

The MELTSPREAD Code for Modeling of Ex-Vessel Core Debris Spreading Behavior

Code Manual – Version3-beta

NE Division

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ABSTRACT

MELTSPREAD3 is a transient one-dimensional computer code that has been developed to predict the gravity-driven flow and freezing behavior of molten reactor core materials (corium) in containment geometries. Predictions can be made for corium flowing across surfaces under either dry or wet cavity conditions. The spreading surfaces that can be selected are steel, concrete, a user-specified material (e.g., a ceramic), or an arbitrary combination thereof. The corium can have a wide range of compositions of reactor core materials that includes distinct oxide phases (predominantly UO_2 , ZrO_2 , and steel oxides) plus metallic phases (predominantly Zr and steel). The code requires input that describes the containment geometry, melt "pour" conditions, and cavity atmospheric conditions (i.e., pressure, temperature, and cavity flooding information). For cases in which the cavity contains a preexisting water layer at the time of RPV failure, melt jet breakup and particle bed formation can be calculated mechanistically given the time-dependent melt pour conditions (input data) as well as the heatup and boiloff of water in the melt impingement zone (calculated). For core debris impacting either the containment floor or previously spread material, the code calculates the transient hydrodynamics and heat transfer which determine the spreading and freezing behavior of the melt. The code predicts conditions at the end of the spreading stage, including melt relocation distance, depth and material composition profiles, substrate ablation profile, and wall heatup. Code output can be used as input to other models such as CORQUENCH that evaluate long term core-concrete interaction behavior following the transient spreading stage. MELTSPREAD3 was originally developed to investigate BWR Mark I liner vulnerability, but has been substantially upgraded and applied to other reactor designs (e.g., the EPR), and more recently to the plant accidents at Fukushima Daiichi. The most recent round of improvements that are documented in this report have been specifically implemented to support industry in developing Severe Accident Water Management (SAWM) strategies for Boiling Water Reactors.

This document is a Code Manual which contains i) a technology review, ii) descriptions of models and correlations, iii) descriptions of the implicit, finite difference numerical solution scheme, iv) a user's guide, and v) a summary of code validation calculations that have been performed to date.

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NOMENCLATURE

А	= spreading area, m^2
B_w	= Width of slot jet impinging upon shell, m
D	= hydraulic diameter of spreading corium layer, m
С	= specific heat, J/kg·K
D_j^k	= binary diffusion coefficient, m^2/s
d_B	= sparging gas bubble diameter, m
e	= specific enthalpy, J/kg
e _{cr,sol}	= specific enthalpy of corium at solidus, J/kg
Δe_{cr}	= crust latent heat of fusion, J/kg
e _{st,sol}	= substrate specific enthalpy at solidus, J/kg
Δe_{st}	= substrate latent heat of fusion, J/kg
Δe^{i}_{dc}	= concrete decomposition enthalpy for dryout of i th concrete
	constituent, J/kg
c	= specific heat at constant pressure, J/(kg·K)
Е	= relative substrate elevation, m
F	= friction factor
F_{CO_2}	= reaction fraction of CO_2 gas sparging through melt layer
F_{H_2O}	= reaction fraction of H_20 vapor sparging through melt layer
g	= gravitational acceleration, m/s^2
h	= collapsed depth of melt layer, m
h^i	= collapsed depth of i th melt constituent, m
h _{adj}	= melt depth adjacent to shell, m
h _{bot}	= heat transfer coefficient at melt bottom surface, $W/m^2 \cdot K$
h _{shell}	= heat transfer coefficient between melt and shell, $W/m^2 \cdot K$
h_{top}	= heat transfer coefficient at melt top surface, $W/m^2 \cdot K$
j	= superficial gas velocity, m/s
<i>j_{nc}</i>	= noncondensable gas superficial velocity, m/s
j _v	= water vapor superficial gas velocity, m/s
k	= thermal conductivity, $W/(m \cdot K)$
Ku	= Kutateladze number
L	= Laplace constant = $\sqrt{\sigma/g(\rho - \rho_g)}$, m
Μ	= molecular weight
\dot{m}_{H_2O}	= mass flux of H_20 vapor due to concrete decomposition, kg/($m^2\cdot s)$
\dot{m}_{CO_2}	= mass flux of CO_2 gas due to concrete decomposition, kg/($m^2 \cdot s$)
<i>ṁ_{vessel}</i>	= mass flux of corium from reactor pressure vessel, kg/($m^2 \cdot s$)

Р	= system pressure, Pa
Pr	= Prandtl number
q"	= heat flux, W/m^2
q_{ox,H_2O}^i	= oxidation energy release for reaction of i th melt constituent with
	H_20 vapor, J/kg
q^i_{ox,CO_2}	= oxidation energy release for reaction of i th melt constituent with
	CO_2 vapor, J/kg
<i>q_{decay}</i>	= decay heat generation rate per unit mass of UO_2 , W/kg
R	= ideal gas constant, $m^2/(s^2 \cdot K)$
Re	= Reynolds number
S	= flow channel width normal to flow, m
t	= time, s
Т	= temperature, K
T _{bot}	= surface temperature at bottom of corium layer, K
T_{top}	= surface temperature at top of corium layer, K
T_{adj}	= melt temperature adjacent to shell, K
U	= velocity, m/s
V_b	= bubble volume, m^3
X_{melt}^i	= weight fraction of i th melt constituent in melt
X_{sf}^i	= weight fraction of i th melt constituent in solidified debris
X ⁱ _{vessel}	= weight fraction of i th melt constituent draining from reactor
	pressure vessel
Ζ	= radial coordinate, m

Superscripts

i	= corium constituent
n	= beginning of timestep quantity
n+l	= end of timestep quantity
r	= iterated quantity

Superscripts

adj	= adjacent to shell
bot	= bottom of corium layer
cond	= conduction heat transfer mode
с	= continuous phase
cr	= crust quantity
CHF	= critical heat flux
d	= dispersed phase

dc	= concrete decomposition quantity
entr	= entrainment
fb	= film boiling heat transfer mode
frz	= value at freezing point
g	= gas
j, k, m	= finite difference nodalization indices
1, w	= water
liq	= value at liquidus
min	= min film boiling point
nb	= nucleate boiling heat transfer mode
rad	= radiation heat transfer mode
rise	= rise time through melt layer
st	= substrate surface
shell	= surface of shell
sol	= value at solidus
sf	= melt/debris surface
sub	= subcooling
struc	= overlaying structure
Т	= terminal rise quantity
top	= top of corium layer
x	= coordinate normal to substrate surface, m
x_{dc}^i	= location of i th concrete decomposition front, m
Vessel	= RPV quantity
Z	= coordinate parallel to substrate surface, m

Greek Symbols

Ω_D	= collision integral
α	= void fraction
α_{adj}	= melt void fraction adjacent to shell
α_{sol}	= solid fraction in melt
$\alpha_{sol,max}$	= maximum solid packing fraction
δ	= crust thickness, m
Δ	= difference
η	= depth of eroded substrate, m
σ_{stef}	= Stefan-Boltzmann constant = $5.67 \cdot 10^{-8} W/m^2 \cdot K$
σ	= surface tension, N/m
$\sigma_{j,k}$	= Lennard-Jones potential parameter
ρ	= density, kg/m^3
μ	= viscosity, kg/(m·s)

- τ = shear stress, N/m²
- λ = Taylor wavelength, m
- \in = radiative emissivity
- θ = shell inclination angle with respect to horizontal, degrees

Section 1

INTRODUCTION

BACKGROUND

The MELTSPREAD code for the analysis of core debris spreading in containments was originally developed^[1,2] and applied^[3,4] to support resolution of the Mark I Boiling Water Reactor (BWR) shell vulnerability issue.^[5] For Beyond Design Basis Accidents (BDBAs) in which molten corium is postulated to breach the reactor pressure vessel (RPV) lower head, a significant question concerns the spreading of the discharged core material. The Mark I containment geometry is typical of that at the Peach Bottom Nuclear Power Station shown in Figures 1-1 and 1-2. Corium discharged from the RPV will initially be confined by the reinforced concrete walls and floor of the pedestal region. However, the pedestal wall incorporates one or more doorways for personnel access which are not sealed with thick hatches. They have doors which would not be expected to provide a significant barrier against corium migration or thermal attack. One of the principal questions addressed in the Mark I shell vulnerability studies was whether the corium, after flowing through the pedestal doorway, would be able to spread all the way to the liner of the primary containment, or whether heat transfer to the structure, underlying concrete, and overlying water would freeze and immobilize the melt short of the liner. If molten corium came in contact with the steel liner, the liner would be at risk.^[6] The principal concern was that failure of the liner would provide a path whereby fission products could bypass the suppression pool and be released directly into the surrounding reactor building. However, if liner integrity is maintained, fission product venting from the containment would take place through the suppression pool with subsequent retention of fission products and reduction of the source term. To support resolution of this issue, MELTSPREAD was specifically developed to address questions related to the extent of core debris spreading, as well as the subsequent heatup of the shell if contacted by the spread material.

Since this work was completed^[1-4], the reactor accidents at Fukushima Daiichi occurred. As a result, the nuclear industry has been reevaluating accident management strategies for both PWRs and BWRs. Specific to BWRs, previous accident management guidance called for flooding the drywell to a level of approximately 1.2 m (4 feet) above the drywell floor once vessel breach has

been determined. While this action can help to submerge ex-vessel core debris, it can also result in flooding the wetwell and thereby render the wetwell vent path unavailable. On this basis, an alternate strategy has been proposed in industry guidance^[7] for responding to the severe accident capable vent Order, EA-13-109.^[8] This alternate strategy aims to throttle the flooding rate to achieve a stable wetwell water level while preserving the wetwell vent path and keeping the core debris covered with water.



Figure 1-1 Illustration of Mark I Configuration (Peach Bottom Units 2 and 3)



Figure 1-2 Illustration of Mark I Configuration Showing Doorway and Sump Pit Locations (Peach Bottom Units 2 and 3)

To inform the development of these Severe Accident Water Management (SAWM) strategies, it became clear that improved analytical tools would be needed in order to realistically model ex-vessel core debris spreading and debris cooling behavior. This most recent version of MELTSPREAD is intended to satisfy the enhanced modeling needs related to core debris spreading; a separate model (i.e., CORQUENCH4^[9]) has been enhanced to satisfy the need for realistic evaluations of long-term debris coolability. The overall focus of this work is to provide *flexible*, analytically capable, and validated models to support development of SAWM strategies that aim to keep ex-vessel core debris covered with water while preserving the BWR wetwell vent path. Specifically, there are gaps in analysis capability for evaluating core melt relocation and cooling behavior that accounts for several important factors that include the effect of water throttling on spreading and long term debris coolability. These gaps have been identified by an industry-lab advisory group as high priority items to address.^[10] Other spreading-related knowledge gaps include: i) the impact of below vessel structure in a BWR on melt relocation from the RPV to the drywell floor, and ii) the potential for melt fragmentation and cooling in water present on the drywell floor.

One specific factor that can impact flooding strategy is the spatial distribution of core melt in containment following vessel failure and melt spreading. For instance, a localized accumulation of melt in the pedestal region of a BWR may require a more specific flooding approach in comparison to the situation in which core melt is spread uniformly over the pedestal and drywell floor areas. In the former case, the localized core melt accumulation could form a dam preventing adequate debris flooding and cooling if the water is not injected directly on top the core debris, whereas in the latter case, effective debris flooding is expected regardless of injection point(s) as long as the injection flowrate is high enough to remove sensible and decay heat from the debris. These spatial distribution questions, coupled with the overall effectiveness of the debris cooling process, may impact the water injection requirements for achieving a balance between water injection flowrate versus boil-off, thereby minimizing extraneous spillover into the wetwell. These types of potential scenarios provide the impetus for an improved core debris spreading model that is the primary focus of this report.

OBJECTIVES AND APPROACH

With the above background, the overall objectives of this work are three-fold:

1) Document the overall modeling strategy as well as the various phenomenological models that are embedded in MELTPSREAD for

calculating ex-vessel core debris spreading under as realistic conditions as possible.

- 2) Provide a user guide for the code to facilitate the utilization of the software by other organizations and individuals that may have an interest.
- 3) Summarize the various validation calculations that have been carried out in order to gauge the predictive capability of the code.

To this end, a phenomenology and literature review is provided to complete this introductory section as precursor to the model descriptions that are provided in Section 2. The numerical methods used to solve the equations governing melt spreading are then described in Section 3. This is followed by instructions on how to assemble the user input file for the code in Section 4. Subsequently, a description of the output text and plotting files is provided in Section 5. Finally, validation calculations, material property subroutines, ancillary model derivations, and a description of supporting software are provided in the appendices.

PHENOMENOLOGY AND LITERATURE REVIEW

As shown in Figure 1-3 for Mark I systems, a significant amount of belowvessel structure exists in the form of control rod drive and instrument tube housings, in addition to a personnel catwalk. Corium draining from the RPV might undergo significant splashing as it relocates through this structure. As shown in Figure 1-4, this could cause the corium to "rain" down on the pedestal floor. An early scoping study was carried out by Chu, Sienicki and Spencer ^[11] to evaluate the potential impacts of this structure on melt arrival conditions on the pedestal floor. This is also an area that is being investigated as part of this work, with analytical models under development^[12] that will eventually be used to assess the impact of melt-structure interaction on overall spreading behavior. Recent findings from Fukushima Units 2-3 support the notion that this core debris holdup in this structure may be substantial, and could impact containment response in general.^[13] Aside from below vessel structure, melt stream interaction with water present on the pedestal floor may lead to fragmentation and quenching that can also impact spreading; see Figure 1-5. This type of behavior has been modeled in the current version of MELTSPREAD and is documented in this report.

As the corium accumulates on the floor and begins to spread, heat transfer from the melt to underlying concrete can lead to concrete decomposition and generation of gases, principally water vapor and carbon dioxide. This process



Figure 1-3 Illustration of Below Vessel Structure in a Mark I System



Figure 1-4 Depiction of Corium Interaction with Below Vessel Structure



Figure 1-5 Melt Pour Interaction with Water Present on the Pedestal Floor

is illustrated in Figure 1-6. As the gases rise through the melt they would be further heated and might undergo chemical reactions with melt constituents. In turn, the gases could cause agitation of the molten core materials. Ultimately, the gases would pass through the upper surface of the melt. As depicted in Figure 1-7, if water is present atop the core material, the gases flowing through the interface between the melt and likely augment the rate of melt-to-water heat transfer through the mechanisms of interfacial area enhancement and melt entrainment into the overlying water layer, as has been demonstrated in numerous reactor material core-concrete interaction experiments.^[14]

As the corium continues to spread, heat transfer to underlying concrete and overlying water may eventually lead to melt freezing. As depicted in Figure 1-8, freezing might occur as a result of crust growth over the substrate surface and crust growth at the melt/water interface. Conversely, sparging non-condensable gases arising from concrete decomposition might continuously break up any crusts that form into segments/platelets that are continuously mixed back into the melt. In this situation, illustrated in Figure 1-9, the corium is expected to freeze as slurry composed of dispersed solid particulate and liquid. Finally, as shown in Figure 1-10, previously frozen and immobilized core debris would form a barrier over which corium subsequently draining from the RPV must spread.



Figure 1-6 Depiction of Corium Spreading Over a Concrete Surface



Figure 1-7 Depiction of Corium Interaction with Overlying Water Layer



Figure 1-8 Depiction of Corium Freezing Through the Mechanism of Crust Formation



Figure 1-9 Depiction of Corium Freezing Through the Mechanism of Bulk Solidification



Figure 1-10 Depiction of Corium Spreading Over Previously Solidified Debris

As the spreading process continues, there is the potential for melt to flow out of the pedestal doorway and come into contact with the containment shell. This process is illustrated in Figures 1-11 and 1-12. Corium contact with the shell is expected to lead to crust growth on the shell surface. Continued flow out of the pedestal doorway might lead to significant shell thermal loading due to impingement heat transfer. There is some circumstantial evidence from Fukushima Unit 1 that this may have occurred, and may have contributed to shell failure.^[13] If water is present in the drywell, shell thermal loading would be mitigated by the "fin effect," i.e., lateral heat conduction along the length of the shell from the region where corium is in contact with the shell to the region where water is in contact with the shell.



Figure 1-11 Depiction of Corium Spreading Out of the Pedestal Doorway



Figure 1-12 Depiction of Corium Interaction with Shell

In summary, for accident sequences in Mark I containments in which corium melts through the RPV lower head, the assessment of the extent of spreading and shell vulnerability involves many complex phenomena. These phenomena include, but are not limited to, gravity driven spreading in a complex flow geometry, transient concrete heatup and decomposition, increases in meltwater heat transfer due to sparging gas flows, freezing and immobilization of corium with subsequent flow over the frozen material, and two-dimensional heatup of the shell, including the "fin effect," should the corium come into contact with the shell. Closely linked to this process is severe accident water management (SAWM) since the distribution of core debris in containment can impact the flooding strategy.

In terms of related analytical studies in the U.S., following initial development and application of MELTSPREAD to the resolution of the Mark I shell vulnerability issue,^[1-5] this model was further refined and an extensive set of validation calculations were carried under sponsorship from the Nuclear Regulatory Commission (NRC).^[15-16] The code was subsequently applied to analyze spreading behavior in the core catcher of the EPR^[17] in support of the licensing process for this reactor in the U.S.^[15-16]

Internationally, extensive model and code development activities were also carried out as part of the European Union (EU) program to address spreading issues associated with the EPR.^[17] At CEA, the THEMA code was developed^{[18-} ¹⁹ to simulate spreading while accounting for the effects of heat transfer and solidification, in addition to ablation of the underlying spreading surface. THEMA uses conservation equations that are locally averaged over the melt This same approach is used in MELTSPREAD, but THEMA has an depth. advantage in that it is able to calculate two dimensional spreading, whereas MELTSPREAD is 1-D. Other three-dimensional codes were developed as part of the EU effort that included axial meshing over the melt depth. These codes include CROCO^[21] developed at IRSN in France, LAVA^[22] developed at GRS in Germany, and CORFLOW^[23] developed by Areva in Germany. One limitation of these codes is that they are computationally intensive with associated long run times. Thus, these codes are not amendable to the analysis of longer term transients. Aside from code development, other modeling activities^[24] have been performed to provide approximate closed form solutions for spreading of high temperature melts, in addition to studies to develop models^[25] that better correlate corium viscosity, which is one of the key variables affecting melt spreading.

More recently, strides have been made in the use of commercial CFD codes to analyze core debris spreading behavior.^[26] Effects accounted for in this approach include radiation heat transfer, decay heat, temperature-dependent viscosity. However, crusting behavior and the potential for concrete decomposition and ablation are not modeled. Like the other methods described above, this approach is computationally intensive and so the ability to apply this method to longer term transients is limited.^[26]

Following closure of the Mark I issue, MELTSPREAD development ceased in the early 1990's, at which time the melt spreading database upon which the code had been originally validated was rather limited. In particular, the database used for initial validation consisted of: i) comparison to an analytical solution for the dam break problem,^[27] iii) water spreading tests in a 1/10 linear scale model of the Mark I containment by Theofanous et al.,^[6] and iii) steel spreading tests by Suzuki et al.^[28] that were also conducted in a Mark I type geometry.

Following this initial work, there was a vast amount of experimental research carried out principally in the EU to support the development and licensing of the EPR concept.^[17] In terms of experiments, large isothermal spreading tests were carried out at CEA with water and glycerol by Veteau et al.^[29] in the Corine test facility. This test series was subsequently expanded to investigate the effects of bottom gas injection on spreading behavior, as well as freezing effects using low temperature eutectic metal melt mixtures.^[29] Spreading tests with high temperature simulant oxide (calcia – boria eutectic) under both wet and dry cavity conditions were also conducted by Dinh et al.^[30] at the Royal Institute of Technology (RIT) in Sweden. In addition, several series of spreading tests with both high temperature steel and oxide simulants were performed at the Karlsruhe Institute of Technology (KIT) by Engel et al.^[31] and Eppinger et al.^[32] in the KATS test facility, and by Foit^[33] and Alsmeyer et al.^[34] using a slightly modified oxide simulant in the ECOKATS facility.

Aside from simulant tests, several reactor material melt spreading programs were performed in the EU to provide prototypic melt spreading data. As reported by Cognet et al.^[35] and Journeau et al.,^[36-37] several corium melt spreading tests were carried out at CEA with varying melt compositions and substrate materials in the VULCANO facility. Two corium tests were also conducted by Magallon and Tromm^[38] as part of the FARO program, one of them under wet cavity conditions. Finally, several large scale spreading tests at up to 2 metric ton melt mass were conducted at Siempelkamp Nuklear in Germany on various types of surface materials (Sappok and Steinwarz^[39] and Steinwarz et al.^[40]).

As previously noted, experiment data from these various simulant and reactor material experiment programs was not available during original MELTSPREAD development, and so one key element of the current workscope was to assess the enhanced version of the code against this expanded database.

Section 2

MODEL DESCRIPTION

The general physical models incorporated into MELTSPREAD3 are described in this section. A summary of principal modeling assumptions and model limitations is shown in Table 2-1. Except where otherwise noted, the local melt thermophysical properties are evaluated based on the local melt constituency and mean layer temperature (See Table 2-1). A description of the thermophysical property subroutines currently implemented in MELTSPREAD3 is provided in appendix B. Details of the numerical methodology used to solve the following equations are provided in Section 3. A depiction of corium spreading over a concrete surface was provided earlier in Figure 1-6. An illustration of the geometry and nomenclature used in the following analysis is shown in Figure 2-1.

GENERAL CONSERVATION EQUATIONS

The relocation model incorporated into MELTSPREAD3 performs a spatially dependent fluid dynamics calculation of the gravity driven motions of a molten mass spreading in a one-dimensional flow channel of varying cross-sectional area. The velocity of the flowing melt is dependent upon the local gravity head of the spreading corium layer. In particular, the fluid velocity is assumed to satisfy the equation

$$\frac{\partial U}{\partial t} + \frac{1}{2} \frac{\partial U^2}{\partial z} = g \frac{\partial}{\partial z} [h + E] - \frac{4\tau}{\rho D}, \qquad (2-1)$$

where

U = velocity,
ρ = melt collapsed density,
g = gravitational acceleration,
h = melt collapsed depth,
D = melt hydraulic diameter = 4h, and
E = substrate elevation.

and τ is the frictional shear stress at the lower surface of the melt which is evaluated through the equation,

$$\tau = \frac{1}{2}\rho f U|U|, \qquad (2-2)$$

Table 2-1 SUMMARY OF MAJOR MODELING ASSUMTIONS INCORPORATED INTO MELTSPREAD3

Assumption	Evaluation	
Spreading is modeled within a prescribed one-dimensional flow channel. For the Mark I configuration, circular nodalization of pedestal; constant spreading angle between pedestal doorway and liner; and channel flow through the remainder of the drywell annulus are assumed.	The degree of approximation introduced by this assumption is dependent, among other things, upon how well the 1-D channel assumption approximates the actual flow path. The assumed flow configuration is qualitatively consistent with water spreading experiments of Theofanous et. al. ^[5] conducted in a 1:10 scale Mark I geometry. Good agreement is obtained between MELTSPREAD3 and measurements of transient water depth at various locations in these tests. ^[5] In general, spreading angle should decrease as	
spreading angle assumed for melt exiting Mark I pedestal doorway and spreading between pedestal doorway and liner.	velocity of melt approaching doorway increases or depth upstream of doorway decreases. Spreading angles as low as 55 degrees observed in water spreading experiments of Theofanous et. al. ^[5] conducted in 1:10 scale Mark I geometry.	
Heat transfer downward into the substrate and immobilized solid material is modeled with local one-dimensional calculations. Multidimensional heat transfer effects are neglected inside the substrate and immobilized material.	Sideward erosion into the substrate is excluded by this assumption which is expected to be good when a limited amount of substrate erosion occurs. As a consequence of the omission of sideward erosion, downward erosion may be overestimated, although the eroded volume is probably underestimated.	
The melt velocity and temperature are assumed uniform over the one-dimensional cross section of the spreading melt layer.	For laminar creeping flows, a laminar profile will exist across the layer thickness. Frictional and heat transfer terms are formulated in terms of mean layer velocity and temperature such that actual axial profile is not required. Due to multi- dimensional effects, local thickness could vary somewhat across lateral extent of melt, but spreading in lateral directions will tend to reduce such variations.	
Downward melt-to-substrate heat transfer coefficient assumed to be the larger of the Bradley bubbling natural convection coefficient and laminar-turbulent Dittus-Boelter forced convection coefficients dependent upon whether local Reynolds number exceeds critical value for onset of turbulence.	Current uncertainty regarding the appropriate form of the downward heat transfer coefficient in dynamic spreading regime; slag thermal resistance effects will decrease the forced convection heat flux.	

Assumption	Evaluation
Unward melt to water heat transfer	Melt viscosity or non Newtonian flow effects
encompasses the full boiling curve through film, transition, and nucleate boiling. The film boiling heat transfer	could retard the passage of gas through the upper surface thereby reducing the area enhancement effects. This would decrease the
coefficient includes effects of thermal radiation, conduction, and coolant subcooling. The upper surface area	upward heat losses resulting in greater spreading extents than are calculated.
assumed to be increased by gas bubbles passing through the surface.	
Upward melt-to-water and melt-to- atmosphere heat transfer coefficients neglect sustained crust formation at the upper surface.	Crust formation will lower the upper surface temperature at which energy radiates from the spreading layer. Crusts will also impede the passage of gas through the surface decreasing the effects of gas sparging-induced area enhancement further reducing upward heat losses. This will result in greater spreading extents then calculated.
When water is absent, energy absorption by the steam/gas mixture above the melt is neglected.	The resultant heatup of the steam/gas mixture will reduce the overall radiation heat transfer loss from the melt upper surface.
When water is absent, radiative heat transfer from the spreading melt to the liner and other overlying structures is neglected.	Heatup of overlying structure, including the Mark I shell, will be underpredicted when the cavity is dry.
Immobilized solid material is not permitted to commence further relocation until the surface temperature exceeds the solidus.	This assumption affects the continued relocation of solidified material that subsequently heats up and remelts. A molten mass that forms inside a mound of immobilized material is not permitted to break out as the result of localized failure of the constraining "crucible" boundary.
Chemical reaction rates are assumed limited by rate of gas release from concrete. Zr, Cr, and Fe oxidize in sequence. Interactions between released melt and oxides from the concrete such as that involving	Slower rates or intermediate reactions would be expected to result in slightly lesser spreading extends/greater depths than calculated.

Table 2-1 SUMMARY OF MAJOR MODELING ASSUMTIONS INCORPORATED INTO MELTSPREAD3 (Cont'd)

Table 2-1 SUMMARY OF MAJOR MODELING ASSUMTIONS INCORPORATED INTO MELTSPREAD3 (Cont'd)

Assumption	Evaluation
Newtonian melt flow is	Although completely molten core materials are expected to
assumed. The Ishii-Zuber	flow as Newtonian fluids, binary melt alloy mixtures and
(24) effective viscosity	core-concrete mixtures exhibit non-Newton behavior below
enhancement is assumed	the liquidus. In this slurry regime, the melt can be
for the flow of slurries.	described with an effective viscosity, but this viscosity is
	shear rate dependent. Due to non-Newtonian effects, melt
	undergoing freezing could exhibit a greater resistance to
	flow than assumed in analysis resulting in lesser spreading
	extents-greater depths than calculated.
Solid volume fraction of	Non-linear relationships between solid fraction and
each phase is assumed to	temperature describe binary metal alloys under non-
increase continuously	equilibrium conditions. The impact of this assumption
between liquidus and	upon the present analysis is probably minor compared with
solidus.	non-Newtonian slurry effects.
Liquidus and solidus	Actual liquidus and solidus temperatures are composition
temperatures of oxide and	dependent and will vary due to the addition of concrete
metal phases are assumed	erosion products into the melt and chemical reactions.
to remain constant	Addition of concrete constituents will decrease the liquidus
throughout calculation.	and solidus temperatures tending to increase the local melt
	superheat above the liquidus. This will result in greater
	spreading extents than calculated.
Calculation of crust	This will not be a significant approximation when the crust
formation upon solid	thickness is small (i.e., convective heat transfer rate is
surfaces neglects decay heat	high); it becomes more of an approximation as the
generation inside crusts.	thickness of the crust increases.



Figure 2-13 Illustration of the Geometry and Nomenclature Used in the Melt Spreading Model
and f is the friction factor. Note in Eq. 2-1 that the effect of voiding in the melt due to sparging concrete decomposition gases has been neglected in the gravity head term. Further note that the non-conservative form of the onedimensional momentum equation is implied because it reduces to Bernoulli's law in the limit of negligible frictional resistance. Consistent with classical theories on gravity currents (e.g., see Benjamin,^[27]) the pressure head driving the flow is assumed to equal the local hydrostatic head. In this manner, solution of Eq. 2-1 in the limit of frictionless flow yields the correct theoretical leading edge spreading velocity^[27] after transient affects have died away (see Appendix C).

Heat transfer from the melt to underlying concrete can lead to release of concrete decomposition gases, principally water vapor and carbon dioxide. The elevation gradient is included to account for the presence of previously solidified debris, as well as the initial profile of the spreading surface that may include large discontinuities such as the presence of a sump. The void fraction in the melt, α , is calculated based on the correlation of Kataoka and Ishii.^[41] The void fraction is specified in terms of a dimensionless gas velocity, j_g^+ , which is defined as follows:

$$j_{g}^{+} = \frac{j_{g}}{\left[\frac{\sigma g \left(\rho - \rho_{g}\right)}{\rho_{g}^{2}}\right]^{\frac{1}{4}}},$$
(2-3)

where

j_g	$= j_{H_20} + j_{co_2},$
j _{H20}	= water vapor superficial gas velocity due to concrete
	decomposition,
<i>j</i> _{co2}	= carbon dioxide superficial gas velocity due to
	concrete decomposition,
$ ho_g$	$= \rho_{H_20} + \rho_{co_2},$
$ ho_{co_2}$	$=\frac{P}{R_{g,CO_2} T_{dc}},$
$ ho_{H_20}$	$=\frac{P}{R_{g,H_2,O} T_{dc}},$
R_{g,CO_2} , $R_{g,H_{2,O}}$	= ideal gas constants for CO_2 and H_2O gases,
T _{dc}	= concrete decomposition temperature,
Р	= drywell annulus pressure,
σ	= melt surface tension.

For

$$j_g^+ < 0.5$$
 (2-4)

a bubbly flow regime exists and the melt void fraction is given by the equation

$$\alpha = \frac{1}{c_0 + \sqrt{2}/j_j^{+}},\tag{2-5}$$

where

$$C_0 = 1.2 - 0.2 \sqrt{\frac{\rho_g}{\rho}} \,. \tag{2-6}$$

For

$$j_g^+ > 0.5,$$
 (2-7)

the flow is churn turbulent and the melt void fraction is given by the equation

$$\alpha = \frac{1}{C_o \, j_g^+ + 0.03 \left(\frac{\rho}{\rho_g}\right)^{0.157} \left(\frac{\mu}{\rho \sigma \sqrt{\sigma/g(\rho - \rho_g)}}\right)^{0.50}} \tag{2-8}$$

where

 μ = melt viscosity.

Spreading is restricted to occur such that the melt depth at the leading edge does not fall below the minimum depth at which surface tension balances gravity; i.e.¹

$$h_{min} = \sqrt{\frac{2\sigma}{\rho g}}.$$
 (2-9)

The friction factor, f, in Eq. 2-2 is dependent upon the local melt Reynolds number which is defined through the equation,

$$Re = \frac{\rho(1-\alpha) D|U|}{\mu}.$$
 (2-10)

For Reynolds numbers below a transition value of 2300, the friction factor is evaluated through the following expression,

¹ The minimum depth is evaluated by setting the gravity head at the leading edge (ρgh) equal to the effective surface tension pressure ($2\sigma/h$).

$$f = \frac{24}{Re}.\tag{2-11}$$

Note that the coefficient on the right hand side of Eq. 2-11 (i.e., 24) is based on the assumption of a fully developed parabolic velocity profile within the melt. Thus, over short flow distances where the velocity profile has not become fully developed, the friction factor will be underestimated through the use of Eq. 2-11. However, the treatment of a developing velocity profile is beyond the scope of this work, and therefore Eq. 2-11 is used to estimate the friction factor whenever the local Reynolds number falls below the transition value of 2300.

For Reynolds numbers above 2300, the friction factor is assumed to be given by the fully developed turbulent flow equation,^[42]

$$f = \frac{1}{4x^2},$$
 (2-12)

where *x* satisfies the transcendental equation,

$$x = 1.74 - \frac{2}{\ln(10)} \ln\left(\frac{2R_{sand}}{D} + \frac{18.7x}{Re}\right).$$
 (2-13)

Equations 2-12 and 2-13 apply to flow over a substrate which may be either hydraulically smooth, or a rough surface characterized by the equivalent sand roughness, R_{sand} .

The collapsed melt depth, h, in Eq. 2-1 is written as a sum of the local melt constituent collapsed depths, h^i . MELTSPREAD3 tracks a total of 16 melt constituents that are summarized in Table 2-2. The metals are treated as a distinct phase from the oxides. The general form of the conservation of mass equation for the i^{th} melt constituent is as follows,

$$S \frac{\partial}{\partial t} (\rho^{i} h^{i}) + \frac{\partial}{\partial z} (S \rho^{i} h^{i} U)$$

= $\beta^{i} S \left[F_{H_{2}O} \gamma^{i}_{H_{2}O} \dot{m}_{H_{2}O} + F_{CO_{2}} \gamma^{i}_{CO_{2}} m_{CO_{2}} \right]$
- $S \rho^{i} \left[x^{i}_{sf} \frac{d\eta}{dt} + x^{i}_{melt} \frac{d\delta}{dt} \right] + S x^{i}_{vessel} \dot{m}_{vessel},$ (2-14)

where

δ	=	crust thickness,
$\gamma^i_{H_2O},\gamma^i_{CO_2}$	=	Stoichiometric constants for the reaction of the i^{th} melt
		constituent with H_2O and CO_2 gases,
x_{sf}^i	=	weight fraction of i^{th} melt constituent in solidified debris,
		steel, or concrete substrate,
x_{melt}^i	=	weight fraction of i^{th} melt constituent in corium,
x_{vessel}^i	=	weight fraction of i^{th} melt constituent in corium draining
		from reactor pressure vessel,
\dot{m}_{vessel}	=	mass flux of corium draining from reactor pressure vessel,
		(+1, oxidizable melt constituents
β^i	=	{-1, oxidized melt constituents
		0.nonoxidizable/nonoxidized constituents.

Table 2-2 MELT CONTITUENTS TRACKED BY MELTSPREAD3

Metals	Oxides
Zr	UO ₂
Cr	ZrO ₂
Fe	FeO
Ni	Fe_2O_3
B_4C	Fe_3O_4
U	NiO
В	Cr_2O_3
	B_2O_3
	Concrete Slag (SiO_2 , MgO , CaO , Al_2O_3)

The third term in Eq. 2-14 account for the mass source and sink effects due to the oxidation of metallic melt constituents in the corium layer. Carbon dioxide and water vapor arising from concrete decomposition are assumed to react with zirconium, chromium, and iron. The oxidation reactions treated in MELTSPREAD3 are summarized in Table 2-3. Also included in this table are the assumed oxidation energy releases for the various reactions. Due to the large oxidation potential for the reaction of zirconium with H_20 and $C0_2$ gases, zirconium is preferentially oxidized before chromium and iron, should zirconium be locally present in the melt layer. If zirconium is absent as an initial condition or the zirconium inventory is exhausted due to oxidation, then chromium is oxidized. Finally, if zirconium and chromium are both locally absent, then iron is oxidized. Note the reaction of zirconium with silicates which arise from concrete ablation is currently not modeled in MELTSPREAD3. The oxidation fractions F_{H_2O} and F_{CO_2} in Eq. 2-14 account for incomplete chemical reaction of the sparging gases as the gas bubbles rise through the melt layer. Assuming rigid isothermal bubbles and binary diffusion, then the mass transfer inside the bubbles obeys a transient diffusion equation which for spherical bubbles is^[43]

$$F_{H_2O} = 1 - \frac{6}{\pi^2} \sum_{n=1}^{\infty} \frac{1}{n^2} \exp\left(\frac{-4n^2 \pi^2 D_{H_2O}^{H_2} t_{rise}}{d_b^2}\right)$$
(2-15)

$$F_{CO_2} = 1 - \frac{6}{\pi^2} \sum_{n=1}^{\infty} \frac{1}{n^2} \exp\left(\frac{-4n^2 \pi^2 D_{CO_2}^{CO} t_{rise}}{d_B^2}\right), \qquad (2-16)$$

where

$D_{H_2O}^{H_2}$	= binary diffusion coefficient for a $H_2 O - H_2$ gas mixture,
$D_{CO_2}^{CO}$	= binary diffusion coefficient for a $CO_2 - CO$ gas mixture,
d_B	= gas bubble diameter,
t _{rise}	= bubble rise time through melt layer.

Table 2-3 SUMMARY OF METAL OXIDATION REACTIONS TREATED IN MELTSPREAD3

Chemical Reaction	Stoichiometric Constant, γ	Enthalpy Release per kilogram of metal reacted, MJ/kg
$Zr + 2H_20 \rightarrow ZrO_2 + 2H_2$	$M_{Zr}/2M_{H_2O}$	6.74
$Zr + 2 CO_2 \rightarrow ZrO_2 + CO$	$M_{Zr}/2M_{CO_2}$	5.84
$2 Cr + 3H_2O \rightarrow Cr_2O_3 + 3H_2$	$2M_{Cr}/3M_{H_2O}$	3.57
$2 Cr + 3CO_2 \rightarrow Cr_2O_3 + 3CO$	$2M_{Cr}/3M_{CO_2}$	2.75
$Fe + H_2O \rightarrow FeO + H_2$	$M_{Fe}/M_{H_2}O$	0.078

The binary diffusion coefficients in Eqs. 2-16 and 2-17 are estimated using the theoretical expression developed by Hirschfelder et al.^[44] that is applicable to low pressure, binary gas mixture systems; i.e.,

$$D_{j}^{k} = 0.001858 T_{dc}^{3/2} \frac{\left(1/M_{j}+1/M_{k}\right)^{1/2}}{P \sigma_{j,k}^{2}\Omega_{D}} (cm^{2}/s), \qquad (2-17)$$

where

M_j , M_k	= molecular weights of binary gas constituents,
$\sigma_{j,k}$	= Lennard-Jones potential parameter,
Ω_D	= collision integral.

The collision integral and Lennard-Jones parameter are tabulated in Reference [43]. The diameter of the gas bubbles sparging through the melt layer is assumed to equal the minimum between the Taylor bubble size and the local depth of the corium layer; i.e.,

$$d_B = \min \begin{cases} \lambda/2; h > \lambda/2\\ h; h \le \lambda/2 \end{cases}$$
(2-18)

where λ is the Taylor wavelength which is defined as,^[45]

$$\lambda = 2\pi \sqrt{\frac{3\sigma}{g(\rho - \rho_g)}}.$$
(2-19)

Note that Eq. 2-19 was developed on the basis of inviscid flow theory.^[45] Thus, for situations in which the local melt viscosity increases substantially, Eqs. 2-18 and 2-19 will lead to an underestimate of the gas bubble diameter.

The bubble rise time, t_{rise} , is evaluated based on the simplying assumption² that the bubbles ascend through the melt layer at the terminal rise velocity,

$$t_{rise=\frac{h}{U_T}}, \qquad (2-20)$$

where

 U_T = bubble terminal rise velocity.

The terminal velocity is assumed to be given by the correlation of Peebles and Garber,^[46]

$$U_T = 1.18 \left(\frac{\sigma g}{\rho}\right)^{1/4}$$
. (2-21)

Depending on the melt-substrate interfacial boundary condition, the fourth term in Eq. 2-14 accounts for mass transfer into the melt layer due to substrate ablation, and/or mass transfer out of the corium layer due to crust formation. Explicit expressions for the ablation and crusting rates for a variety of melt/substrate interfacial boundary conditions are provided in the next subsection. The fifth term in Eq. 2-14 accounts for local, time-dependent mass addition to the melt layer due to drainage from the reactor pressure vessel. As depicted in Figure 1-3, a significant amount of below vessel structure exists in

 $^{^2}$ Note that Eq. 2-20 will under-predict the bubble rise time in shallow melt depths where the bubbles do not have time to attain the terminal rise velocity. In this case, the oxidation fractions (Eqs. 2-16 and 2-17) will be under-predicted. However, a more detailed treatment of this problem is beyond the scope of this work.

the form of control rod drive and instrument tube housings, in addition to a personnel catwalk. Corium draining from a localized breach in the reactor pressure vessel may undergo significant splashing and holdup due to freezing as it passes through this structure, causing the corium to "rain" down on the pedestal floor. To account for this behavior, MELTSPREAD3 permits melt addition to the spreading layer over a distributed as well as localized area, but the current version does not explicitly calculate the extent of dispersion or holdup. Standalone models are under development to treat this type of behavior,^[12] and these models may be incorporated into MELTSPREAD3 in the future. In addition, water present on the floor could cause melt fragmentation and thereby reduce the temperature of the subsequently spreading material, or fragmentation could lead to a rubble bed on top of the spread debris. A model for evaluating this type of behavior are described later in this section.

The spreading melt constituents are assumed to be in local thermodynamic equilibrium at a single, local layer specific enthalpy. Within the layer, the metals are treated as a distinct phase from the oxides with user-specified liquidus and solidus temperatures for each phase. The enthalpy is obtained from the solution of the conservation of enthalpy equation,

$$S\frac{\partial}{\partial t}(\rho h e) + \frac{\partial}{\partial z}(S\rho h e U) = -Sh_{bot}(T - T_{bot})$$
$$-Sh_{top}(T - T_{top}) + S\rho h x_{melt}^{UO_2} \dot{q}_{decay} + S\dot{m}_{vessel} e_{vessel}$$
$$-S\rho \left[e_{sol,st} \frac{d\eta}{dt} + e_{cr,sol} \frac{d\delta}{dt} \right] + SF_{H_2O} \dot{m}_{H_2O} \sum i \gamma_{H_2O}^i q_{ox,H_2O}^i$$
$$SF_{CO_2} \dot{m}_{CO_2} \sum i \gamma_{CO_2}^i q_{ox,CO_2}^i - Q_{shell} D(z - z_{shell}), \qquad (2-22)$$

where

е	= melt specific enthalpy,
T _{bot}	= surface temperature at bottom of melt layer,
h _{bot}	= heat transfer coefficient at bottom of melt layer,
T _{top}	= surface temperature at top of melt layer,
h_{top}	= heat transfer coefficient at top of melt layer,
<i>q_{decay}</i>	= decay heat rate per kg UO_2 in melt,
e _{vessel}	= specific enthalpy of corium release from reactor pressure
e _{cr,sol}	 crust specific enthalpy at solidus,
e _{sol,st}	 substrate specific enthalpy at solidus,
q_{ox,H_2O}^i	= oxidation energy release per unit mass of i^{th} melt
	constituent oxidized by H_2O vapor,

and $T_{sf}(y)$ is the surface temperature variation along the submerged portion the shell. An illustration of the coordinate system and nomenclature used in the shell heatup model (described in detail later in this Section) is provided in Figure 2-2.



Figure 2-14 Illustration of the Geometry and Nomenclature Used in the Shell Heatup Model

The local enthalpy in the melt layer is checked to determine if the enthalpy has fallen below the solidus value. If so, the melt is immobilized and added to previously solidified melt and concrete in the calculation.

If the enthalpy of the core debris lies between the liquidus and solidus, the melt is modeled as slurry with enhanced effective viscosity due to the presence of solids in the melt. There are two modeling options for treating the increase in viscosity due to buildup of solid material. The first is a correlation developed by Ishii and Zuber,^[47]

$$\mu_{slurry} = \mu_c \left(1 - \frac{\alpha_{sol}}{\alpha_{sol,max}} \right)^{-2.5\alpha_{sol,max} \left(\frac{\mu_d + 0.4\mu_c}{\mu_d + \mu_c} \right)}, \qquad (2-23)$$

where

α_{sol}	= solid fraction in melt,
$\alpha_{sol,max}$	= maximum solid packing fraction,
μ_c	= melt continuous phase viscosity,
μ_d	= melt dispersed phase viscosity.

Additional details on the method for evaluating the slurry viscosity based on the local melt constituency, solid fraction, and temperature is provided in Appendix B.

Although initial validation of MELTSPREAD was carried using the Ishii-Zuber correlation for predicting melt viscosity, initial applications to the expanded database indicated that spreading behavior was much better reproduced using the correlation developed by Ramacciotti et al.^[25] In this model, the apparent melt viscosity in the freezing range is correlated as:

$$\mu_{slurry}=\mu_0 e^{2.5C_R \alpha_{sol}},\tag{2-24}$$

where μ_o is the viscosity at the melt liquidus, a_{sol} is the melt solid fraction, and C_R is a user-supplied empirical constant that depends upon experiment conditions and varies between 4 and $8^{[25]}$ As is evident from Eq. 2-24, accurate knowledge of the melt solid-fraction variation between the liquidus-solidus is important when using this viscosity correlation. Two options are provided for assessing the solid fraction variation: i) the fraction can be modeled assuming a linear variation between the liquidus and solidus, or ii) a user-supplied solid fraction versus temperature table can be provided. Additional details are provided in Section 4 and Appendix B.

HEAT TRANSFER AT MELT LOWER SURFACE

A source of uncertainty in the analysis of melt spreading is the applicable heat transfer coefficient at the melt lower surface. At this surface, the user has three modeling options for the heat transfer coefficient, which include: (i) forced convection, (ii) bubble agitation, or (iii) the larger of the forced convection and bubble agitation models. The forced convection heat transfer coefficient is assumed to be given by the fully developed pipe flow correlation,^[48]

$$h_{bot} = \begin{cases} 7.6 \frac{k}{D}; Re < 2300\\ 0.023 Re^{0.8} Pr^{0.4} \frac{k}{D}; Re \ge 2300 \end{cases},$$
(2-25)

where

k = melt thermal conductivity,

and the local Reynolds number is evaluated through Eq. 2-10. The melt Prandlt number is defined as

$$Pr = \frac{c\mu_c}{k} \tag{2-26}$$

where

c = melt specific heat at constant pressure.

Equation 2-25 is applied to cases in which the local melt enthalpy lies above the liquidus, and also to cases in which the melt enthalpy lies between the liquidus and solidus. When the melt enthalpy lies in the freezing transition range, buildup of solidified particulate in the melt may act to suppress turbulent fluctuations thereby lowering the effective forced convection heat transfer coefficient. To first order, this effect is accounted for by the increase in effective melt viscosity as calculated through either Eq. 2-23 or 2-24.

The bubble agitation heat transfer coefficient is currently calculated using the revised periodic contact model of Kao and Kazimi,^[49] or Kutateladze's bubble agitation model^[50] as revised by Bradley^[51] for the interaction of core materials with concrete. Kao and Kazimi's heat transfer coefficient is given by the relationship,

$$h_{bot} = C_o \left(\frac{k}{L}\right) \left[\frac{\sqrt{k\rho c}}{\sqrt{k_f \rho_f c_f}} \left(\frac{T - T_1}{T - T_{dc}}\right)\right]^2 \left[\frac{c_f (T - T_{dc})}{e_{dc}}\right] \tau , \qquad (2-27)$$

where

 C_0 = empirical constant = 2.08,

- k_f = thermal conductivity of ablated substrate,
- ρ_f = density of ablated substrate,
- c_f = specific heat at constant pressure of ablated substrate,

$$e_{dc}$$
 = substrate decomposition enthalpy,

L = Laplace constant =
$$\sqrt{\frac{\sigma}{g(\rho - \rho_g)}}$$
,

and T_I is given through the equation,

$$T_{I} = \left(\frac{\sqrt{k\rho c} T + \sqrt{k_{st}\rho_{st}c_{st}} T_{dc}}{\sqrt{k\rho c} + \sqrt{k_{st}\rho_{st}c_{st}}}\right)\tau, + \left(\frac{\sqrt{k\rho c} T + \sqrt{k_{f}\rho_{f}c_{f}} T_{dc}}{\sqrt{k\rho c} + \sqrt{k_{f}\rho_{f}c_{f}}}\right)(1-\tau),$$
(2-28)

where

 $\begin{array}{ll} k_{st} & = \text{substrate thermal conductivity,} \\ \rho_{st} & = \text{substrate density,} \\ c_{st} & = \text{substrate specific heat, and} \\ \tau & = \frac{e_{dc}}{e_{dc} + c_f \left(\frac{T_I - T_{dc}}{3}\right)}. \end{array}$

When bubble agitation heat transfer is specified, Eq. 2-27 can be applied to the concrete and solidified debris substrate surfaces. For the cases of solidified debris and steel surfaces, the decomposition temperature and enthalpy are taken equal to the solidus temperature and latent heat of fusion, respectively. If the substrate interface temperature has not reached or has fallen below the decomposition temperature, or the substrate is not locally degassing, the bubble agitation heat transfer coefficient is set equal to zero and the downward heat transfer coefficient is evaluated using the forced convection expression defined in Eq. 2-25.

Bradley's modification^[51] to Kutateladze's bubble agitation heat transfer coefficient^[50] is given through the equation

$$h_{bot} = \begin{cases} 1.5 \cdot 10^{-3} C_i \left(\frac{k}{L}\right) (Ku)^{2/3}; j_g < j_{tr} \\ 1.5 \cdot 10^{-3} C_i \left(\frac{k}{L}\right) (Ku)^{2/3} \left(\frac{j_g}{j_{tr}}\right)^{-1/2}; j_g \ge j_{tr} \end{cases},$$
(2-29)

where

Ku
$$= \frac{Pc j_g}{kg} ,$$
$$j_{tr} = 4.3 \cdot 10^{-4} \frac{\sigma}{\mu} ,$$

and C_i is a constant which accounts for the effects of transient interaction of core materials with concrete. For ablating concrete, C_i represents the effects of thermal resistance across the rising slag layer in which case $Ci \simeq 0.29$. Bradley's model is implemented into MELTSPREAD3 in an identical manner.

At the melt lower surface, a variety of boundary conditions are treated to encompass a range of melt-substrate interaction conditions. A summary of these boundary conditions is provided in Table 2-4, while physical depictions of these states are provided in Figure 2-3. The index NBCINT (acronym for the <u>Number of the Boundary Condition at the INT</u>erface) is the internal variable used in MELTSPREAD3 to denote the various boundary conditions summarized in Table 2-4. For the purpose of consistency, the equations governing the interfacial heat transfer for these various boundary conditions are described using this notation below.

For the case NBCINT = 1, which corresponds to a convective boundary condition, the energy balance at the melt/substrate interface is of the form,

$$h_{bot}(T - T_{st}) = -k_{st} \frac{\partial T_{st}}{\partial x} |_{x=o} . \qquad (2-30)$$

For the case NBCINT = 2, which corresponds to crust growth with no ablation of underlying substrate, the interfacial boundary condition when decay heat in the crust is negligible (See table 2-1) is of the form,

$$k_{cr}\left(\frac{T_{sol,cr}-T_{sf}}{\delta_{cr}}\right) = -k_{st}\frac{\partial T_{st}}{\partial x}|_{x=o} , \qquad (2-31)$$

where

k _{cr}	= crust thermal conductivity,
T _{sol,cr}	= solidus temperature of crusting material,
δ_{cr}	= crust thickness.

The crust thickness, δ_{cr} , is governed by the equation,

$$\rho_{cr} \,\Delta e_{cr} \frac{d\delta_{cr}}{dt} = k_{cr} \frac{(T_{sol,cr} - T_{sf})}{\delta_{cr}} - h_{bot} \big(T - T_{sol,cr} \big), \tag{2-32}$$

where

 $\rho_{cr} = crust density,$ $\Delta e_{cr} = crust latent heat of fusion.$

For the case NBCINT = 3, the downward heat transfer to the underlying substrate is assumed to be limited by thin crust segments. For this case, the melt/substrate boundary condition is given through the equation,

$$h_{bot}(T - T_{sol,cr}) = -k_{st} \frac{\partial T_{st}}{\partial x} |_{x=o}$$
(2-33)

NBCINT*	Boundary Condition Type
1	Convective boundary condition; heat transfer coefficient, h
2	Crust growth, no substrate ablation
3	Thin crust, no substrate ablation
4	Ablating substrate, no crust, ablated substrate continuously
	mixed into melt
5	Ablating substrate, no crust, ablated substrate remain as film
	over substrate surface
6	Porous crust growth over ablating substrate; substrate drains
	through crust into melt
7	Thin porous crust over ablating substrate
8	Non-porous crust growth over ablating substrate; ablated
	substrate remains as film beneath crust
9	Thin non-porous crust over ablating substrate; ablated
	substrate remains as film beneath crust

Table 2-4 SUMMA	RY OF MEL	F/SUBSTRATE	INTERFACIAL	BOUNDARY	CONDITIONS	TREATED II	N MELTSPREAD3
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*Denotes boundary condition index; same parameter used internal to the code.







Figure 2-15 Depiction of Various Melt/Substrate Interaction Boundary Conditions Treated by MELTSPREAD3











Figure 2-3 Depiction of Various Melt/Substrate Interaction Boundary Conditions Treated by MELTSPREAD3 (Cont'd.)

If the melt/substrate or crust/substrate interface temperature exceeds the substrate solidus temperature, then an ablation calculation is initiated. For the case NBCINT = 4, which corresponds to the situation in which the ablated material is continuously mixed into the melt, the interfacial boundary condition is given through the equation,

$$T_{st} \mid_{x=0} T_{sol,st},$$
 (2-34)

and the substrate ablation rate is governed by the equation,

$$\rho_{st} \Delta e_{st} \frac{d\eta}{dt} = -k_{st} \frac{\partial T_{st}}{\partial x} |_{x=0} - h_{bot} \left(T - T_{sol,st} \right), \qquad (2-35)$$

where

$ ho_{st}$	= substrate density,
Δe_{st}	= substrate latent heat of fusion,
T _{sol,st}	= substrate decomposition or solidus temperature,
η	= depth of ablated substrate.

For the case NBCINT = 5, which corresponds to the situation in which the substrate is ablating in the absence of crust formation and the ablated substrate remains on the surface as a film, the boundary condition at the substrate surface is given by the equation,

$$T_{st} \mid_{x=0} T_{sol,st}.$$
 (2-36)

The substrate ablation and film growth rates are given by the equations,

$$\rho_{st} \,\Delta e_{st} \frac{d\eta}{dt} = -k_{st} \frac{\partial T_{st}}{\partial x} \mid_{x=0} - k_f \,\left(\frac{T_I - T_{sol,st}}{\delta_f}\right),\tag{2-37}$$

$$\rho_f \, \frac{d\delta_f}{dt} = -\rho_{st} \frac{d\eta}{dt} \, , \qquad (2-38)$$

where

 $T_I = \text{melt/film interfacial temperature},$

and subscript f denotes properties of the ablated substrate film. The interface temperature, T_I , between the melt and film is found through the following energy balance,

$$h_{bot}(T - T_1) = h_f\left(\frac{T_1 - T_{sol,st}}{\delta_f}\right), \qquad (2-39)$$

i.e.,

$$T_I = \frac{1}{h_{bot} + k_f / \delta_f} \left\{ h_{bot} T + \frac{k_f}{\delta_f} T_{sol,st} \right\}.$$
 (2-40)

With this equation, T_l can be eliminated from Eq. 2-37 to obtain

$$\rho_{st} \Delta e_{st} \frac{d\eta}{dt} = -k_{st} \frac{\partial T_{st}}{\partial x} |_{x=0} - \frac{k_f h_{bot}}{\delta_f h_{bot} + k_f} \left(T - T_{sol,st} \right).$$
(2-41)

For the case NBCINT = 6, which corresponds to the situation in which the substrate is ablating in the presence of porous crust formation and the ablated substrate continuously drains through the porous crust, the substrate boundary condition is given through the equation,

$$T_{st}|_{x=0} = T_{sol,st}$$
 (2-42)

The simultaneous equations for the rate of crust growth and the rate of substrate ablation are of the form,

$$\rho_{cr} \,\Delta e_{cr} \frac{d\delta_{cr}}{dt} = -k_{cr} \left(\frac{T_{sol,cr} - T_{sol,st}}{\delta_{cr}} \right) - h_{bot} \left(T - T_{sol,cr} \right), \qquad (2-43)$$

$$\rho_{st} \,\Delta e_{st} \frac{d\eta}{dt} = -k_{cr} \left(\frac{T_{sol,cr} - T_{sol,st}}{\delta_{cr}} \right) - k_{st} \frac{\delta T_{st}}{\delta x} \,|_{x=0}. \tag{2-44}$$

For the case NBCINT = 7, which corresponds to a thin porous crust over ablating substrate, the substrate boundary condition is given through the equation,

$$T_{st} \mid_{x=0} = T_{sol,st} \,. \tag{2-45}$$

The substrate ablation rate is governed by the equation,

$$\rho_{st} \Delta e_{st} \frac{d\eta}{dt} = -k_{st} \frac{\partial T_{st}}{\partial x} |_{x=0} - h_{bot} \left(T - T_{sol,cr} \right).$$
(2-46)

For the case NBCINT = 8, which corresponds to non-porous crust growth over ablating substrate and the ablated substrate is retained as a molten film beneath the crust, the substrate boundary condition is given through the equation,

$$T_{st}|_{x=0} = T_{sol,st}$$
. (2-47)

The simultaneous equations governing the rate of crust growth, the rate of substrate ablation, and the rate of molten film formation are of the form,

$$\rho_{cr} \,\Delta e_{cr} \frac{d\delta_{cr}}{dt} = k_{cr} \left(\frac{T_{sol,cr} - T_I}{\delta_{cr}} \right) - h_{bot} \left(T - T_{sol,cr} \right) \,, \tag{2-48}$$

$$\rho_{st} \,\Delta e_{st} \frac{d\eta}{dt} = -k_{st} \frac{\partial T_{st}}{\partial x} \,|_{x=0} - k_f \,\left(\frac{T_I - T_{sol,st}}{\delta_f}\right), \tag{2-49}$$

$$\rho_f \frac{d\delta_f}{dt} = -\rho_{st} \frac{d\eta}{dt} \quad , \tag{2-50}$$

where

$T_I = \text{crust/film interfacial temperature.}$

The interface temperature T_I is eliminated through an energy balance of the form,

$$k_{cr}\left(\frac{T_{sol,cr}-T_I}{\delta_{cr}}\right) = k_f\left(\frac{T_I-T_{sol,st}}{\delta_f}\right) , \qquad (2-51)$$

i.e.,

$$T_I = \frac{T_{sol,cr}(k_{cr}/\delta_{cr}) + T_{sol,st}(k_f/\delta_f)}{k_{cr}/\delta_{cr} + k_f/\delta_f} \quad . \tag{2-52}$$

With Eqs. 2-51 and 2-52, Eqs. 2-48 and 2-49 may be rewritten as,

$$\rho_{cr} \,\Delta e_{cr} \frac{d\delta_{cr}}{dt} = k_{eff} \left(\frac{T_{sol,cr} - T_{sol,st}}{\delta_{cr}} \right) - h_{bot} \left(T - T_{sol,cr} \right), \tag{2-53}$$

$$\rho_{st} \,\Delta e_{st} \frac{d\eta}{dt} = -k_{st} \frac{\partial T_{st}}{\partial x} \mid_{x=0} - k_{eff} \left(\frac{T_{sol,cr} - T_{sol,st}}{\delta_{cr}} \right), \tag{2-54}$$

where k_{eff} is the effective thermal conductivity across crust and film and is written as

$$k_{eff} = \frac{k_{cr}k_f}{k_{cr}\delta_f/\delta_{cr}+k_f},$$
(2-55)

For the case NBCINT = 9, which corresponds to a thin nonporous crust over ablating substrate and the ablated substrate is retained as a molten film beneath the crust, the substrate boundary condition is given through the equation,

$$T_{st}|_{x=0} = T_{sol,st}$$
 (2-56)

The equation governing the substrate ablation rate is of the form,

$$\rho_{st} \,\Delta e_{st} \frac{d\eta}{dt} = -k_{st} \frac{\partial T_{st}}{\partial x} \mid_{x=0} - h_{bot} \left(T - T_{sol,cr} \right), \tag{2-57}$$

where the following energy balance has been employed to express the conduction heat transfer rate across the molten substrate film in terms of the heat convected to the thin crust,

$$k_f \ \frac{(T_{sol,cr} - T_{sol,st})}{\delta_f} = h_{bot} \left(T - T_{sol,cr} \right). \tag{2-58}$$

MELTSPREAD3 has been set up to perform a mechanistic calculation of the melt/substrate interfacial heat transfer for various boundary conditions based on user-supplied options which determine the physical modeling assumptions employed in the analysis. Flexibility is desirable due to modeling uncertainties regarding the appropriate form of the heat transfer boundary condition at the melt/substrate interface (See Table 2-1). The boundary condition progression calculated by MELTSPREAD3 is illustrated by the flow diagram shown in Figure 2-4. The progression is based on user-supplied modeling assumptions as well as the local thermal conditions at the melt/substrate interface. The modeling assumptions currently available in MELTSPREAD3 are summarized below.

Crust Formation Versus Bulk Freezing

This option allows the user to specify crust formation at the substrate surface, or melt flow with no crust formation until the melt specific enthalpy falls below the solidus value at which point melt is immobilized and added to previously solidified melt and concrete in the calculation. For the case of flow over concrete surfaces, the bulk freezing option is motivated by the uncertainty regarding continued crust formation and stability in the presence of sparging concrete decomposition gases. For the case of flow over steel surfaces, crust formation on the substrate will most likely occur. Note that regardless of the choice of bulk freezing or crust formation, if the melt enthalpy locally falls below the solidus value, the melt is immobilized and incorporated into the local volume fraction of the corium oxide phase. If the volume fraction of the oxide phase is greater than 64%³ and the enthalpy of the mixture has fallen below the enthalpy evaluated at the oxide phase solidus temperature, then the corium is immobilized. If this condition is not met, then the corium mixture is immobilized when the mixture enthalpy falls below the enthalpy evaluated at the metal phase solidus temperature.

³ This is the maximum random close packing fraction based on computer simulations and experiments; see <u>https://en.wikipedia.org/wiki/Random_close_pack</u>.

Growing Crust Versus Thin Crust Segments

If crust growth is selected, this option allows the user to specify continuous crust growth at the substrate surface versus heat transfer limited by thin crust segments. However, for this case the bulk freezing check described above is still performed, and the core debris is immobilized if the conditions for bulk freezing are met.

Porous Crust Versus Non-Porous Crust

If the crust option is chosen and the underlying substrate reaches the melting temperature, a substrate ablation calculation is automatically invoked. The crust porosity option allows the user to specify whether the ablated substrate material will penetrate through the crust into the overlying melt layer, or be retained as a molten film beneath the crust. For the case of flow over concrete, any crust that forms and adheres to the surface will, by necessity, be porous as a result of the venting of concrete decomposition gases. Otherwise, the gas would simply pressurize and eventually break the crust. Additionally, concrete slag has a much lower density than corium and therefore buoyancy forces will most likely cause the slag to rise through the crust pores into the overlying melt. In contrast, for flow over steel plate surfaces, the presence of steel may act to locally suppress (or divert) concrete decomposition gases, should concrete be present beneath the steel. In this case, the corium crust may be non-porous, and the ablated steel will be trapped beneath the crust. Although available as a user option, scoping calculations indicate that this boundary condition is at best highly transient, as any slag that forms acts as an insulator between the melt and ablating surface. Thus, the buildup of this additional thermal resistance quickly causes ablation to stop, and so the process is inherently self-limiting. Thus, this boundary condition option is felt to be physically unrealistic.

Mixing Versus Non-Mixing of Ablated Material

If the bulk freezing option is chosen and the substrate surface temperature reaches the melting temperature, a substrate ablation calculation is automatically invoked. The mixing option allows the user to specify whether the ablated material is continuously mixed into the melt or locally remains as a molten film over the surface. For the case of flow over concrete, sparging decomposition gases are expected to rapidly mix the slag into the melt layer and. Moreover, and based on the discussion provided immediately above, mixing of ablated material is felt to be the physically realistic boundary condition option.



Figure 2-4. Boundary Condition Progression Based on Thermal Conditions and User-Supplied Modeling Assumptions.

HEAT TRANSFER AT MELT UPPER SURFACE

Crust formation can also be specified at the melt upper surface. However, a time-dependent crust growth calculation is currently not performed. If noncondensable gases are locally sparging the melt, it is assumed that the gas flux breaks up any crust which may form into segments/platelets that are continuously mixed into the melt, thereby effectively negating the limiting heat transfer effects of crust formation. For this case the melt layer upper surface temperature will approximately equal the bulk temperature. In reality, as the local superficial gas velocity decreases, a point will be reached^[52] at which pool agitation forces are no longer sufficient to preclude incipient crust formation, and a stable insulating crust will develop which separates the melt from the overlying medium (See Table 2-1). Thus, the upward heat transfer rate calculated using this modeling approach likely represents an upper bound.

With these assumptions, the heat flux at the top of the melt is given through the equation

$$q_{top} = h_{top,med}(T - T_{med}) , \qquad (2-59)$$

where

T_{med} = temperature of overlying medium,
 h_{top,med} = heat transfer coefficient from the melt upper surface to the overlying medium.

Explicit forms for $h_{top,med}$ are provided later in this section. If the local gas flux is zero, then a thin crust is assumed to form at the melt upper surface. For this case, the heat transfer from the bulk melt to the upper surface is given through the equation,

$$q_T = h_{top,melt} \left(T - T_{sol,cr} \right) \,, \tag{2-60}$$

where

 $h_{top,melt}$ = heat transfer coefficient from melt to upper surface.

The heat transfer coefficient $h_{top,melt}$ is set equal to that given by Eq. 2-24 for forced convection at the melt lower surface.

As a user option, the heat transfer from the melt upper surface may be assumed to be limited by a thin crust regardless of the presence of sparging concrete decomposition gases. For this case, the local check on the gas flux is bypassed and the upper heat transfer is calculated according to Eq. 2-60.

At the melt upper surface, heat transfer to either an overlying water layer or direct heat transfer to the containment atmosphere is treated. If water is absent, the heat transfer is calculated assuming radiation off the top of the melt. For this case, the heat transfer coefficient is given through the equation,

$$h_{top} = \frac{\sigma_{stef}}{1/\epsilon + 1/\epsilon_{struc} - 1} (T^2 + T_{struc}^2) (T + T_{struc}) , \qquad (2-61)$$

where

 σ_{stef} = Stefan-Boltzmann constant = 5.67 $\cdot 10^{-8} W/m^2 K$, ϵ = melt emissivity, ϵ_{struc} = emissivity of overlying structure, T_{struc} = temperature of overlying structure.

Currently there is no calculation of the heatup of the overlying structure due to thermal radiation off the top of the melt. Thus, T_{struc} is constant at a user-specified value over the duration of the calculation. Additionally, energy absorption by the steam/gas mixture above the melt is not treated. The resultant gas heatup will reduce the overall radiant heat transfer from the melt upper surface (See Table 2-1).

In Mark I containments, the downcomers limit the water height in the pedestal and drywell regions by allowing for spillover into the steam suppression pool (see Figure 1-1). If water is present in the drywell, a local check on the height of the melt layer relative to the downcomer height is performed. If the melt height exceeds the downcomer height, radiant heat transfer to overlying structure is assumed and the heat transfer coefficient is calculated through Eq. 2-60.

For flooded cavity conditions, if the local melt height is less than the local water height as set by the downcomer height in the simple water model, or as calculated by the detailed water inventory model that is described later in this section, then heat transfer from the melt upper surface is calculated along a full boiling curve. As the melt is cooled and solidified, the local surface temperature may fall below the minimum film boiling temperature. In this case, the surface will quench and a nucleate boiling regime will be encountered. Heat transfer in this regime is modeled using Rohsenow's correlation.^[53] The nucleate boiling heat flux is given through the equation,

$$q_{nb} = \frac{\mu_l h_{lv} c_{sf}^{-3}}{\sqrt{\frac{\sigma_l}{g(\rho_l - \rho_v)}}} \left(\frac{c_l \Delta T_{sat}}{h_{lv}}\right)^3 \left(\frac{k_l}{c_l \mu_l}\right)^{5.1} , \qquad (2-62)$$

where

C_{sf}	= empirical constant for a given surface and boiling liquid,
μ_l	= water viscosity,
h_{lv}	= water latent heat of vaporization,
σ_l	= water surface tension,
$ ho_l$	= water density,
$ ho_v$	= water vapor density,
c _l	= water specific heat at constant pressure,
k _l	= water thermal conductivity,
ΔT_{sat}	$= T_{sf} - T_{sat}$, and
T _{sat}	= water saturation temperature.

The empirical constant C_{sf} in Eq. 2-62 varies widely for different heater surface/boiling liquid combinations.^[53] For the purposes of this work, the constant is assumed to equal the value reported for water and stainless steel;^[53] i.e., $C_{sf} \simeq 0.02$.

The critical heat flux is evaluated using the correlation of Ivey-Morris,^[54] which accounts for bulk liquid subcooling. The critical heat flux is given through the equation,

$$q_{CHF} = q_{CHF,sat} \left[1 + 0.1 \left(\frac{\rho_l}{\rho_v} \right)^{3/4} \frac{c_l \Delta T_{sub}}{h_{lv}} \right], \qquad (2-63)$$

where

 ΔT_{sub} = bulk liquid subcooling,

and $q_{CHF,sat}$ is the critical heat flux for saturated liquid and is evaluated using the correlation developed by Zuber,^[54]

$$q_{CHF} = 0.14 \,\rho_{\nu} h_{l\nu} \left(\frac{\rho_{\nu}^2}{g \,\sigma_l(\rho_l - \rho_{\nu})} \right)^{1/4} \,. \tag{2-64}$$

The surface superheat at which the critical heat flux is reached is found by equating Eqs. 2-62 and 2-63. This yields,

$$\Delta T_{CHF} = \left(\frac{q_{CHF}}{\alpha_{nb}}\right)^3 , \qquad (2-65)$$

where

$$\alpha_{nb} = \frac{h_{lv}\mu_l}{\sqrt{\frac{\sigma_l}{g(\rho_l - \rho_v)}}} C_{sf}^{-3} \left(\frac{c_l}{h_{lv}}\right)^3 \left(\frac{k_l}{c_l\mu_l}\right)^{5.1} \quad .$$
(2-66)

The surface superheat at the minimum film boiling point is modeled using the correlation of Henry.^[56] The correlation is of the form,

$$\Delta T_{min} = \Delta T_{min,B} + 0.42 \left(\Delta T_{min,B+} \Delta T_{sub} \right) \left[\sqrt{\frac{(k\rho c)_l}{(k\rho c)_{sf}}} \cdot \frac{h_{lv}}{c_{sf} \Delta T_{min,B}} \right]^{0.6}, \qquad (2-67)$$

where $\Delta T_{min,B}$ is the minimum film boiling temperature given by Berenson's model,^[57]

$$\Delta T_{min,B} = 0.127 \ \frac{h_{lv}\rho_v}{k_v} \left[\frac{g(\rho_l - \rho_v)}{\rho_l + \rho_v}\right]^{2/3} x \left[\frac{\sigma_l}{g(\rho_l + \rho_v)}\right]^{1/2} x \left[\frac{\mu_v}{g(\rho_l - \rho_v)}\right]^{1/3} , \qquad (2-68)$$

where

 k_v = water vapor thermal conductivity, μ_v = water vapor viscosity.

In the transition boiling regime, the heat flux is assumed to vary linearly between the critical heat flux and the film boiling heat flux evaluated at the minimum film boiling temperature,

$$q_{tran} = q_{CHF} + \frac{(q_{fb,min} - q_{CHF})}{\Delta T_{min} - \Delta T_{CHF}} \left(\Delta T_{sat} - \Delta T_{CHF}\right) , \qquad (2-69)$$

where

 $q_{fb,min}$ = film boiling heat flux evaluated at ΔT_{min} .

The film boiling heat flux at the minimum film boiling temperature is obtained through the model described below.

Due to the extremely high temperatures associated with prototypic reactor materials in a molten state, initial film boiling heat transfer is anticipated for the case of corium spreading beneath an overlying water layer. Prediction of the film boiling heat flux for this case is complicated by the presence of sparging concrete decomposition gases which may influence the rate of melt-towater heat transfer. A model has been developed as part of this work to describe this process.

The approach is to extend in an integrated fashion the film boiling model of Berenson^[57] to account for additional phenomena perceived to be important in the prediction of melt-to-water heat transfer. These phenomena include (but are not necessarily limited to) radiant heat transfer across the vapor film, bulk liquid subcooling, and interfacial area enhancement due to sparging gas. A depiction of these processes was given in Figure 1-7.

The overall heat transfer coefficient between the melt and overlying coolant layer is written as

$$h_{tot} = A_*(h_{cond} + h_{rad}) ,$$
 (2-70)

where

$$h_{rad} = \sigma_{stef} \epsilon (T^2 + T_{sat}^2) (T + T_{sat}) , \qquad (2-71)$$

$$h_{cond} = \frac{k_v}{\delta_g} , \qquad (2-72)$$

 A_* = dimensionless interfacial area enhancement,

 δ_q = gas film thickness.

The conduction heat transfer coefficient across the film, h_{cond} , accounts for subcooling and implicitly includes the effects of radiation heat transfer, which acts to thicken the vapor film. The quantity A_* is the dimensionless area enhancement that accounts for the effects of surface deformation due to sparging gas. The radiation view factor between the melt and overlying water layer is set equal to unity based on the assumption that the vapor film thickness will be small in comparison to the length scale of the melt surface deformations due to gas sparging. An energy balance at the liquid-vapor interface yields the following expression for the net steam superficial gas velocity into the film:

$$j_{\nu} = \frac{A_*}{\rho_{\nu} h_{l\nu}} \left\{ \frac{k_{\nu}}{\delta} \Delta T_{sat} + h_{rad} \Delta T_{sat} - h_{sub} \Delta T_{sub} \right\}, \qquad (2-73)$$

where $h_{sub}\Delta T_{sub}$ is the interfacial cooling heat flux due to bulk liquid subcooling. This term accounts for suppression of the steam generation rate at the interface due to energy transport into the bulk liquid when the liquid is subcooled.

In order to solve for δ_g , an additional equation is required. Following Berenson's approach,^[57] the radial steam velocity in the film is related to the pressure drop across the film as

$$\frac{dP}{dr} = \frac{C\mu_v}{\delta_g^2},\tag{2-74}$$

where C = 12 for the no-slip boundary condition at the film-liquid interface, or C = 3 for the no-shear boundary condition. Upon noting that two nodes (bubbles) are growing in an area of the gas/liquid interface equal to λ^2 at any time (Sunas et. al^[58]), the film radial gas velocity is found as

$$\nu = \left(\frac{\lambda^2/2 - \pi r^2}{2\pi r \delta_g}\right) j_\nu,\tag{2-75}$$

where

$$\lambda = 2\pi \sqrt{\frac{\sigma_l}{g(\rho_1 - \rho_e)}} \,. \tag{2-76}$$

the expression for the film thickness is obtained by integration on Eq. 2-74 over the Taylor bubble site. The resultant pressure differential across the film is evaluated in terms of the combined hydrostatic and surface tension pressures associated with the presence of the bubble at the Taylor instability site (Berenson^[57]). These considerations yield the following transcendental equation for the gas film thickness in the presence of gas injection, radiation, and subcooling,

$$\delta_g^3 = \frac{C_2^4 \mu_v}{\rho_v h_{lv} g(\rho_1 - \rho_v)} \sqrt{\frac{\sigma_l}{(\rho_1 - \rho_v)}} \left\{ A_* \left[k_v \frac{\Delta T_{sat}}{\delta_g} + h_{rad} \Delta T_{sat} - h_{sub} \Delta T_{sub} \right] \right\}$$
(2-77)

where C_2 is an empirical constant. Berenson's equation for the film thickness is obtained by setting $h_{rad} = 0$ and $h_{sub} = 0$ in Eq. 2-77. In order to recover Berenson's equation for the film thickness in these limits, C_2 is set equal to 2.35.

Introduction of Berenson's equation for the film thickness as a scale for δ_g in Eq. 2-77 yields the following dimensionless expression,

$$\delta_*^3 = A_* \left(\frac{1}{\delta_*} + \beta_{rad} - \beta_{sub} \right) , \qquad (2-78)$$

where

$$\delta_*^3 = \frac{\delta_g}{\delta_B}; \ \delta_B = 2.35 \left[\frac{k_\nu \mu_\nu \Delta T_{sat}}{\rho_\nu g(\rho_1 - \rho_\nu) h_{l\nu}} \sqrt{\frac{\sigma_l}{g(\rho_1 - \rho_\nu)}} \right]^{1/4}, \tag{2-79}$$

$$\beta_{rad} = \frac{h_{rad}}{k_v / \delta_B} \,, \tag{2-80}$$

$$\beta_{sub} = \frac{h_{sub} \Delta T_{sub}}{k_v \Delta T_{sat} / \delta_B}.$$
(2-81)

Eq. 2-78 is a quartic equation for δ_* which can be solved to yield

$$\delta_* = \frac{1}{2} \left\{ \left[2[\alpha^2 + 4]^{1/2} - \alpha \right]^{1/2} - sgn \varepsilon \alpha^{1/2} \right\} A_*^{1/4} \quad , \tag{2-82}$$

where

$$\alpha = \left[e + \frac{\varepsilon^2}{2}\right]^{1/3} - \left[e - \frac{\varepsilon^2}{2}\right]^{1/3},$$
(2-83)

$$e = \left[\frac{\varepsilon^4}{4} + \left(\frac{4}{3}\right)^3\right]^{1/2},$$
 (2-84)

$$sgn \varepsilon = \begin{cases} 1, \ \beta_{sub} - \beta_{rad} \ge 0\\ -1, \ \beta_{sub} - \beta_{rad} < 0 \end{cases},$$
(2-85)

and $\varepsilon \equiv (\beta_{sub} - \beta_{rad})/A_*$. Equation 2-82 is the dimensionless correction to Berenson's expression for the vapor film thickness for radiation and subcooling.

Bulk liquid subcooling will act to suppress the vapor generation rate and thereby reduce the vapor film thickness. The present approach is to assume that bubble departure at the nodes of the Taylor instability will periodically replenish the subcooled liquid adjacent to the interface. This approach was originally employed by Szekely^[59] in the analysis of the interfacial heat transfer between two immiscible fluid layers, and more recently by Kao and Kazimi^[49] in

the development of their periodic contact model for the analysis of molten coreconcrete interaction (MCCI). h_{sub} is thus estimated as

$$h_{sub} = \frac{2_{kl}\sqrt{f}}{\sqrt{\pi\alpha_1}} \tag{2-86}$$

and, therefore,

$$\beta_{sub} = C_3 \left(\frac{2_{kl} \Delta T_{sub} \sqrt{f}}{\sqrt{\pi \alpha_1} k_v \, \Delta T_{sat} / \delta_B} \right)^n.$$
(2-87)

The bubble departure frequency, f, is assumed to equal the critical wave frequency of the Taylor instability^[60]

$$f = \frac{1}{2\pi} \left[\frac{\sigma_l}{(\rho_1 + \rho_e)} \left(g \, \frac{(\rho_1 - \rho_e)}{\sigma_l} \right)^{3/2} \right]^{1/2} \tag{2-88}$$

The empirical constants C_3 and n in Eq. 2-87 are introduced to account for the fact that condensation due to subcooling acts to suppress the growth rate of the Taylor instability^[61] below that predicted by Eq. 2-88. No attempt to model the effects of condensation on wave frequency are made here.

Although there is a considerable amount of experiment data available in the literature regarding subcooled film boiling over spheres and cylinders, little information has been reported for the case of subcooled film boiling over flat plates. In the absence of such data, a preliminary adjustment of the constants in Eq. 2-87 was made according to the horizontal cylinder data of Sakurai et. al.^[62] The results of this comparison indicate that $C_3 \simeq 2.0$ and $n \simeq 0.5$.

The dimensionless interfacial are enhancement, A_* , is estimated through the following argument. For a two-phase flow, the bubble number flux transverse to the pool is j/V_b , where V_b = bubble volume. If the bubbles have a residence time of t_r on the surface of the pool prior to rupture, then the number of bubbles per unit area observable on the surface at any given time will be jt_r/V_b . The projected surface area covered by a bubble on the surface is πR^2 ; if the local surface area of the perturbed interface due to bubble impact is denoted A_{dome} , then the dimensionless surface area is found as

$$A_* = 1 + \left(\frac{jt_r \pi R^2}{V_b}\right) \left(\frac{A_{dome}}{\pi R^2} - 1\right).$$
(2-89)

The sparging gas bubbles are assumed to be brought to rest at the surface of the melt with the bubble centroid at an elevation of R above the surface from a terminal rise velocity of U_T . This geometric picture is drawn from the

immersible fluid layer mixing experiments of Greene et. al.^[63] If it is assumed that the residence time of the bubbles on the surface is proportional to the time required to bring the bubble to rest, then $t_r \simeq 2R/U_T$. The surface area of the distended interface under these geometric assumptions is $4\pi R^2$. With these assumptions, Eq. 2-89 becomes,

$$A_* = 1 + 4.5 \, \frac{j}{u_r} \tag{2-90}$$

where U_T has been previously defined in Eq. 2-21. Equation 2-90 has a similar functional dependency to Greene's empirically-based correlation^[64-65] for the augmentation in film boiling heat flux due to sparging gas.

As is evident from Eqs. 2-70 and 2-90, for reactor core materials, interfacial area enhancement due to sparging decomposition gases will cause rapid escalation in the film boiling heat flux with increasing superficial gas velocity. This tendency cannot proceed indefinitely. For situations in which the film boiling heat flux exceeds the critical heat flux, rapid vapor generation will begin to levitate the water away from the deformed corium surface. At this point, the assumption that the length scale of the corium surface deformations due to sparging gas are large in comparison to the gas film thickness may no longer be valid. Thus, the melt/water interfacial area augmentation predicted by Eq. 2-90 is capped at 3.0 within the code.

WATER INVENTORY MODEL

The previous section outlined the various models that have been implemented in MELTSPREAD3 to calculate heat transfer to overlying water. The code has also been structured to provide a detailed water inventory modeling capability. As for the melt spreading analysis, the overall approach is to solve coupled mass, momentum, and energy equations for the water layer overlying the melt to calculate local depths, velocities, and boiloff rates while factoring in the potential for water injection as well as spillover into downcomers that may exist in the cavity. The underlying material can consist of either spreading core debris, or uncovered containment floor. The velocity of the flowing water is dependent upon the local gravity head of the water layer. In particular, the fluid velocity is assumed to satisfy the equation,

$$\frac{\partial U_w}{\partial t} + \frac{1}{2} \frac{\partial U_w^2}{\partial z} = g \frac{\partial}{\partial z} [H_w + E] - \frac{4\tau_w}{\rho_l D_w}, \qquad (2-91)$$

where:

U_w	= local water spreading velocity,
H_w	= local collapsed water depth,
D_w	= equivalent water hydraulic diameter = $4H_{\omega}$,
E	= local substrate elevation,

and τ_w is the frictional shear stress at the water-debris interface that is evaluated through the equation,

$$\tau_w = \frac{1}{2} \rho_l f_w U_w |U_w|, \qquad (2-92)$$

where f_w is the water flow friction factor. As for the core debris, water spreading is restricted to occur such that the depth at the leading edge does not fall below the minimum depth at which surface tension balances gravity,

$$H_{w,min} = \sqrt{\frac{2\sigma_l}{\rho_l g}} . \tag{2-93}$$

The friction factor f_w in Eq. 2-92 is dependent upon the local water flow Reynolds number which is defined through the equation,

$$Re = \frac{\rho_l D |U_w|}{\mu_l} \,. \tag{2-94}$$

Given the Reynolds number definition, the friction factor is calculated using the correlations defined in Eqs. 2-11 through 2-13 for core debris. The equivalent sand roughness R_{sand} in Eqs. 2-13 is set within the code to $R_{sand} = 1$ cm for core debris to reflect observed surface imperfections^[14] in this type of material that has been cooled by overlying water. One modeling limitation in the current approach for calculating frictional flow resistance of water spreading over core debris is that the effect of particle beds has not been considered. These types of porous structures that could be formed by melt jet fragmentation and/or melt eruptions would clearly increase the flow resistance, but this effect is not addressed in the current analysis.

The general form of the conservation of mass equation for the water layer is as follows,

$$S \frac{\partial}{\partial t}(\rho_l H_w) + \frac{\partial}{\partial z}(S\rho_l H_w U_w) = S\dot{m}_w', \qquad (2-95)$$

where

 $\dot{m}_{w}^{"}$ = net local *influx* of water from extraneous sources.

The coolant mass conservation equation is thus of the form:

$$\dot{m}_w = \dot{m}_w A = \dot{m}_{inj} - \dot{m}_{st} - \dot{m}_{dc} \tag{2-96}$$

where A is local surface area and subscript *inj* denotes injected water, *st* denotes coolant steaming rate due to heat transfer from the core debris, and *dc* denotes the local gravity-driven mass flowrate into downcomers that may be present on the containment floor. The rate of local coolant loss due to boiling is expressed as

$$\dot{m}_{st} = \begin{cases} \frac{q_{wat}A}{h_{lv}}; & T_w = T_{sat} \\ 0; & T_w < T_{sat} \end{cases}$$
(2-97)

where $q_{wat}^{"}$ is the local heat flux from the debris to the overlying coolant and is evaluated based on the local boiling heat transfer conditions that are active at the time; expressions were provided in the previous section.

As noted, water flow into downcomers (i.e., spillover points) can be calculated at specified locations as a user option. The available flow area for water to enter each downcomer is calculated as the water height above the downcomer inlet times a 'cord length', C_{dc} that is specified as part of the user input. For instance, if the downcomer is a circular pipe with a horizontally oriented opening, then the cord length would simply be the pipe diameter. The water flow velocity is calculated using a simple 1-D quasi-steady solution to Bernoulli's equation that relates the flow velocity over the edge to the local water height above the edge; i.e., $u_{dc} = \sqrt{2g\Delta H}$, where $\Delta H = H_w - H_{dc}$ is the water height over the top of the downcomer inlet. With this background, then by conservation of mass the water mass flowrate into each downcomer is given by

$$\dot{m}_{dc} = \begin{cases} \rho_l \sqrt{2g} C_{dc} \Delta H^{3/2}; \ H_w \ge H_{dc} \\ 0; \qquad H_w < H_{dc} \end{cases}$$
(2-98)

As noted earlier, the effect of coolant voiding on pool swell and onset of spillover into the downcomers is not accounted for in this simplified model.

A water conservation of energy equation is solved to evaluate local coolant heatup for situations in which the coolant is subcooled. The water specific enthalpy is obtained from the solution of the equation,

$$S\frac{\partial}{\partial t}(\rho_l H_w e_w) + \frac{\partial}{\partial z}(S\rho_l H_w e_w U_w) = S(q_{wat}^{"} + \dot{m}_{inj}^{"} e_{inj} - \dot{m}_{dc}^{"} e_w)$$
(2-99)

where:

e_w	= water specific enthalpy,
e_{inj}	= injection water specific enthalpy,
$\dot{m}^{''}_{inj}$	= local mass flux of water injection, and
$\dot{m}_{dc}^{"}$	= local mass flux of water into spillover points.

MELT JET BREAKUP MODEL

A melt jet breakup model (Figure 1-5) has been implemented to evaluate the effect of fragmentation in a water pool beneath the RPV on subsequent spreading behavior. The model requires melt pour rate and RPV hole diameter vs. time as inputs, as well as the RPV elevation distance above the pedestal floor. With that information, the code calculates melt jet thinning and acceleration as it falls towards the water pool beneath the RPV under the force of gravity. In particular, given the time-dependent melt fall height z, the melt jet radius and velocity at impact with the top of the water are given through the following equations:

$$R(z) = R_o \left(1 + \frac{2gz}{U_o^2} \right)^{-1/4}$$
(2-100)

$$U(z) = U_o \left(1 + \frac{2gz}{U_o^2} \right)^{1/2}$$
(2-101)

Where R is denotes radius, and subscript 'o' denotes conditions at the RPV exit. The code treats $R_o(t)$ as a user input. The exit velocity from the RPV is thus evaluated from the simple expression

$$U_{o} = \frac{\dot{Q}}{\pi R_{0}^{2}}$$
(2-102)

where

Q = melt volumetric pour rate from RPV.

Once the jet impacts the water, the extent of jet fragmentation is calculated using correlations available in the literature. The approach utilized is the same as that recommended in the OECD/NEA Technical Note on ex-vessel debris coolability;^[66] i.e., the potential for coarse jet breakup is calculated based on the Saito correlation,^[67] with the potential for fine jet breakup calculated using the Epstein correlation^[68] that is based on Kelvin-Helmholtz instability theory. The theoretical jet penetration distance is then set equal to the lesser of these predictions. The Saito correlation is based on jet breakup due to gravity and inertial effects; his expression for maximum jet penetration distance *L* is given by^[67]

$$L/D\big)_{Saito} = 2.1 \left(\frac{\rho_m}{\rho_l} Fr\right)^{1/2}$$
(2-103)

where *Fr* is the Froude number that is defined as

$$Fr = \frac{U^2}{2Rg} \tag{2-104}$$

In contrast to the Saito correlation, the Epstein model assumes that jet fragmentation occurs due to Kelvin-Helmholtz instability at the interface between the penetrating jet and blanketing steam layer. The correlation is of the form: ^[68]

$$L/D)_{Epstein} = \frac{\sqrt{3}}{2} \left(1 + \frac{\rho_{\nu}}{\rho} \right) \left(\frac{\rho}{\rho_{\nu}} \right)^{1/2}$$
(2-105)

This model is applicable to high Weber number ($We = \rho U^2 D/\sigma$) melt flow conditions.

The potential for melt stream breakup is then determined by calculating the Saito and Epstein limits through Eqs. 2-103 and 2-105, and then taking the lesser of these two values. Thus, at low entry velocities, breakup is controlled by inertia and gravitational effects, whereas at high flowrates, inertia and surface tension effects control the jet breakup process.

With the theoretical penetration distance L known through the above methodology, the jet is assumed to be completely fragmented and cooled if the theoretical penetration distance is less than the local water depth. Conversely, if the water depth is too shallow to completely fragment the melt jet, then the fraction of the jet fragmented is calculated on the basis of the ratio of the actual water depth to the depth required for complete fragmentation. Assuming an idealized geometry in which the coherent jet remains circular and the erosion mass flux from the jet surface remains constant over the penetration distance L, then the following equation for the fraction of core debris fragmented when the water pool depth x_p is < L is derived,

$$F_{frag} = \frac{2x_p}{L} \left(1 - \frac{x_p}{2L} \right) \tag{2-106}$$

Two modeling options are provided for assessing the impact of jet fragmentation on the melt arrival conditions on the pedestal floor. In the first approach, any particulate formed due to fragmentation is assumed to re-mix with the melt, which acts to lower (through a thermal equilibration calculation) the effective melt temperature at impact with the floor. This increases viscosity which acts to lower the spreading velocity. In the second approach, the debris fragmented from the jet is assumed to be rendered as a particle bed that resides on top of the remaining coherent melt material that subsequently impacts the containment floor and spreads. The assumption is made that the cooling of the remaining coherent jet is minimal, and this material impacts and spreads at the vessel exit temperature. Thus, in this scenario melt temperature is the same, but the melt mass available for spreading is reduced. Based on physical observations from reactor material jet fragmentation tests (i.e. Argonne Corium Coolant Mixing (CCM)^[69] and FARO tests conducted at ISPRA^[70]), the latter scenario is deemed to be most likely.

In the analysis, the time-dependent water depth over the core debris is calculated including the effects of local boil-off from the jet cooling process, as well as elevation changes due to accumulation of coherent melt that is not fragmented below the water surface.

CONCRETE DRYOUT MODEL

In the underlying substrate, a one-dimensional transient heat conduction equation is solved to obtain the local substrate enthalpy,

$$\rho_{st} \frac{\partial e_{st}}{\partial t} = \frac{\partial}{\partial x} \left(k_{st} \frac{\partial e_{st}}{\partial x} \right) + \rho_{st} x_{st}^{UO_2} \dot{q}_{decay}.$$
(2-107)

Equation 2-107 is applied to both concrete and steel substrates (or a combination thereof), as well as solidified core materials. The concrete property routines incorporated into MELTSPREAD3 implicitly account for the decomposition enthalpies associated with the generation of water vapor (evaporable H_2O and decomposition of $Ca(OH)_2$), as well as the generation of carbon dioxide (decomposition of $CaCO_3$ and $M_gCa(CO_3)_2$). The concrete decomposition reactions and the corresponding decomposition temperatures at which these reactions occur are summarized in Table 2-5.

Table 2-5 SUMMARY OF THE PRINCIPAL CONCRETE DECOMPOSITION REACTION TREATED IN MELTSPREAD3

Compound	Formula	Decomposition Reaction	Decomposition Temperature ^[71]
Free Water	H ₂ 0		Saturation Temperature
Dolomite	$CaMg(CO_3)_2$	$CaMg(CO_3)_2 \rightarrow CaO + MgO + 2CO_2$	1033
Calcite	CaCO ₃	$CaCO_3 \rightarrow$	1172
(Calcium Carbonate)		$CaO + CO_2$	
Calcium Hydroxide	<i>Ca</i> (<i>OH</i>) ₂	$Ca(OH_2) \rightarrow$	853
		$CaO + H_2O$	

In concrete regions, the front locations for each of the decomposition processes satisfies the equation,

$$\rho_{st}\Delta e_{st,dc}^{i}\frac{dx_{dc}^{i}}{dt} = -\frac{k_{st}\partial T_{st}}{\partial x}|_{x_{dc}^{i}-\epsilon} + \frac{k_{st}\partial T_{st}}{\partial x}|_{x_{dc}^{i}+\epsilon}, \qquad (2-108)$$

where

 $\Delta e_{st,dc}^i$ = enthalpy change due to decomposition of the i-th concrete constituent,

 x_{dc}^i = location of the i-th concrete dryout front,

and superscript i denotes the four compounds shown in Table 2-5. The concrete degassing rate for evaporable H_2O is therefore,

$$\dot{m}_{free\,H_{20}} = x_{free\,H_{20}}\rho_{st}\,\frac{dx_{dc}{}^{free\,H_{20}}}{dt},\tag{2-109}$$

where

 x_{free,H_20} = weight fraction free H_20 in concrete.

Similar expressions apply to the decomposition of $Ca(OH)_2$, $CaCO_3$, and $MgCa(CO_3)_2$. The maximum specific enthalpy attained in the concrete is locally monitored and stored such that the correct degassing rate is predicted on reheating of concrete which has undergone quenching following the onset of decomposition.

The user has the option of specifying a general concrete composition. The available constituents are: SiO_2 , MgO, CaO, FeO, Fe_2O_3 , Fe_3O_4 , Na_2O , K_2O , TiO_2 , CO_2 , H_2O , Al_2O_3 , Fe and Cr. In addition, three default concrete compositions are provided; these are: limestone-common sand, siliceous, and limestone-limestone. The assumed chemical compositions for these concretes are summarized in Table 2-6, while the solidus/liquidus temperatures^[72] are provided in Table 2-7.

SHELL HEATUP MODEL

If the melt spreading region propagates to the structural boundary (the containment shell in Mark I containments), a local, two-dimensional, transient heatup calculation can be invoked. The physical situation is depicted in Figure 1-12. The governing equation for the shell heatup calculation is of the form,

Constituent	Limestone/Common Sand Concrete		Limestone/Common Sand Concrete Siliceous Concrete		Limestone/Limestone Concrete	
	Weight	Mole	Weight	Mole	Weight	Mole
	Percent	Percent	Percent	Percent	Percent	Percent
SiO_2	28.8	22.8	69.7	60.7	7.0	5.2
MgO	9.8	11.6	0.7	0.9	7.3	8.2
CaO	26.4	22.4	13.7	12.8	42.4	34.0
Fe_2O_3	1.6	0.5	1.0	0.3	0.8	0.2
Al_2O_3	3.6	1.7	4.0	2.1	1.9	0.8
Na ₂ O	1.1	0.8	0.7	0.6	-	-
K ₂ O	0.6	0.3	1.4	0.8	0.4	0.2
TiO ₂	0.1	0.1	0.8	0.5	0.1	0.1
CO_2	21.8	23.4	1.00	1.2	33.2	34.0
H ₂ O	6.2	16.4	6.91	20.0	6.9	17.3

Table 2-6 ASSUMED COMPOSITION OF DEFAULT CONCRETES IN WEIGHT AND MOLE PERCENTS

Table 2-7 SOLIDUS/LIQUIDUS^[72] AND DECOMPOSITION TEMPERATURES FOR DEFAULT CONCRETES

Concrete Type	Solidus Temperature (K)	Liquidus Temperature (K)	Assumed Decomposition Temperature (K)
Limestone-Common Sand	1393	1568	1568
Siliceous	1403	1523	1523
Limestone-Limestone	1495	2577	1800

$$\frac{\rho \partial e}{\partial t} = \frac{\partial}{\partial x} \left(\frac{k \partial T}{\partial x} \right) + \frac{\partial}{\partial y} \left(\frac{k \partial T}{\partial y} \right).$$
(2-110)

where the coordinate system for Eq. 2-110 was shown previously in Figure 2-2.

If the local shell surface temperature lies below the melt freezing temperature, stable crust growth on the submerged portion of the shell is calculated according to the equation,

$$\rho_{cr} \Delta e_{cr} \frac{d\delta_{cr}(y)}{dt} = k_{cr} \left(\frac{T_{sol,cr} - T_{sf}(y)}{\delta_{cr}(y)} \right) - h_{shell} \left(T_{adj} - T_{frz,cr} \right), \tag{2-111}$$

where

 $T_{frz,cr}$ = crust freezing temperature, $T_{sf}(y)$ = local shell surface temperature beneath growth crust.

Modeling options for the crust freezing temperature, $T_{frz,cr}$, are described in Section 4.

To provide the user with flexibility to model situations in which the crust is postulated to not be mechanically stable, the crust calculation may be overridden in which case the local surface heat flux over the submerged portion of the shell is calculated from the equation,

$$q_{shell} = h_{shell} \left(T_{adj} - T_{sf}(y) \right). \tag{2-112}$$

A source of uncertainty in the analysis of the shell thermal loading due to spreading melt is the applicable heat transfer coefficient between the melt and the shell, h_{shell} . The user currently has three modeling options for the heat transfer coefficient, which include: (i) forced convection, (ii) bubble-driven recirculation, or (iii) sum of forced convection and bubble-driven recirculation heat transfer coefficients. The convective heat transfer coefficient between the melt and shell is modeled using a slot jet impingement heat transfer correlation,^[73]

$$h_{shell} = 1.101 \, Re^{0.368} Pr^{0.42} \frac{k}{D} \tag{2-113}$$

where

Re $= \frac{2B_w \rho V_{adj}}{\mu}$ B_w = impinging slot jet width, V_{adj} = melt velocity impinging on shell.

As described in Section 4, the impinging slot jet width, B_w , is a user-specified constant.

The bubble-driven recirculation heat transfer coefficient is calculated using the model of Theofanous et. al.,^[74] which is given by the equation,

$$h_{shell} = 0.037 \, Re^{0.8} Pr^{0.33} \frac{k}{h_{adj}} \,, \tag{2-114}$$

where

 $\begin{array}{ll} \operatorname{Re} & = \frac{\rho h_{adj} U_L}{\mu} \\ U_L & = \operatorname{melt} \mbox{ (single phase) recirculation velocity adjacent to shell,} \\ h_{adj} & = \operatorname{melt} \mbox{ height adjacent to shell.} \end{array}$

Theofanous, et. al.^[74] developed the following upper-bound correlation for U_L based on the melt sparging rate adjacent to the shell,
$$U_L = \begin{cases} U_L = 17.0 \ j_{adj}; & j_{adj} < 6 \ cm/sec \\ U_L = 1.02 \ m/sec; \ j_{adj} \ge 6 \ cm/sec \end{cases},$$
(2-115)

 j_{adj} = melt sparging rate adjacent to shell.

MELTSPREAD3 currently does not have the capability of performing an explicit ablation calculation should the shell surface temperature reach the steel melting temperature. The carbon steel property routines incorporated into MELTSPREAD3 implicity account for the latent heat of fusion should the shell temperature reach the liquidus (see Appendix B). Thus, for situations in which the melting temperature is reached, the ablated steel is effectively treated as a stationary molten film across which the heat transfer occurs by transient conduction.

Should corium freeze over the substrate adjacent to the shell, then heat transfer from the solidified melt may significantly influence the shell thermal response. In this situation, a detailed analysis would involve solving a twodimensional transient heat conduction equation in both the shell and solidified melt region adjacent to the shell. An analysis of this type is beyond the current scope of work. In the region of the shell which is below the solidified melt depth, the current approach is to apply the interfacial heat transfer coefficient applicable to the case in which two semi-infinite slabs at different temperatures are brought into intimate contact; i.e.,^[75]

$$h_{shell,cr} = k_{cr} \left[\frac{\pi k_{cr} (t - t_{freeze})}{\rho_{cr} c_{cr}} \right]^{-1/2} , \qquad (2-116)$$

where

 t_{freeze} = time at which melt freezes adjacent to shell.

Given Eq. 2-116, the local thermal loading on the shell due to the presence of solidified debris is evaluated based on the average debris temperature adjacent to the shell, $T_{cr,adj}$, and the local shell surface temperature, $T_{sf}(y)$ (See Figure 2-2). Note that as $t - t_{freeze} \rightarrow \infty$, Eq. 2-116 predicts $h_{shell,cr} \rightarrow 0$, which is not a physically realistic solution for long times if the decay heat level in the frozen material adjacent to the shell is significant. To account for this situation, the effective conduction length scale in Eq. 2-116 is capped at $\frac{1}{2}$ the spreading grid cell size adjacent to the shell, i.e.,

$$h_{shell,cr} = \frac{k_{cr}}{X_L}; t - t_{freeze} \ge \frac{\rho_{cr}c_{cr}X_L^2}{\pi k_{cr}}, \qquad (2-117)$$

 $X_L = \frac{1}{2}$ the spreading grid cell size adjacent to the shell.

The spreading grid cell size is depicted in Figure 2-2. A complete description of the spreading discretization scheme leading to the definition of the numerical grid cell size adjacent to the shell is provided in the next section.

If water is absent, the heat transfer from the shell above the melt surface is calculated assuming radiation heat transfer to overlying structure. The heat transfer coefficient is of the form,

$$h_{shell,atm} = \frac{\sigma_{stef}}{1/\epsilon_{shell} + 1/\epsilon_{struc} - 1} \left(T_{sf}^2 + T_{struc}^2\right) \left(T_{sf} + T_{struc}\right) , \qquad (2-118)$$

where

 ϵ_{shell} = shell radiation emissivity.

Heating of the shell above the melt surface due to radiation heat transfer from the melt adjacent to the shell is currently not modeled.

If water is present in the drywell, a local check on the melt height relative to the water is performed. If the local melt height exceeds the water height, a radiation boundary condition is applied. If the local height is less than the water height, heat transfer is calculated along a full boiling curve. In the nucleate boiling regime, heat transfer is calculated using Rohsenow's correlation^[53] with a correction for shell inclination according to the correlation on Jung et. al. ^[76]. The nucleate boiling heat flux is given by the equation,

$$q_{nb,shell} = \frac{\mu_l h_{lv} c_{sf,i}^{-1/r}}{\sqrt{\frac{\sigma_l}{g(\rho_l - \rho_v)}}} \left(\frac{c_l \Delta T_{sat}}{h_{lv}}\right)^{1/r} \left(\frac{k_l}{c_l \mu_l}\right)^{1.7/r} , \qquad (2-119)$$

where $C_{sf,i}$ and r are correlated in terms of shell inclination. The correlations are given as ^[76]

$$\frac{c_{sf,i}}{c_{sf}} = 1.0 - 2.41.10^{-4}\theta, \qquad (2-120)$$

$$r = 0.256 - 1.514 x \, 10^{-4} \theta + 1.778 \cdot 10^{-5} \theta^2 - 7.16 x \, 10^{-8} \theta^3, \tag{2-121}$$

and C_{sf} in Eq. 2-120 is assumed to equal the reported value^[53] for stainless steel; i.e., $C_{sf} = 0.02$.

The critical heat flux from the shell surface is modeled using Zuber's saturated boiling correlation^[55] that is given by Eq. 2-63. The shell surface superheat at which the critical heat flux is reached is obtained by equating Eqs. 2-63 and 2-119, which yields

$$\Delta T_{CHF}^{shell} = \left(\frac{q_{CHF,sat}}{\alpha_{nb,shell}}\right)^r , \qquad (2-122)$$

where

$$\alpha_{nb,shell} = \frac{\mu_l h_{lv} c_{sf,i}^{-1/r}}{\sqrt{\frac{\sigma_l}{g(\rho_l - \rho_v)}}} \left(\frac{c_l}{h_{lv}}\right)^{1/r} \left(\frac{k_l}{c_l \mu_l}\right)^{1.7/r}.$$
(2-123)

The surface superheat at the minimum film boiling point is modeled using the correlation of Henry, ^[56] which is given by Eq. 2-67.

In the transition boiling regime, the surface heat flux is assumed to vary linearly between the critical heat flux and the film boiling heat flux evaluated at the minimum film boiling temperature. The correlation for the transition boiling heat flux is given by Eq. 2-69.

In the film boiling regime the heat transfer coefficient is modeled using the equation of Berenson^[57] with a correction for shell inclination according to the experiment data of Sauer et. al.^[77]. The film boiling heat transfer coefficient is thus defined as,^[57]

$$h_{fb,shell} = 0.425 F_i \left[\frac{k_v^3 h_{lv} \rho_v g(\rho_l - \rho_v)}{\mu_v \Delta T_{sat} \sqrt{\frac{\sigma}{g(\rho_l - \rho_v)}}} \right]^{1/4} , \qquad (2-124)$$

where F_i is a correction factor for shell inclination and is obtained by a curve fit to the data of Sauer et. al., ^[77]

$$F_i = 1 + 4.514 x \, 10^{-3} \, \theta \, . \tag{2-125}$$

Section 3

NUMERICAL METHODOLOGY

The numerical methodology for solving the system of equations described in the previous section is discussed here. The approach is to utilize an implicit, Eulerian finite difference numerical scheme which removes numerical stability limitations corresponding to material convection, heat diffusion, and heat transfer between the melt and underlying substrate or overlying medium.

DIFFERENCED FORM OF MELT CONSERVATION OF MOMENTUM EQUATION

The nomenclature for the spreading mesh cells is illustrated in Figure 3-1. In formulating the finite difference equations for the spreading melt, a staggered mesh is employed in which velocities are defined at the edges of the numerical grid cells, and other variables such as the layer depths and enthalpies (temperatures) are defined at cell centers. Thus, the fundamental velocity, $U_{j-1/2}$, in Figure 3-1 is that at the edge of the j th and j-1 st cells.

The substrate surface is assumed to be discretized into j = 1, 2, ..., J numerical grid cells. At interior grid cell interfaces, for which $2 \le j \le J$, the finite difference approximation to the conservation of momentum equation (Eq. 2-1) is of the form,

$$\frac{U_{j-1/2}^{n+1} - U_{j-1/2}^{n}}{\delta t} + \frac{1}{2} \frac{\delta z_{j}}{\delta z_{j} \delta z_{j-1}} \left(1 + sqn(u)\right) U_{j-1/2}^{n+1} \left(U_{j-1/2}^{n+1} - U_{j-3/2}^{n+1}\right)
+ \frac{1}{2} \frac{\delta z_{j-1}}{\delta z_{j} \delta z_{T}} \left(1 - sqn(u)\right) U_{j-1/2}^{n+1} \left(U_{j+1/2}^{n+1} - U_{j-1/2}^{n+1}\right)
= \frac{-g}{\left(\delta z_{j} + \delta z_{j-1}\right)} \left[\frac{h_{j}^{n+1}}{1 - \alpha_{j}^{n}} + E_{j}^{n} - \frac{h_{j-1}^{n+1}}{1 - \alpha_{j-1}^{n}} - E_{j-1}^{n}\right] - \frac{1}{2} f_{j-1/2} \frac{U_{j-1/2}^{n+1}}{h_{j}^{n}} \left|U_{j-1/2}^{n+1}\right|$$
(3-1)

where

 $\begin{array}{ll} \delta t &= \text{timestep size,} \\ n &= \text{superscript denoting beginning of timestep value,} \\ n+1 &= \text{superscript denoting end of timestep value,} \\ sgn\left(u\right) = \begin{cases} +1, \ U_{j-1/2}^{n+1} > 0 \\ -1, \ U_{j-1/2}^{n+1} < 0 \end{cases} \\ \delta z_T &= \delta z_j + \delta z_{j-1} + sgn(u) \left(\delta z_j + \delta z_{j-1}\right), \\ \delta z &= \text{spreading grid cell size,} \end{cases}$

- j = subscript denoting center on jth numerical grid cell,
- j-1 = subscript denoting center of j-1 st numerical grid cell, and

j-1/2 = subscript denoting common edge of jth and j-1 st numerical grid cells.



Figure 3-16 Illustration of Geometry and Nomenclature for Differencing of Melt Spreading Equations

Note that the advection term in Eq. 2-1 has been conservatively differenced using the donor cell method as developed by Hotchkiss.^[78] This method is adopted due to the inherent numerical stability in comparison to other differencing techniques, such as the central difference approximation, and is also applicable to fixed as well as variable mesh sizes.

Equation 3-1 is solved assuming no flow across the system boundaries. Thus, the boundary conditions on the discretized momentum equation are, for j=1,

$$U_{J-1/2}^{n+1} = 0, (3-2)$$

and for j=J+1,

$$U_{l+1/2}^{n+1} = 0. (3-3)$$

The local velocities are calculated from Eqs. 3-1 through 3-3 in conjunction with an approximate conservation of mass equation which neglects the effects of crust growth, substrate ablation, and oxidation reactions on the local melt height.

Employing the donor cell method for differencing of the convective mass flux term, the finite difference approximation to the simplified conservation of mass equation is of the form,

$$\frac{A_{j}}{\delta_{t}} \left[h_{j}^{n+1} - h_{j}^{n} \right] + S_{j-1/2} \langle -U_{j-1/2}^{n+1}, 0 \rangle h_{j}^{n+1} + S_{j+1/2} \langle U_{j+1/2}^{n+1}, 0 \rangle h_{j}^{n+1}
-S_{j-1/2} h_{j-1}^{n+1} \langle U_{j-1/2}^{n+1}, 0 \rangle - S_{j+1/2} h_{j+1}^{n+1} \langle U_{j+1/2}^{n+1}, 0 \rangle = \frac{A_{j}}{\rho_{l}} (\dot{m}_{vessel})_{j},$$
(3-4)

$$(\dot{m}_{vessel_j})$$
 = local corium mass flux the RPV,

and the operator, <;;>, denotes the largest of the two possible arguments; i.e.,

$$\langle U_{j+1/2}^{n+1}, 0 \rangle = \begin{cases} U_{j+1/2}^{n+1}, U_{j+1/2}^{n+1} > 0\\ 0, & U_{j+1/2}^{n+1} < 0 \end{cases}$$
(3-5)

The constraint that the melt depth at the leading edge does not fall below the minimum depth at which surface tension balances gravity (Eq. 2-9) is applied to the differenced form of the equations by performing a local check on the melt depth relative to the minimum spreading depth. If h_j^{n+1} and h_{j-1}^{n+1} are less than h_{min} , then $U_{j-1/2}$ is set equal to zero.

Care must be exercised in solving Eqs. 3-1 and 3-4 over substrate surfaces with large physical discontinuities in elevation that exist as an initial condition. This situation is depicted in Figure 3-2. Let the elevation discontinuity lie between the j-1 st and j th numerical grid cells and assume that $E_j > E_{j-1}$. For this case, there will be flow across the cell boundary if the following condition is satisfied,

$$\frac{h_{j-1}}{1-\alpha_{j-1}} + E_{j-1} > E_j. \tag{3-6}$$

If the condition defined by Eq. 3-6 is not satisfied, then the cell edge velocity across the substrate discontinuity is set equal to zero, $U_{j-1/2} = 0$. If Eq. 3-6 is satisfied, then flow across the cell boundary is calculated with the gravity head evaluated as in Eq. 3-1. It is important to note the following two points: i) if the conditional check defined by Eq. 3-6 is not applied and $h_{j-1}/(1 - \alpha_{j-1}) + E_{j-1} < E_j$, then an artificial adverse pressure drop across the discontinuity will be applied resulting in an accumulation of material as depicted in Figure 3-3; and ii) the conditional check defined in Eq. 3-6 is applied only to initial discontinuities in the substrate elevation (i.e., the condition is not applied to discontinuities which arise as a result of melt freezing).



Figure 3-17 Illustration of Flow Over Large Elevation Discontinuities in Substrate Surface



Figure 3-18 Illustration of Artificial Back Flow at Large Discontinuities in Substrate Surface

DIFFERENCED FORM OF MELT CONSERVATION OF MASS AND ENERGY EQUATIONS

Given the local melt velocities as calculated through Eqs. 3-1 through 3-5, the detailed conservation of mass and energy equations are then solved to obtain the end of timestep melt constituency and enthalpy. The mass and energy equations are formulated numerically using an Eulerian finite difference scheme in which convective terms are differenced using the donor cell differencing approach. This numerical scheme will give rise to so-called "Eulerian mixing" effects which will tend to artificially equilibrate melt depths and temperatures more rapidly than purely physical processes, and will also somewhat reduce the peak calculated depths and temperatures. The degree of approximation introduced by Eulerian mixing depends upon the shape of the depth and temperature profiles, as well as the numerical grid cell size.

The finite difference approximation to the detailed conservation of mass equation for the i th melt constituent (Eq. 2-14) is of the form,

$$\frac{A_{j}}{\delta_{t}} \Big[(h_{j}^{i})^{n+1} - (h_{j}^{i})^{n} \Big] - S_{j-1/2} \langle U_{j-1/2}^{n+1}, 0 \rangle (h_{j-1}^{i})^{n+1} + S_{j-1/2} \langle -U_{j-1/2}^{n+1}, 0 \rangle (h_{j}^{i})^{n+1} \\
+ S_{j+1/2} \langle U_{j+1/2}^{n+1}, 0 \rangle (h_{j}^{i})^{n+1} - S_{j+1/2} \langle -U_{j+1/2}^{n+1}, 0 \rangle (h_{j+1}^{i})^{n+1} \\
= \frac{\beta^{i} A_{j}}{\rho_{l}^{i}} \Big[(F_{H_{2}} 0)_{j}^{n+1} \gamma_{H_{2}0}^{i} (\dot{m}_{H_{2}0})_{j}^{n+1} + (F_{CO_{2}})_{j}^{n+1} \gamma_{CO_{2}}^{i} (\dot{m}_{CO_{2}})_{j}^{n+1} \Big] \\
- \frac{A_{j} \rho_{s}^{i}}{\rho_{l}^{i}} \Big[\left(x_{sf}^{i} \frac{d\eta}{dt} \right)_{j}^{n+1} + \left(x_{melt}^{i} \frac{d\delta}{dt} \right)_{j}^{n+1} \Big] + \frac{A_{j} x_{vessel}^{i}}{\rho_{l}^{i}} (\dot{m}_{vessel})_{j}^{n+1}.$$
(3-7)

Specific expressions for the differenced form of the concrete decomposition gas mass fluxes, $(\dot{m}_{H_20})_j^{n+1}$ and $(\dot{m}_{C02})_j^{n+1}$, and the differenced form of the crust growth and substrate ablation rates, $\left(\frac{d\delta}{dt}\right)_j^{n+1}$ and $\left(\frac{d\eta}{dt}\right)_j^{n+1}$, are given later in this section. The total local collapsed melt height is related to the individual melt constituent heights through the equation,

$$h_j = \sum_{i=1}^{16} h_j^i.$$
(3-8)

Employing the donor cell method for differencing of the convective energy flux term, the finite difference approximation to the conservation of mass equation (Eq. 2-22) is of the form,

$$\frac{A_{j}}{\delta t} \Big[(\rho h e)_{j}^{n+1} - (\rho h e)_{j}^{n} \Big] - S_{j-1/2} \langle U_{j-1/2}^{n+1}, 0 \rangle (\rho h e)_{j-1}^{n+1} + S_{j-1/2} \langle -U_{j-1/2}^{n+1}, 0 \rangle (\rho h e)_{j}^{n+1} + S_{j+1/2} \langle U_{j+1/2}^{n+1}, 0 \rangle (\rho h e)_{j}^{n+1} - S_{j+1/2} \langle -U_{j+1/2}^{n+1}, 0 \rangle (\rho h e)_{j+1}^{n+1} = -A_{j} (h_{bot})_{j}^{n+1} (T_{j}^{n+1} - (T_{bot})_{j}^{n+1}) \\ -A_{j} (h_{top})_{j}^{n+1} \left(T_{j}^{n+1} - (T_{top})_{j}^{n+1} \right) + A_{j} \rho_{j} (h_{j})^{n+1} (\dot{q}_{decay})^{n+1} (x_{melt}^{UO_{2}})_{j}^{n+1} \\ +A_{j} (\dot{m}_{vessel})_{j}^{n+1} e_{vessel}^{n+1} - A_{j} \rho \left[e_{ablation} \left(\frac{d\eta}{dt} \right)_{j}^{n+1} + e_{crust} \left(\frac{d\delta}{dt} \right)_{j}^{n+1} \right] \\ +A_{j} (F_{H_{2}O})_{j}^{n+1} (\dot{m}_{cO_{2}})_{j}^{n+1} \sum_{i} \gamma_{H_{2}O}^{i} q_{ox,H_{2}O}^{i} + A_{j} (F_{CO_{2}})_{j}^{n+1} (\dot{m}_{cO_{2}})_{j}^{n+1} \sum_{i} \gamma_{CO_{2}}^{i} q_{ox,CO_{2}} \\ -S_{j+1/2} D (j - J_{adj}) \sum_{k=1}^{N_{sub}} l_{k} h_{shell}^{n+1} (T_{j}^{n+1} - (T_{shell}^{n+1})_{k})$$

$$(3-9)$$

where

 N_{sub} = number of shell nodes submerged by melt, J_{adj} = spreading node adjacent to shell outside pedestal doorway, and

$$D(j - J_{adj}) = \begin{cases} 0, \ j \neq J_{adj} \\ 1, \ j = J_{adj} \end{cases}$$

Equations 3-7 and 3-9 are solved in regions of the substrate surface in which molten corium exits. In regions where corium has not spread or material has previously frozen and no molten corium currently exists over the solidified melt, the local melt enthalpy is set equal to zero. Heat transfer in regions of solidified corium is treated through the substrate heatup equations which are described next.

DIFFERENCED FORM OF SUBSTRATE HEATUP/DECOMPOSITION EQUATION

The grid cell nomenclature for the substrate heatup and decomposition calculation is shown in Figure 3-4. At each spreading grid cell location, j, the underlying substrate is discretized into m = 1, 2, ..., M, numerical grid cells. For purposes of brevity, the subscript J will not be shown in the following equations with the understanding that one set of these equations is solved at each spreading grid cell location.

The general form of the finite difference approximation to the substrate conservation of energy equation, Eq. 2-107, is

$$\frac{V_m \rho_m^{n+1}}{\delta t} (e_m^{n+1} - e_m^n) = C_{m-1/2}^{n+1} (T_{m-1}^{n+1} - T_m^{n+1})$$

$$-C_{m+1/2}^{n+1} (T_m^{n+1} - T_{m+1}^{n+1}) + \rho_m^{n+1} (\dot{q}_{decay})_m^{n+1} V_m (x_{st}^{UO_2})_m,$$
(3-10)

where

$$V_m = \delta x_{m,m-1/2} + \delta x_{m,m+1/2},$$

$$C_{m-1/2}^{n+1} = \frac{k_m^{n+1}k_{m-1}^{n+1}}{k_m^{n+1}\delta x_{m-1,m+1/2} + k_{m-1}^{n+1}\delta x_{m-1,m-1/2}},$$

$$C_{m+1/2}^{n+1} = \frac{k_m^{n+1}k_{m+1}^{n+1}}{k_{m+1}^{n+1}\delta x_{m,m+1/2} + k_m^{n+1}\delta x_{m+1,m-1/2}}.$$

Equation 3-10 is applied to both concrete and steel surfaces as well as solidified melt, with material properties set accordingly. At the bottom of the numerical grid, an adiabatic boundary condition is assumed for which the following equation is satisfied:

,

$$\frac{V_m \rho_M}{\delta t} (e_M^{n+1} - e_M^n) = C_{M-1/2}^{n+1} (T_{M-1}^{n+1} - T_M^n) + \rho_M^{n+1} V_M (\dot{q}_{decay})_M^{n+1} + \rho_M^{n+1} V_M (\dot{q}_{decay})_M^{n+1} (x_{st}^{UO_2})_M$$
(3-11)



Figure 3-19 Illustration of Geometry and Nomenclature for Differencing of Substrate Heatup Equations

At the melt/substrate interface, the specific form of the discretization equation is dependent upon the current interfacial boundary condition. For the case of a convective boundary condition, the equation,

$$\frac{V_1 \rho_1^{n+1}}{\delta t} (e_1^{n+1} - e_1^n) = h_{bot}^{n+1} (T^{n+1} - T_1^{n+1}) - C_{1-1/2}^{n+1} (T_1^{n+1} - T_2^{n+1}) + (\dot{q}_{decay})_1^{n+1} \rho_1^{n+1} V_1 (x_{st}^{UO_2})$$
(3-12)

is satisfied for the cell adjacent to the melt, where

$$V_1 = \delta x_{1,1+1/2}$$
.

For the case of a growing stable crust at the surface with no ablation of the underlying substrate, the equation,

$$\frac{V_{1}\rho_{1}^{n+1}}{\delta t}(e_{1}^{n+1}-e_{1}^{n}) = k_{cr}^{n+1}\frac{(T_{sol,cr}-T_{1}^{n+1})}{\delta_{cr}^{n+1}} - C_{1+1/2}^{n+1}(T_{1}^{n+1}-T_{2}^{n+1})
+ (\dot{q}_{decay})_{1}^{n+1}\rho_{1}^{n+1}V_{1}(x_{st}^{UO_{2}}),$$
(3-13)

is satisfied for the cell adjacent to the crust. The end of timestep crust depth, δ_{cr}^{n+1} , is obtained by first multiplying Eq. 2-31 through by δ_{cr} to obtain

$$\frac{\rho_{cr}\Delta e_{cr}}{2} \left. \frac{d\delta_{cr}^2}{dt} = -\delta_{cr} k_{cr} \left. \frac{\partial T}{\partial x} \right|_{x=\delta_{cr}} - \delta_{cr} h_{bot} \left(T - T_{sol,cr} \right). \tag{3-14}$$

Expressing the heat conduction across the crust in terms of the primitive variables and differencing the resultant expression yields:

$$\frac{\rho_{cr}\Delta e_{cr}}{2\delta t} \left[(\delta_{cr}^{n+1})^2 - (\delta_{cr}^n)^2 \right] = k_{cr}^{n+1} \left(T_{sol,cr} - T_1^{n+1} \right) - \delta_{cr}^{n+1} h_{bot}^{n+1} \left(T^{n+1} - T_{sol,cr} \right)$$
(3-15)

Equation 3-15 is a quadratic equation for δ_{cr}^{n+1} . The physically realistic root of this equation is

$$\delta_{cr}^{n+1} = h_{bot}^{n+1} \frac{(T^{n+1} - T_{sol,cr})}{2\zeta_{cr}} + \frac{\Gamma_{cr}^{n+1}}{2}, \qquad (3-16)$$

where

$$\Gamma_{cr}^{n+1} = \left[(h_{bot}^{n+1}) \left(T^{n+1} - T_{sol,cr} \right)^2 + 4 \left((\delta_{cr}^n)^2 + \frac{k_{cr}^{n+1}}{\zeta_{cr}} \left(T_{sol,cr} - T_1^{n+1} \right) \right) \right]^{1/2}, \quad (3-17)$$

$$\zeta_{cr} = \frac{\rho_{cr} \Delta e_{cr}}{2\delta t} \tag{3-18}$$

The finite difference approximation to the crust growth rate equation, Eq. 2-31, is of the form,

$$\rho_{cr}^{n+1} \Delta e_{cr} \frac{d\delta_{cr}}{dt} \Big)^{n+1} = k_{cr}^{n+1} \frac{(T^{n+1} - T_{sol,cr})}{\delta_{cr}^{n+1}} - h_{bot}^{n+1} (T^{n+1} - T_{sol,cr}).$$
(3-19)

Equation 3-19 is used to evaluate the local melt deposition rate due to crust formation in Eqs. 3-7 and 3-9.

For the case in which the downward heat transfer is limited by thin crust segments and no ablation of the underlying substrate is occurring, the equation,

$$\frac{V_{1}\rho_{1}^{n+1}}{\delta t}(e_{1}^{n+1}-e_{1}^{n}) = h_{bot}^{n+1}(T^{n+1}-T_{sol,cr}) - C_{1+1/2}^{n+1}((T_{1}^{n+1}-T_{2}^{n+1}) + \rho_{1}^{n+1}V_{1}(\dot{q}_{decay})_{1}^{n+1}(x_{st}^{UO_{2}})_{1}$$
(3-20)

is satisfied.

For cases in which substrate ablation is occurring, the calculation is performed with a fixed Eulerian numerical grid. This method is motivated by the requirement of tracking the concrete dryout fronts which would be complicated if the mesh structure were to be redefined at the end of each timestep due to ablation of the substrate. The ablation calculation is functionally identical to the crust growth calculation with the exception that the ablating substrate node is retained in the node indexing scheme for the substrate as opposed to being defined as a separate entity as is done for the case of crust growth. This semantic distinction is made because it is computationally convenient to retain the ablating node in the substrate indexing scheme for tracking of the concrete dryout fronts; the method is described later in this section. The nodal structure for the substrate ablation calculation is illustrated in Figure 3-5. For this case, the surface node is treated as isothermal at the substrate ablation temperature, i.e.,



$$T_1^{n+1} = T_{sol,st} \ . \tag{3-21}$$

Figure 3-20 Illustration of Substrate Ablation Nodalization Scheme

The energy balance for the second node is of the form,

$$\frac{V_2 \rho_2^{n+1}}{\delta t} (e_2^{n+1} - e_2^n) = k^{n+1} \frac{\left(T_{sol,st} - T_2^{n+1}\right)}{\eta^{n+1}}$$
$$-C_{2-1/2}^{n+1} (T_2^{n+1} - T_3^{n+1}) + \left(\dot{q}_{decay}\right)_2^{n+1} \rho_2^{n+1} V_2 \left(x_{st}^{UO_2}\right)_2 \tag{3-22}$$

$$\bar{k}^{n+1} = \begin{cases} \frac{k_1^{n+1}k_2^{n+1}\eta^{n+1}}{k_2^{n+1}(\eta^{n+1} - \delta x_{2,2-1/2}^0) + k_1^{n+1}\delta x_{2,2-1/2}^0}, & \text{if } \eta^{n+1} > \delta x_{2,1/2}^0\\ k_1^{n+1}, & \text{if } \eta^{n+1} \le \delta x_{2,1/2}^0 \end{cases}$$
(3-23)

As depicted in Figure 3-5, to avoid numerical singularities as $\eta^{n+1} \rightarrow 0$ due to ablation, the calculation must be "mapped" to the next node into the substrate. The relaxation criterion and procedure is discussed in Section 4.

The specific form of the difference equations for the end of timestep ablation depth and ablation rate are dependent upon the boundary condition at the melt/substrate interface. The various ablation boundary conditions treated in MELTSPREAD3 have been previously summarized in Table 2-4.

For the case NBCINT=4, which corresponds to the situation in which the substrate is ablating and the ablated material is continuously mixed off the interface, the expression for the end of timestep ablation depth is found from Eq. 2-34 as

$$\eta^{n+1} = \frac{h_{bot}^{n+1}(T^{n+1} - T_{sol,st})}{2\zeta_{st}} + \frac{\Gamma_{st}^{n+1}}{2}, \qquad (3-24)$$

where

$$\Gamma_{st}^{n+1} = \left(\left(h_{bot}^{n+1} \frac{(T^{n+1} - T_{sol,st})}{\zeta_{st}} \right)^2 + 4 \left((\eta^n)^2 + \frac{\bar{k}^{n+1}}{\zeta_{st}} (T_{sol,st} - T_2^{n+1}) \right) \right)^{1/2}$$
(3-25)

$$\zeta_{st} = \frac{\rho_{st} \Delta e_{st}}{2\delta t} \,. \tag{3-26}$$

The finite difference approximation to the ablation rate equation is of the form,

$$\rho_{st}\Delta e_{st} \frac{d\eta}{dt}\Big]^{n+1} = \bar{k}^{n+1} \left(\frac{T_{sol,st} - T_2^{n+1}}{\eta^{n+1}}\right) - h_{bot}^{n+1} \left(T^{n+1} - T_{sol,st}\right).$$
(3-27)

Equation 3-27 is used to evaluate the rate at which ablated substrate is transported into the bulk melt in Eqs. 3-7 and 3-9.

For the case NBCINT=5, which corresponds to substrate ablation and the ablated substrate remains as a molten film on the surface, the expressions for the end of timestep molten film and ablation depths are found from Eqs. 2-37 and 2-40 as

$$\delta_f^{n+1} = \delta_f^n + \frac{\rho_{st}}{\rho_f} (\eta^{n+1} - \eta^n).$$
(3-28)

$$\eta^{n+1} = \bar{h}^{n+1} \left(\frac{T^{n+1} - T_{sol,st}}{2\zeta_{st}} \right) + \frac{\Gamma_{st}^{n+1}}{2} , \qquad (3-29)$$

$$\Gamma_{st}^{n+1} = \left[\left(\bar{h}^{n+1} \frac{(T^{n+1} - T_{sol,st})}{\zeta_{st}} \right)^2 + 4 \left((\eta^n)^2 + \bar{k}^{n+1} \frac{(T_{sol,st} - T_2)}{\zeta^{st}} \right) \right]^{1/2}, \tag{3-30}$$

$$\bar{h}^{n+1} = \frac{k_f^{n+1} h_{bot}^{n+1}}{\delta_f^{n+1} h_{bot}^{n+1} + k_f^{n+1}} \,. \tag{3-31}$$

The finite difference approximation to the ablation rate equation for this case is of the form,

$$\rho_{st} \Delta e_{st} \frac{d\eta}{dt} \Big]^{n+1} = \bar{k}^{n+1} \left(\frac{T_{sol,st} - T_2^{n+1}}{\eta^{n+1}} \right) - \bar{h}^{n+1} \left(T^{n+1} - T_{sol,st} \right) \,. \tag{3-32}$$

For the case NBCINT=6, which corresponds to porous crust growth over ablating substrate and the ablated substrate continuously drains through the crust, the expressions for the end of timestep crust and ablation depths are found from Eqs. 2-42 and 2-43 as

$$\delta_f^{n+1} = -\frac{h_{bot}^{n+1}(T^{n+1} - T_{sol,cr})}{2\zeta_{cr}} + \frac{\Gamma_{st}^{n+1}}{2}, \qquad (3-33)$$

$$\eta^{n+1} = -k_{cr}^{n+1} \frac{(T_{sol,cr} - T_{sol,st})}{2\zeta_{st}\delta_{cr}^{n+1}} + \frac{\Gamma_{st}^{n+1}}{2} , \qquad (3-34)$$

where

$$\Gamma_{cr}^{n+1} = \left[\left(\frac{h_{bot}^{n+1}(T^{n+1} - T_{sol,cr})}{\zeta_{cr}} \right)^2 + 4 \left((\delta_{cr}^n)^2 + \frac{k_{cr}^{n+1}(T_{sol,cr} - T_{sol,st})}{\zeta_{cr}} \right) \right]^{1/2} , \qquad (3-35)$$

$$\Gamma_{st}^{n+1} = \left[\left(k_{cr}^{n+1} \frac{(T_{sol,cr} - T_{sol,st})}{\delta_{cr}^{n+1} \zeta_{st}} \right)^2 + 4 \left((\eta^n)^2 + \bar{k}^{n+1} \frac{(T_{sol,st} - T_2^{n+1})}{\zeta_{st}} \right) \right]^{1/2}.$$
 (3-36)

The finite difference approximations to the crust and ablation rate equations are

$$\rho_{cr}\Delta e_{cr} \frac{d\delta_{cr}}{dt}\Big]^{n+1} = k_{cr}^{n+1} \frac{(T_{sol,cr} - T_{sol,st})}{\delta_{cr}^{n+1}} - h_{bot}^{n+1} (T^{n+1} - T_{sol,cr})$$
(3-37)

$$\rho_{st} \Delta e_{st} \frac{d\eta}{dt} \Big]^{n+1} = \bar{k}^{n+1} \frac{(T_{sol,st} - T_2^{n+1})}{\eta^{n+1}} - k_{cr}^{n+1} \frac{(T_{sol,cr} - T_{sol,st})}{\delta_{cr}^{n+1}} \,. \tag{3-38}$$

For the case NBCINT=7, which corresponds to a thin porous crust over ablating substrate, the end of timestep ablation depth is found from Eq. 2-45 as

$$\eta^{n+1} = -h_{bot}^{n+1} \frac{(T^{n+1} - T_{sol,cr})}{2\zeta_{st}} + \frac{\Gamma_{st}}{2}, \qquad (3-39)$$

$$\Gamma_{st}^{n+1} = \left[\left(\frac{h_{bot}^{n+1}(T^{n+1} - T_{sol,cr})}{\zeta_{st}} \right)^2 + 4 \left((\eta^n)^2 + \frac{\bar{k}^{n+1}(T_{sol,st} - T_2^{n+1})}{\zeta_{st}} \right) \right]^{1/2}.$$
 (3-40)

The difference approximation to the ablation rate equation is,

$$\rho_{st}\Delta e_{st} \frac{d\eta}{dt}\Big]^{n+1} = \bar{k}^{n+1} \frac{\left(T_{sol,st} - T_2\right)^{n+1}}{\eta^{n+1}} - h_{bot}^{n+1} \left(T^{n+1} - T_{sol,cr}\right) \,. \tag{3-41}$$

For the case NBCINT=8, which corresponds to crust growth over ablating substrate and the ablated material is retained as a molten film beneath the crust, the expressions for the end of timestep crust, ablation, and molten film depths are found from Eqs. 2-47 as

$$\delta_{cr}^{n+1} = \frac{h_{bot}^{n+1}(T^{n+1} - T_{sol,cr})}{2\zeta_{cr}} + \frac{\Gamma_{cr}^{n+1}}{2} , \qquad (3-42)$$

$$\eta^{n+1} = -\frac{\bar{k}_{cr}(T_{sol,cr} - T_{sol,st})}{2\delta_{cr}^{n+1}\zeta_{st}} + \frac{\Gamma_{st}^{n+1}}{2}, \qquad (3-43)$$

$$\delta_f^{n+1} = \delta_f^n + \frac{\rho_{st,l}^{n+1}}{\rho_{st,l}^{n+1}} (\eta^{n+1} - \eta^n) , \qquad (3-44)$$

where

$$\bar{k}_{cr}^{n+1} = \frac{k_{cr}^{n+1}k_f^{n+1}\delta_{cr}^{n+1}}{k_{cr}^{n+1}\delta_f^{n+1} + k_f^{n+1}\delta_{cr}^{n+1}},$$
(3-45)

$$\Gamma_{cr}^{n+1} = \left[\left(\frac{h_{bot}^{n+1}(T^{n+1} - T_{sol,cr})}{\zeta_{cr}} \right)^2 + 4 \left((\delta^{n+1})^2 + \frac{\bar{k}_{cr}^{n+1}(T_{sol,cr} - T_{sol,st})}{\zeta_{cr}} \right) \right]^{1/2},$$
(3-46)

$$\Gamma_{st}^{n+1} = \left[\left(\frac{\bar{k}_{cr}^{n+1}(T_{sol,cr} - T_{sol,st})}{\delta_{cr}^{n+1}\zeta_{st}} \right)^2 + 4 \left((\eta^n)^2 + \bar{k}^{n+1} \frac{(T_{sol,st} - T_2^{n+1})}{\zeta_{st}} \right) \right]^{1/2} .$$
(3-47)

The difference approximations to the crust and ablation rate equations are found as

$$\rho_{cr}\Delta e_{cr} \frac{d\delta_{cr}}{dt}\Big]^{n+1} = \frac{\bar{k}_{cr}^{n+1}(T_{sol,cr} - T_{sol,st})}{\delta_{cr}^{n+1}} - h_{bot}^{n+1}(T^{n+1} - T_{sol,cr}) , \qquad (3-48)$$

$$\rho_{st} \Delta e_{st} \frac{d\eta}{dt} \Big]^{n+1} = \frac{\bar{k}^{n+1} (T_{sol,st} - T_2^{n+1})}{\zeta^{n+1}} - \frac{\bar{k}_{cr}^{n+1} (T_{sol,cr} - T_{sol,st})}{\delta_{cr}^{n+1}} \,. \tag{3-49}$$

For the case NBCINT=9, which corresponds to a thin crust over ablating substrate and the ablated substrate material is retained as a molten film beneath the thin crust, the expression for the end of timestep ablation and molten film depths are found from Eqs. 2-25 and 2-53 as

$$\eta^{n+1} = -h_{bot}^{n+1} \frac{(T^{n+1} - T_{sol,cr})}{2\zeta_{st}} + \frac{\Gamma_{st}^{n+1}}{2} , \qquad (3-50)$$

$$\delta_f^{n+1} = \delta_f^{n+1} + \frac{\rho_{st,s}}{\rho_{st,l}} (\eta^{n+1} - \eta^n) , \qquad (3-51)$$

where

$$\Gamma_{st}^{n+1} = \left[\left(\frac{h_{bot}^{n+1}(T^{n+1} - T_{sol,cr})}{\zeta_{st}} \right)^2 + 4 \left((\eta_n)^2 + \frac{\bar{k}^{n+1}(T_{sol,st} - T_2^{n+1})}{\zeta_{st}} \right) \right]^{1/2} .$$
(3-52)

The difference approximation to the ablation rate equation is

$$\rho_{st} \Delta e_{st} \frac{d\eta}{dt} \Big]^{n+1} = \bar{k}^{n+1} \frac{(T_{sol,st} - T_2^{n+1})}{\eta^{n+1}} - h_{bot}^{n+1} \left(T^{n+1} - T_{sol,cr} \right) \,. \tag{3-53}$$

In concrete regions, MELTSPREAD3 tracks the rate of propagation of the dryout fronts in order to calculate the local degassing rate. The concrete property routines account for the decomposition enthalpies associated with the generation of water vapor and carbon dioxide (See Appendix B). The decomposition reactions were summarized in Table 2-5. Thus, the propagation rate of the decomposition isotherms determines the degassing rate. Assume that the dryout isotherm for the i th decomposition process lies between the m th and m+1 st nodes. For the case of piece-wise linear inter-nodal temperature variation, the location of the isotherm between the two nodes is given through the equation,

$$x_{dc}^{i} = l_{m,m+1} \frac{T_{dc}^{i} - T_{m}^{n+1}}{T_{m+1}^{n+1} - T_{m}^{n+1}},$$
(3-54)

where

$$T_{dc}^i$$
 = decomposition temperature for i th decomposition process, and $l_{m,m+1} = \delta x_{m,m+1/2} + \delta x_{m+1,m-1/2}$

Differentiating Eq. 3-54 with respect to time yields the following expression for the propagation rate of the dryout front in terms of the rate of change in local node specific enthalpies,

$$\frac{dx_{dc}^{i}}{dt} = \frac{1_{m,m+1}}{(T_{m+1}^{n+1} - T_{m}^{n+1})^{2}} \left\{ \left(T_{dc}^{i} - T_{m+1}^{n+1} \right) W_{m}^{n+1} \frac{de}{dt} \right)_{m}^{n+1} + \left(T_{m+1}^{n+1} - T_{dc}^{i} \right) W_{m+1}^{n+1} \frac{de}{dt} \right)_{m+1}^{n+1} \right\},$$
(3-55)

$$W_{m}^{n+1} = \frac{dT}{de} \int_{m}^{n+1} W_{m+1}^{n+1} = \frac{dT}{de} \int_{m+1}^{n+1} W_{m+1}^{n+1} = \frac{dT}{de} \int_{m+1}^{n+1} \frac{de}{dt} \int_{m+1}^{n+1} = \frac{1}{\rho_{m+1}^{n+1} V_{m+1}} \left\{ C_{m+1,m-1/2}^{n+1} (T_m^{n+1} - T_{m+1}^{n+1}) - C_{m+1,m+1/2}^{n+1} (T_{m+1}^{n+1} - T_{m+2}^{n+1}) + \rho_{m+1}^{n+1} (\dot{q}_{decay}) \int_{m+1}^{n+1} V_{m+1} \right\},$$

$$(3-56)$$

$$-C_{m+1,m+1/2}^{n+1} (T_{m+1}^{n+1} - T_{m+2}^{n+1}) + \rho_{m+1}^{n+1} (\dot{q}_{decay}) \int_{m+1}^{n+1} V_{m+1} \right\},$$

$$(3-57)$$

and

$$CON_{m}^{n+1} = \begin{cases} C_{m,m-1/2}^{n+1}(T_{m-1}^{n+1} - T_{m}^{n+1}); \ m \ge 3\\ C_{m,m-1/2}^{n+1}(T_{m-1}^{n+1} - T_{m}^{n+1}); \ m = 2 \ and \ NBCINT \le 3\\ h_{bot}^{n+1}(T^{n+1} - T_{1}^{n+1}); \ m = 1 \ and \ NBCINT = 1\\ \frac{k_{cr}^{n+1}(T_{sol,cr} - T_{1}^{n+1})}{\delta_{cr}^{n+1}}; \ m = 1 \ and \ NBCINT = 2\\ h_{bot}^{n+1}(T^{n+1} - T_{sol,cr}); \ m = 1 \ and \ NBCINT = 3\\ \overline{k}^{n+1}\frac{(T_{sol,st} - T_{2})}{\eta^{n+1}}; \ m = 2 \ and \ NBCINT > 3 \end{cases}$$

For the case in which substrate ablation is occurring, then the (Eulerian) location of the dryout front relative to a fixed coordinate system is given by the equation

$$x_{dc}^{i} = l_{m,m+1}^{o} + \eta^{n+1} \left(\frac{T_{dc}^{i} - T_{m+1}^{n+1}}{T_{m+1}^{n+1} - T_{sol,st}} \right)$$
(3-58)

where

 $l^o_{m,m+1}$ = inter-nodal spacing prior to concrete ablation.

Differentiation of Eq. 3-58 with respect to time yields the following expression for the propagation rate of the dryout front,

$$\frac{dx_{dc}^{i}}{dt} = \left(\frac{T_{dc}^{i} - T_{m+1}^{n+1}}{T_{m+1}^{n+1} - T_{sol,st}^{n+1}}\right) \frac{d\eta}{dt} \right)^{n+1} - \frac{\eta^{n+1} W_{m+1}^{n+1} \left(T_{dc}^{i} - T_{m+1}^{n+1}\right)}{\left(T_{m+1}^{n+1} - T_{sol,st}\right)^{2}} \frac{de}{dt} \right)_{m+1}^{n+1}$$
(3-59)

For each dryout or decomposition front, a local check is performed to determine if the dryout/decomposition front lies in a concrete region and that the local enthalpy has previously exceeded the enthalpy at which the i th concrete constituent is completely dried out. For situations in which both of these criteria are met, the expression for the local end of timestep water vapor mass flux is found through Eqs. 3-55 and 3-59 as

$$\left(\dot{m}_{H_{2}O}\right)^{n+1} = <\rho_m^{n+1}, \rho_{m+1}^{n+1} >_{free H_{2}O} x_{free H_{2}O} \frac{dx_{dc}^{free H_{2}O}}{dt} \right)^{n+1}$$

+< $\rho_m^{n+1}, \rho_{m+1}^{n+1} >_{Ca(OH)_2} x_{Ca(OH)_2} \frac{dx_{dc}^{Ca(OH)_2}}{dt} \right)^{n+1} ,$ (3-60)

where

$$\begin{split} x_{free\,H_20}, x_{Ca(OH)_2} &= \text{concrete weight percents of } H_20 \text{ in the form of free} \\ &\text{water and bound in } Ca(OH)_2, \text{ respectively,} \\ &< \rho_m^{n+1}, \rho_{m+1}^{n+1} > \quad = \begin{cases} \rho_m^{n+1}; \left(x_{dc}^i\right)^{n+1} \leq \delta x_{m,m+1/2} \\ \rho_{m+1}^{n+1}; \left(x_{dc}^i\right)^{n+1} > \delta x_{m,m+1/2} \end{cases} \end{split}$$

Subject to the same criteria as applied to Eq. 3-60, the local CO_2 gas mass flux is found through the equation

$$\left(\dot{m}_{CO_2}\right)^{n+1} = <\rho_m^{n+1}, \rho_{m+1}^{n+1} >_{CaCO_3} x_{CaCO_3} \frac{dx_{dc}^{CaCO_3}}{dt} \right)$$
$$+ <\rho_m^{n+1}, \rho_{m+1}^{n+1} >_{Mg \ Ca(CO_3)_2} x_{Mg \ Ca(CO_3)_2} \frac{dx_{dc}^{Mg \ Ca(CO_3)_2}}{dt} \right)^{n+1}$$
(3-61)

Equations 3-60 and 3-61 are used to evaluate the water vapor and CO_2 gas mass flux terms in Eqs. 3-7 and 3-9.

DIFFERENCED FORM OF SHELL HEATUP EQUATIONS

The index nomenclature for the shell heatup calculation is illustrated in Figure 3-6. The shell is assumed to be discretized into j=1, 2,...,J nodes normal to the shell surface, and k=1, 2,..., K nodes parallel to the shell surface. For interior grid cells, for which $2 \le j \le J$ and $2 \le k \le K$, the finite difference approximation to the shell transient heat conduction equation, Eq. 2-102, is

$$\frac{\rho_{j,k}^{n+1}}{\delta t} V_{j,k} \left(e_{j,k}^{n+1} - e_{j,k}^{n} \right) = l_k C_{j-\frac{1}{2},k}^{n+1} \left(T_{j,k-1}^{n+1} - T_{j,k}^{n+1} \right) - l_k C_{j+\frac{1}{2},k}^{n+1} \left(T_{j,k}^{n+1} - T_{j+1,k}^{n+1} \right) + l_j C_{j,k-1/2}^{n+1} \left(T_{j,k-1}^{n+1} - T_{j,k}^{n+1} \right) - l_j C_{j,k+1/2}^{n+1} \left(T_{j,k}^{n+1} - T_{j,k+1}^{n+1} \right)$$
(3-62)

$$V_{j,k} = l_j l_k$$
, (3-63)

$$C_{j+1/2}^{n+1} = \frac{2 k_{j,k}^{n+1} k_{j+1,k}^{n+1}}{l_{j,k} k_{j+1,k}^{n+1} + l_{j+1,k} k_{j,k}^{n+1}}$$
(3-64)

and $C_{j-1/2,k}$, $C_{j,k-1/2}$, and $C_{j,k+1/2}$ have similar definitions. At the shell rear surface, j=J, an adiabatic boundary condition is assumed for which the following equation is satisfied,

$$\frac{\rho_{j,k}^{n+1}V_{j,k}}{\delta t} \left(e_{j,k}^{n+1} - e_{j,k}^{n} \right) = l_k C_{j-\frac{1}{2},k}^{n+1} \left(T_{j,k-1}^{n+1} - T_{j,k}^{n+1} \right) - l_j C_{j,k-1/2}^{n+1} \left(T_{j,k-1}^{n+1} - T_{j,k}^{n+1} \right) + l_j C_{j,k+1/2}^{n+1} \left(T_{j,k}^{n+1} - T_{j,k+1}^{n+1} \right)$$
(3-65)



Figure 3-21 Illustration of Shell Nodalization Scheme

At the top and bottom of the nodalized shell region (the length of the shell to be nodalized is a user-specified constant, as described in Section 5), adiabatic boundary conditions are also assumed. For k=1, the equation,

$$\frac{\rho_{j,1}^{j+1}V_{j,1}}{\delta t} \left(e_{j,1}^{n+1} - e_{j,1}^{n} \right) = l_1 C_{j-1/2,1}^{n+1} \left(T_{j-1,1}^{n+1} - T_{j,1}^{n+1} \right) - l_1 C_{j+1/2,1}^{n+1} \left(T_{j,1}^{n+1} - T_{j+1,1}^{n+1} \right) - l_j C_{j,1+1/2} \left(T_{j,1}^{n+1} - T_{j,2}^{n+1} \right),$$
(3-66)

is satisfied, whereas at k=K the equation,

...

$$\frac{\rho_{j,K}V_{j,K}}{\delta t} \left(e_{j,k}^{n+1} - e_{j,K}^{n} \right) = l_K C_{j-1/2,K}^{n+1} \left(T_{j-1,K}^{n+1} - T_{j,K}^{n+1} \right) - l_K C_{j+1/2,K}^{n+1} \left(T_{j,K}^{n+1} - T_{j+1,K}^{n+1} \right) - l_j C_{j,K-1/2}^{n+1} \left(T_{j,K-1}^{n+1} - T_{j,K}^{n+1} \right),$$
(3-67)

is satisfied.

On the inside surface of the shell, the specific form of the boundary condition is dependent upon whether frozen corium, molten corium, water, or containment atmosphere is locally present. If molten corium is present, the form of the boundary condition is further dependent upon whether or not crust growth is specified on the shell surface.

For j=1 under situations in which dry atmosphere, water, frozen corium, or molten corium (crust growth not specified) is adjacent to the shell, the equation

$$\frac{\rho_{1,k}^{n+1}V_{1,k}}{\delta t} \left(e_{1,k}^{n+1} - e_{1,k}^{n} \right) = l_k h^{n+1} \left(T_{bound}^{n+1} - T_{1,k}^{n+1} \right) - l_k C_{1-1/2,k}^{n+1} \left(T_{1,k}^{n+1} - T_{2,k}^{n+1} \right) + l_1 C_{1,k-1/2}^{n+1} \left(T_{1,k-1/2}^{n+1} - T_{1,k}^{n+1} \right) - l_1 C_{1,k+1/2}^{n+1} \left(T_{1,k}^{n+1} - T_{1,k+1}^{n+1} \right), \quad (3-68)$$

is satisfied, where

$$T_{bound}^{n+1} = \begin{cases} T_{struc}; dry \ atmosphere \ locally \ present, \\ T_{sat}; \ water \ locally \ present, \\ T_{adj}^{n+1}; \ melt \ locally \ present, \\ T_{froz,adj}^{n+1}; \ frozen \ melt \ locally \ present, \\ \end{cases}$$

$$h^{n+1} = \begin{cases} h_{shell,atm}^{n+1}; \ dry \ atmosphere \ locally \ present, \\ h_{shell,wat}^{n+1}; \ water \ locally \ present, \\ h_{shell}^{n+1}; \ melt \ locally \ present, \\ \end{cases}$$

If the crust growth on the shell is specified and melt has locally covered the shell, then for j=1 the equation,

$$\frac{\rho_{1,k}^{n+1}V_{1,k}}{\delta t} \left(e_{1,k}^{n+1} - e_{1,k}^{n} \right) = l_k k_{cr}^{n+1} \frac{\left(T_{sol,cr}^{n+1} - T_{1,k}^{n+1} \right) - l_k C_{1+1/2,k}^{n+1} \left(T_{1,k}^{n+1} - T_{2,k}^{n+1} \right)}{+ l_1 C_{1,k-1/2}^{n+1} \left(T_{1,k}^{n+1} - T_{1,k}^{n+1} \right) - l_1 C_{1,k+1/2}^{n+1} \left(T_{1,k}^{n+1} - T_{1,k+1}^{n+1} \right)}$$
(3-69)

is satisfied, where

 $\delta_{cr,k}^{n+1}$ = local crust thickness on shell.

The end of timestep crust depth is determined through the equation

$$\left(\delta_{cr,k}\right)^{n+1} = -h_{shell}^{n+1} \frac{\left(T_{adj}^{n+1} - T_{sol,cr}\right)}{2\zeta_{cr}} + \frac{\Gamma_{cr,k}^{n+1}}{2}$$
(3-70)

where

$$\zeta_{cr} = \frac{\rho_{cr} \Delta e_{cr}}{2\delta t},\tag{3-71}$$

$$\Gamma_{cr,k}^{n+1} = \left[\left(\frac{h_{shell}^{n+1} \left(T_{adj}^{n+1} - T_{sol,cr} \right)}{\zeta_{cr}} \right)^2 + 4 \left(\left(\delta_{cr,k}^n \right)^2 + \frac{k_{cr}^{n+1}}{\delta_{cr}} \left(T_{sol,cr} - T_{1,k}^{n+1} \right) \right) \right]^{1/2}.$$
 (3-72)

DIFFERENCED FORM OF WATER CONSERVATION EQUATIONS

As for the solution of the melt conservation of momentum equation, a staggered mesh for the water conservation of energy equation is employed; the nomenclature is the same as that shown in Figure 3-1. At interior grid cell interfaces, for which $2 \le j \le J$, the finite difference approximation to the conservation of momentum equation (Eq. 2-307) is of the form,

$$\frac{U_{w,j-1/2}^{n+1} - U_{w,j-1/2}^{n}}{\delta t} + \frac{1}{2} \frac{\delta z_{j}}{\delta z_{j} \delta z_{j-1}} \left(1 + sqn(u)\right) U_{w,j-1/2}^{n+1} \left(U_{w,j-1/2}^{n+1} - U_{w,j-3/2}^{n+1}\right) \\
+ \frac{1}{2} \frac{\delta z_{j-1}}{\delta z_{j} \delta z_{T}} \left(1 - sqn(u)\right) U_{w,j-1/2}^{n+1} \left(U_{w,j+1/2}^{n+1} - U_{w,j-1/2}^{n+1}\right) \\
= \frac{-g}{\left(\delta z_{j} + \delta z_{j-1}\right)} \left[\frac{H_{w,j}^{n+1}}{1 - \alpha_{j}^{n}} + E_{j}^{n} - \frac{H_{w,j-1}^{n+1}}{1 - \alpha_{j-1}^{n}} - E_{j-1}^{n}\right] - \frac{1}{2} f_{j-1/2} \frac{U_{w,j-1/2}^{n+1}}{H_{w,j}^{n}} \left|U_{w,j-1/2}^{n+1}\right|$$
(3-73)

Equation 3-73 is solved assuming no flow across the system boundaries. Thus, the boundary conditions on the discretized momentum equation are, for j=1,

$$U_{w,J-1/2}^{n+1} = 0, (3-74)$$

and for j=J+1,

$$U_{w,l+1/2}^{n+1} = 0. (3-75)$$

The local velocities are calculated from Eqs. 3-73 to through 3-75 in conjunction with the conservation of mass equation, the differenced form of which is developed below.

Employing the donor cell method for differencing of the convective mass flux term, the finite difference approximation to the water conservation of mass equation (Eq. 2-95) is of the form,

$$\frac{A_{j}}{\delta_{t}} \left[H_{w,j}^{n+1} - H_{w,j}^{n} \right] + S_{j-1/2} \langle -U_{w,j-1/2}^{n+1}, 0 \rangle H_{w,j}^{n+1} + S_{j+1/2} \langle U_{w,j+1/2}^{n+1}, 0 \rangle H_{w,j}^{n+1}
-S_{j-1/2} H_{w,j-1}^{n+1} \langle U_{w,j-1/2}^{n+1}, 0 \rangle - S_{j+1/2} H_{w,j+1}^{n+1} \langle U_{w,j+1/2}^{n+1}, 0 \rangle = \dot{m}_{w,j}^{n+1} / \rho_{l}$$
(3-76)

The operator, $\langle \cdot, \cdot \rangle$, is again noted to denote the largest of the two arguments,

$$\langle U_{w,j+1/2}^{n+1}, 0 \rangle = \begin{cases} U_{w,j+1/2}^{n+1}, & U_{w,j+1/2}^{n+1} > 0\\ 0, & U_{w,j+1/2}^{n+1} < 0 \end{cases}$$
(3-77)

The constraint that the water depth at the leading edge does not fall below the minimum depth at which surface tension balances gravity (Eq. 2-93) is also applied to the differenced form of the equations by performing a local check on the water depth relative to the minimum spreading depth. If $H_{w,j}^{n+1}$ and $H_{w,j-1}^{n+1}$ are less than $H_{w,min}$, then $U_{w,j-1/2}$ is set equal to zero.

As for the case of melt spreading, care must be exercised in solving Eqs. 3-73 and 3-77 over substrate surfaces with large physical discontinuities in elevation that exist as an initial condition; see discussion surrounding Figures 3-2 and 3-3, and Eq. 3-6.

Given the local water velocities as calculated through solution of Eqs. 3-73 to 3-77, the water conservation of energy equation is then then solved to obtain the end of timestep nodal water temperatures. The finite difference approximation to the conservation of energy equation (Eq. 2-99) is of the form,

$$\frac{A_{j}}{\delta t} \Big[(\rho_{l}H_{w}e_{w})_{j}^{n+1} - (\rho_{l}H_{w}e_{w})_{j}^{n} \Big] - S_{j-1/2} \langle U_{w,j-1/2}^{n+1}, 0 \rangle (\rho_{l}H_{w}e_{w})_{j-1}^{n+1} \\
+ S_{j-1/2} \langle -U_{w,j-1/2}^{n+1}, 0 \rangle (\rho_{l}H_{w}e_{w})_{j}^{n+1} + S_{j+1/2} \langle U_{w,j+1/2}^{n+1}, 0 \rangle (\rho_{l}H_{w}e_{w})_{j}^{n+1} \\
- S_{j+1/2} \langle -U_{w,j+1/2}^{n+1}, 0 \rangle (\rho_{l}H_{w}e_{w})_{j+1}^{n+1} = A_{j} (q_{wat}^{"})_{j}^{n+1} + (\dot{m}_{inj}e_{inj})_{j}^{n+1} \\
- (\dot{m}_{dc}e_{w})_{j}^{n+1} \qquad (3-78)$$

FORWARD ELIMINATION SOLUTION SCHEME: MELT SPREADING EQUATIONS

The local variables to be determined from the difference equations developed in the previous section are the melt enthalpy (temperature), melt height, melt constituency, melt velocity, substrate enthalpy (temperature), substrate decomposition (degassing) rate, crust growth rate, and/or the substrate ablation rate. For flooded cavity conditions in which the detailed water inventory model is invoked, the water velocity and temperature distributions also need to be determined.

At the start of the calculation for the current timestep, the cell edge velocities are first determined through the simultaneous solution of Eqs. 3-1 through 3-4 by performing an iterative calculation on the linearized form of these equations. The cell edge velocities are expanded as,

$$U_{j-1/2}^{r+1} = U_{j-1/2}^r + \delta U_{j-1/2}, \qquad (3-79)$$

where

 $\delta U_{j-1/2}$ = incremental change in cell edge velocity, r = iteration step.

Similar expressions apply at the j+1/2 and j-3/2 cell edges. The end of timestep melt depth in Eq. 3-1 is forward eliminated in terms of the incremental changes in cell edge velocities. Substitution of Eq. 3-79 into Eq. 3-4 and linearization of the resultant expression yields,

$$h_j^{r+1} = h_j^n + F_j^r + G_j^r \delta U_{j-1/2} + H_j^r \delta U_{j+1/2}$$
(3-80)

where

$$F_{j} = \frac{\delta t}{A_{j}} \left\{ \frac{(\dot{m}_{vessel})_{j}^{n+1}}{\rho_{j}^{r}} + S_{j-1/2} < U_{j+1/2}^{r}, 0 > h_{j-1}^{r} + S_{j+1/2} < -U_{j+1/2}^{r}, 0 > h_{j+1}^{r} - S_{j-\frac{1}{2}} < -U_{j-\frac{1}{2}}^{r}, 0 > h_{j}^{r} - S_{j+\frac{1}{2}} < U_{j+\frac{1}{2}}^{r}, 0 > h_{j}^{r} \right\},$$
(3-81)

$$G_{j} = \frac{\delta t \, S_{j-1/2}}{A_{j}} \{ h_{j-1}^{r} < sgn(U_{j-1/2}^{r}), 0 > -h_{j}^{r} < -sgn(U_{j-1/2}^{r}), 0 > \}, \qquad (3-82)$$

$$H_{j} = \frac{\delta t \, S_{j+1/2}}{A_{j}} \{ h_{j+1}^{r} < sgn(U_{j+1/2}^{r}), 0 > -h_{j} < -sgn(U_{j+1/2}^{r}), 0 > \}.$$
(3-83)

The forward elimination for h_{j-1}^{n+1} is obtained by setting j=j-1 in Eqs. 3-74 through 3-77. Substitution of Eqs. 3-73 through 3-77 into the momentum equation, Eq. 3-1, and linearizing the resulting expression yields, for j=2,...,J,

$$O_j^r \,\delta U_{j-1/2} + P_j^r \,\delta U_{j+1/2} + Q_j^r \delta U_{j-3/2} + R_j = 0, \qquad (3-84)$$

$$O_{j}^{r} = \frac{1}{\delta t} + \frac{\delta z_{j} \left(1 + sgn(U_{j-1/2}^{r})\right)}{2\delta z_{7} \delta z_{j-1}} \cdot \left(2U_{j-1/2}^{r} - U_{j-3/2}^{r}\right) \\ + \frac{\delta z_{j-1} \left(1 - sgn(U_{j-1/2}^{r})\right)}{2\delta z_{j} \delta z_{T}} \cdot \left(U_{j+1/2}^{r} - 2U_{j-1/2}^{r}\right) \\ + \frac{sgn(U_{j-1/2}^{r})}{2\delta z_{j} \delta z_{T}} f_{j-1/2}^{r} U_{j-1/2}^{r} + \frac{g}{(s-1)^{2}} \left(\frac{G_{j}^{r}}{2} - \frac{H_{j-1}^{r}}{2}\right), \quad (3-85)$$

$$+\frac{g_{j-1/2}}{h_{j}^{n}}f_{j-1/2}^{r}U_{j-1/2}^{r}+\frac{g}{(\delta z_{j}+\delta z_{j-1})}\left(\frac{u_{j}}{1-\alpha_{j}^{n}}-\frac{u_{j-1}}{1-\alpha_{j-1}^{n}}\right),$$
(3-85)

$$P_{j}^{r} = \delta z_{j-1} \frac{\left(1 - sgn\left(U_{j-1/2}^{r}\right)\right)}{2\delta z_{j}\delta z_{T}} U_{j-1/2}^{r} + \frac{g H_{j}^{r}}{\left(1 - \alpha_{j}^{n}\right)(\delta z_{j} + \delta z_{j-1})}, \qquad (3-86)$$

$$Q_{j}^{r} = -\delta z_{j} \frac{\left(1 + sgn\left(U_{j-\frac{1}{2}}^{r}\right)\right)}{2\delta z_{j-1}\delta z_{T}} U_{j-\frac{1}{2}}^{r} - \frac{g G_{j-1}^{r}}{\left(1 - \alpha_{j-1}^{n}\right)(\delta z_{j} + \delta z_{j-1})}, \qquad (3-87)$$

$$R_{j}^{r} = \frac{U_{j-1/2}^{r} - U_{j-1/2}^{n}}{\delta t} + \frac{\delta z_{j} \left(1 + sgn(U_{j-1/2}^{r})\right)}{2\delta z_{7} \delta z_{j-1}} U_{j-1/2}^{r} \left(U_{j-1/2}^{r} - U_{j-3/2}^{r}\right)$$
$$\frac{\delta z_{j-1} \left(1 - sgn(U_{j-1/2}^{r})\right)}{2\delta z_{j} \delta z_{7}} U_{j-1/2}^{r} \left(U_{j+1/2}^{r} - U_{j-3/2}^{r}\right)$$
$$+ \frac{1}{2} \frac{f_{j-1/2}^{r}}{h_{j}^{n}} U_{j-1/2}^{r} \left|U_{j-1/2}^{r}\right| + \frac{g}{(\delta z_{j} + \delta z_{j-1})} \left(\frac{h_{j}^{r} + F_{j}^{r}}{1 - \alpha_{j}^{n}} + E_{j}^{n} - \frac{h_{j-1}^{r} + F_{j-1}^{r}}{1 - \alpha_{j}^{n}} - E_{j-1}^{n}\right).$$
(3-88)

For j=1, the coefficients for the no flow boundary condition are

$$O_1^r = 1$$
,
 $P_1^r = 0$, (3-89)
 $Q_1^r = 0$,
 $R_1^r = 0$.

Similarly, for j=J+1, the coefficients are of the form

$$O_{j+1}^r = 1$$
,
 $P_{J+1}^r = 0$, (3-90)
 $Q_{J+1}^r = 0$,
 $R_{J+1}^r = 0$.

Equation 3-84 constitutes a linear set of equations, in the form of a tri-diagonal matrix, for the incremental changes in the cell edge velocities. Given the current estimate of the edge velocities and melt heights, Eq. 3-84 is solved to obtain the incremental velocity changes. The end of timestep velocities are then updated through Eq. 3-79. Given the updated velocities, Eq. 3-4 is then solved to obtain the updated melt heights. This procedure is repeated until the incremental velocity changes decrease below user-specified convergence criteria (See Section 4).

Given the end of timestep velocities, the coupled set of mass and energy equations for the substrate, shell, and melt are then solved. For these equations, the end of timestep variables are expanded, using the material functional relationships between enthalpy and temperature, in terms of the incremental specific enthalpy changes of all of the melt and structure cells in a Newton-Raphson iterative approach. The end of timestep solutions in the substrate and shell regions are forward-eliminated in terms of the incremental changes in the melt specific enthalpy. Given the forward elimination functions in these regions, the detailed melt conservation of mass and energy equations are then solved. With the incremental changes in bulk melt enthalpy determined, the end of timestep solutions in the substrate and shell are then found by backwards substitution.

The general equations for the expansion of the substrate transient heat conduction equation are of the form

$$e_m^{r+1} = e_m^r + \delta e_m , (3-91)$$

$$T_m^{r+1} = T_m^r + W_m^r \delta e_m , (3-92)$$

where the derivative of temperature with respect to enthalpy material function, W_m^r has been defined under Eq. 3-55. Sustitution of Eqs. 3-91 and 3-92 into Eq. 3-10 yields the expression

$$O_m^r \delta e_m = P_m^r \delta e_{m+1} + Q_m^r \delta e_{m-1} + R_m^r , \qquad (3-93)$$

where

$$O_m^r = \frac{V_m \rho_m^r}{\delta t} + \left(C_{m-1/2}^r + C_{m+1/2}^r\right) W_m^r , \qquad (3-94)$$

$$P_m^r = C_{m+1/2}^r W_{m+1}^r , (3-95)$$

$$Q_m^r = C_{m-1/2}^r W_{m-1}^r , (3-96)$$

$$R_m^r = \frac{V_m \rho_m^r}{\delta t} (e_m^r - e_m^n) + C_{m-1/2}^r (T_{m-1}^r - T_m^r) - C_{m+\frac{1}{2}}^r (T_m^r - T_{m-1}^r) + \rho_m^r V_m (\dot{q}_{decay})_m^{n+1} (X_{st}^{UO_2})_m .$$
(3-97)

For the case m=M, the specific form of the coefficients for the adiabatic node are,

$$O_M^r = \frac{V_m \rho_M^r}{\delta t} + C_{M-1/2}^r W_M^r , \qquad (3-98)$$

$$P_M^r = 0$$
, (3-99)

$$Q_M^r = C_{M-1/2}^r W_{M-1} , \qquad 3-100)$$

$$R_{M}^{r} = \frac{V_{M}\rho_{M}^{r}}{\delta t} (e_{M}^{r} - e_{M}^{r}) + C_{M-1/2}^{r} (T_{M-1}^{r} - T_{M}^{r}) + \rho_{M}^{r} V_{M} (\dot{q}_{decay})_{M}^{n+1} (X_{st}^{UO_{2}})_{M}.$$
 (3-101)

For m = 1, the linearized form of the nodal equation is dependent upon the specific boundary conditions at the melt/substrate interface. For cases in which substrate ablation is not occurring (NBCINT=1, 2, 3; See Table 2-4), the linearized form of the cell energy balance at the substrate surface is,

$$O_1^r \,\delta e_1 = P_1^r \,\delta e_2 + R_1^r + S^r \,\delta e_{melt} \tag{3-102}$$

where

 δe_{melt}^{j} = incremental change in melt specific enthalpy at j-th spreading node,

$$O_{1}^{r} = \begin{cases} \frac{V_{1}\rho_{1}^{r}}{\delta t} + \left(C_{1+1/2}^{r} + h_{bot}^{r}\right)W_{1}^{r}; & NBCINT = 1\\ \frac{V_{1}\rho_{1}^{r}}{\delta t} + \left(\frac{k_{cr}^{r}}{\delta_{cr}^{r}} + k_{cr}\frac{(T_{sol,cr} - T_{1}^{r})}{(\delta_{cr}^{r})^{2}}(d_{1}^{cr})^{r} + C_{1-1/2}^{r}\right)W_{1}^{r}; & NBCINT = 2\\ \frac{V_{1}\rho_{1}^{r}}{\delta t} + C_{1+1/2}^{r}W_{1}^{r}; & NBCINT = 3 \end{cases}$$
(3-103)

$$P_1^r = C_{1+1/2}^r W_2^r , (3-104)$$

$$Q_1^r = 0$$
, (3-105)

$$R_{1}^{r} = \begin{cases} -\frac{\rho_{1}^{r} V_{1}}{\delta t} (e_{1}^{r} - e_{1}^{n}) - C_{1+\frac{1}{2}}^{r} (T_{1}^{r} - T_{2}^{r}) + h_{bot} (T^{r} - T_{1}^{r}) \\ +\rho_{1}^{r} V_{1}^{r} (\dot{q}_{decay})_{1}^{n+1} (X_{st}^{UO_{2}})_{1}; & NBCINT = 1 \\ -\frac{\rho_{1}^{r} V_{1}}{\delta t} (e_{1}^{r} - e_{1}^{n}) + \frac{k_{cr} (T_{sol,cr} - T_{1}^{r})}{\delta_{cr}^{r}} - C_{1+\frac{1}{2}}^{r} (T_{1}^{r} - T_{2}^{r}) \\ +\rho_{1}^{r} V_{1} (\dot{q}_{decay})_{1}^{n+1} (X_{st}^{UO_{2}})_{1}; & NBCINT = 2 \\ -\frac{\rho_{1}^{r} V_{1}}{\delta t} (e_{1}^{r} - e_{1}^{n}) + h_{bot}^{r} (T^{r} - T_{sol,st}) - C_{1+1/2} (T_{1}^{r} - T_{2}^{r}) \\ +\rho_{1}^{r} V_{1} (\dot{q}_{decay})_{1}^{n+1} (X_{st}^{UO_{2}})_{1}; & NBCINT = 3 \end{cases}$$

$$S^{r} = \begin{cases} W_{melt}^{r} h_{bot}^{h}; & NBCINT = 1 \\ -\frac{k_{cr} (T_{sol,cr} - T_{1}^{r})}{(\delta_{cr}^{r})^{2}} ((d_{melt}^{cr})^{r} W_{melt}^{r}; & NBCINT = 2 \\ W_{melt}^{r} h_{bot}^{h}; & NBCINT = 3 \end{cases}$$

$$(3-107)$$

$$(d_1^{cr})^r = \frac{d\delta_{cr}}{dT_1} \Big) , \qquad (3-108)$$

$$(d_{melt}^{cr})^r = \frac{d\delta_{cr}}{dT_1} r^r , \qquad (3-109)$$

The derivative functions for the various boundary conditions, d_1^{cr} and d_{melt}^{cr} , are tedious and are therefore tabulated in Appendix A. In the derivation of Eq. 3-102 the end of timestep melt enthalpy and temperature have been linearized through the equations

$$e^{r+1} = e^r + \delta e_{melt} , \qquad (3-110)$$

$$T^{r+1} = T^r + W^r_{melt} \delta e_{melt} , \qquad (3-111)$$

where

$$W_{melt}^r = \frac{dT}{de} \Big)^r . aga{3-112}$$

It is again noted that, for the purposes of brevity, the subscript denoting the j^{th} spreading cell has been omitted from the substrate equations.

Note that in the development of Eq. 3-102, the bottom heat transfer coefficient has not been expanded in terms of the fluid cell specific enthalpy change or the incremental change in substrate surface temperature. It is assumed that such an expansion is not required to obtain a solution for large timesteps and that the heat transfer coefficient may therefore be formulated in terms of variables at the end of the rth iteration.

For cases in which the substrate is ablating, the surface node is treated as isothermal and therefore the incremental change in specific enthalpy over the timestep is zero for this cell. For m=2, the linearized form of the heat conduction equation is

$$O_2^r \delta e_2 = P_2^r \delta e_3 + R_2^r + S^r \,\delta e_{melt} \,\,, \tag{3-113}$$

where

$$O_2^r = \frac{\rho_2^r V_2}{\delta t} + \left[\frac{\bar{k}^r}{\eta^r} + \bar{k}^r \frac{(T_{sol,st} - T_2^r)}{(\eta^r)^2} (d_2^{st})^r + C_{2+1/2}^r\right] W_2^r , \qquad (3-114)$$

$$P_2^r = C_{2+1/2}^r W_3^r , (3-115)$$

$$Q_2^r = 0$$
, (3-116)

$$R_{2}^{r} = -\frac{\rho_{2}V_{2}}{\delta t}(e_{2}^{r} - e_{2}^{n}) + \frac{\bar{k}^{r}(T_{sol,st} - T_{2}^{r})}{\eta^{r}} - C_{2+\frac{1}{2}}^{r}(T_{2}^{r} - T_{3}^{r}) + \rho_{2}^{r}V_{2}(\dot{q}_{decay})_{2}^{n+1}(X_{st}^{UO_{2}})_{2}$$
(3-117)

$$S^{r} = -\bar{k}^{r} \frac{(T_{sol,st} - T_{2}^{r})}{(\eta^{r})^{2}} (d_{melt}^{st})^{r} W_{melt}^{r} , \qquad (3-118)$$

$$(d_2^{st})^r = \frac{d\eta}{dT_2} \Big)^r$$
, (3-119)

$$(d_{melt}^{st})^r = \frac{d\eta}{dT} \Big)^r . aga{3-120}$$

The derivative functions d_2^{st} and d_{melt}^{st} are tabulated in Appendix A. Given the current estimate of the end of timestep data, Eqs. 3-93 through 3-120 constitute a linear set of equations relating the incremental changes in substrate specific enthalpy to the incremental change in the local melt specific enthalpy. In order to solve the melt conservation equations including the (implicit) effects of end-of-timestep variation in substrate enthalpy, the incremental changes in substrate enthalpy are forward eliminated through an expansion of the form,

$$\delta e_m = \theta_m^0 + \theta_m^1 \delta e_{melt} , \qquad (3-121)$$

where θ_m^0 and θ_m^1 are the substrate forward elimination coefficients. Substitution of Eq. 3-121 into Eq. 3-93 yields the following set of equations,

$$0_m^r \theta_m^l = P_m^r \theta_{m+1}^l + Q_m^r \theta_{m-1}^l + \binom{R_m^r; l=0}{0; l=1}; l = 0, 1.$$
(3-122)

For the case m=M, the forward elimination coefficients satisfy the equation

$$0_{M}^{r}\theta_{M}^{l} = Q_{M}^{r}\theta_{M+1}^{l} + \begin{pmatrix} R_{M}^{r}; l=0\\0; l=1 \end{pmatrix}; l = 0, 1.$$
(3-123)

For the case m=1 under situations in which substrate ablation is not occurring (NBCINT=1,2,3), the forward elimination coefficients satisfy the equations

$$0_l^r \theta_1^l = P_1^r \theta_2^l + \begin{pmatrix} R_1^{1;l=0} \\ S^r; l=1 \end{pmatrix}; l = 0, 1.$$
(3-124)

For cases in which the substrate is ablating (NBCINT>3), the forward elimination coefficients for the (isothermal) surface node satisfy the equation,

$$\theta_1^l = 0, \ l = 0,1. \tag{3-125}$$

For the second node, the coefficients satisfy the equation,

$$0_2^r \,\theta_2^l = P_2^r \theta_3^l + \binom{R_2^r}{s^r}; l = 0,1 \ . \tag{3-126}$$

Equations 3-122 through 3-126 constitute two simple sets of tri-diagonal matrices which are solved in a straightforward manner. The forward elimination scheme then allows the end of timestep substrate enthalpy variables to be expressed in terms of current estimate data plus additional (linear) terms which account for incremental changes in local melt specific enthalpy.

To evaluate the end of timestep ablation and crust growth rate mass source/sink terms in the melt conservation equation, Eqs. 3-7 and 3-9, the substrate surface and melt temperatures in the governing equations for these processes are linearly expanded in terms of material function derivatives, W_m and W_{melt} . The general form of the expansion for the crust growth rate equation is

$$\frac{d\delta_{cr}}{st}\Big)^{r+1} = \frac{d\delta_{cr}}{dt}\Big)^r + \sigma^0 + \sigma^1 \delta e_{melt}, \qquad (3-127)$$

where σ^0 and σ^1 are the crust growth forward elimination coefficients. The general form of the ablation rate equation is,

$$\left.\frac{d\eta}{dt}\right)^{r+1} = \frac{d\eta}{dt}\right)^r + \tau^0 + \tau^1 \delta e_{melt} \ . \tag{3-128}$$

For example, through differentiation and expansion of the crust growth rate equation for the case NBCINT=2, Eq. 3-16, the forward elimination coefficients are found as,

$$\sigma^0 = (f_1^{cr})^r W_1^r \,\theta_1^0 \,, \tag{3-129}$$

$$\sigma^{1} = (f_{melt}^{cr})^{r} W_{melt}^{r} + (f_{1}^{cr}) W_{1}^{r} \theta_{1}^{1} , \qquad (3-130)$$

where

$$f_1^{cr} = \frac{d}{dT_1} \left(\frac{d\delta_{cr}}{dt} \right) , \qquad (3-131)$$

$$f_{melt}^{cr} = \frac{d}{dT} \left(\frac{d\delta_{cr}}{dt} \right) \,. \tag{3-132}$$

The crust growth rate derivative functions, f_1^{cr} and f_{melt}^{cr} , as well as the analogous derivative functions for the substrate ablation rate, f_2^{st} and f_{melt}^{st} , are tabulated in Appendix A. The forward elimination coefficients for the various boundary conditions are summarized in Table 3-1. Note that the coefficients are non-zero only for cases in which there is mass transport into, or out of, the overlying melt layer.

To evaluate the end of timestep concrete degassing rate, the melt and substrate enthalpies and temperature are also expanded in term of the material function derivatives. The results of the expansion yield, for the ith concrete decomposition front,

$$\frac{dx_{dc}^{i}}{dt}\Big)^{r+1} = \frac{dx_{dc}^{i}}{dt}\Big)^{r} + \Omega_{0}^{i} + \Omega_{1}^{i} \,\delta e_{melt} \,. \tag{3-133}$$

where Ω_0^i and Ω_1^i are the forward elimination coefficients. These functions are derived and tabulated in Appendix A. Note that these coefficients are non-zero

only if the degassing isotherm lies in concrete and the concrete has not previously exceeded the dryout enthalpy for the ith decomposition process.

NBCINT	σ^0	σ^1	$ au^0$	τ ¹
1	0	0	0	0
2	$f_1^{cr} W_1 \theta_1^0$	$f_{melt}^{cr} W_{melt} + f_1^{cr} W_1 \theta_1^1$	0	0
3	0	0	0	0
4	0	0	$f_2^{st}W_2\theta_2^0$	$f_{melt}^{st}W_{melt} + f_2^{st}W_2\theta_2^1$
5	0	0	0	0
6	0	$f_{melt}^{cr} W_{melt}$	0	$f_{melt}^{st}W_{melt} + f_2^{st}W_2\theta_2^1$
7	0	0	$f_2^{st}W_2\theta_2^0$	$f_{melt}^{st}W_{melt} + f_2^{st}W_2\theta_2^1$
8	0	0	0	0
9	0	0	0	0

Table 3-1 SUMMARY OF FORWARD ELIMINATION COEFFICIENT FOR VARIOUS BOUNDARY CONDITIONS

The differenced form of the shell heatup equation, Eq. 3-62, is currently written as fully implicit in both the spatial coordinates perpendicular and parallel to the shell surface. Direct solution techniques for discretization equations in two dimensions are available (King^[79]). However, when MELTSPREAD was originally developed,^[1-2] these methods were deemed unacceptable due to the large computation time associated with these methods.^[80] The approach thus used is to solve the equations implicitly in the coordinate perpendicular to the shell surface, while treating the heat transfer terms parallel to the shell surface explicitly. This approach effectively reduces the full two-dimensional problem into a number of simpler one-dimensional problems. However, the explicit approach introduces a Courant numerical stability constraint on the timestep of the form,^[80]

$$\frac{k}{\rho \, c_p} \, \frac{\delta t}{(l_k)^2} < \frac{1}{4} \, . \tag{3-134}$$

In the problem setup for spreading in Mark I containments, (cf. Section 4), this condition must be adhered to in the selection of the timestep and vertical shell mesh size.

Linearization of the discretized form of the shell transient heat conduction equation, Eq. 3-62, in the spatial coordinate normal to the shell surface yields, for $2 \le j \le J-1$ and $2 \le k \le K-1$,

$$O_{j,k}^r \,\delta e_{j,k} = P_{j,k}^r \,\delta e_{j+1,k} + Q_{j,k}^r \delta e_{j-1,k}^r + R_{j,k}^r \,\,, \tag{3-135}$$

$$O_{j,k}^{r} = \frac{\rho_{j,k}^{r} V_{j,k}}{\delta t} + l_{k} \left(C_{j-\frac{1}{2},k}^{r} + C_{j+\frac{1}{2},k}^{r} \right) W_{j,k}^{r} + l_{j} \left(C_{j,k-1/2}^{r} + C_{j,k+1/2}^{r} \right) W_{j,k}^{r} , \quad (3-136)$$

$$P_{j,k}^r = l_k \ C_{j+1/2,k}^r \ W_{j+1/2,k}^r \ , \tag{3-137}$$

$$Q_{j,k}^r = l_k C_{j-1/2,k}^r W_{j-1/2,k}^r , \qquad (3-138)$$

$$R_{j,k}^{r} = -\frac{\rho_{j,k}^{r} V_{j,k}}{\delta t} \left(e_{j,k}^{r} - e_{j,k}^{n} \right) + l_{k} C_{j-\frac{1}{2},k}^{r} \left(T_{j-1,k}^{r} - T_{j,k}^{r} \right) - l_{k} C_{j+1/2,k}^{r} \left(T_{j,k}^{r} - T_{j+1,k}^{r} \right) + l_{j} C_{j,k-1/2}^{r} \left(T_{j,k-1}^{r} - T_{j,k}^{r} \right) - l_{j} C_{j,k+1/2}^{r} \left(T_{j,k}^{r} - T_{j,k+1}^{r} \right)$$
(3-139)

and, for example,

$$W_{j,k} = \frac{\partial T}{\partial e} \Big)_{j,k} \tag{3-140}$$

The linearized form of the nodal matrix coefficients at the (assumed) adiabatic back boundary of the shell, j=J, are found from Eq. 3-65 as,

$$O_{J,k}^{r} = \frac{\rho_{J,k}^{r} V_{J,k}}{\delta t} + l_{k} C_{J-1/2,k}^{r} + l_{J} (C_{J,k1/2}^{r} + C_{J,k+1/2}^{r}) W_{J,k}^{r} , \qquad (3-141)$$

$$P_{J,k}^r = 0 (3-142)$$

$$Q_{J,k}^r = l_k \ C_{J-1/2,k}^r \ W_{J-1,k}^r \ , \tag{3-143}$$

$$R_{J,k}^{r} = -\frac{\rho_{J,k}^{r} V_{J,k}}{\delta t} \left(e_{J,k}^{r} - e_{J,k}^{n} \right) + l_{K} C_{J-1/2,k}^{r} \left(T_{J-1,k}^{r} - T_{J,k}^{r} \right) + l_{J} C_{J,k-1/2} \left(T_{J,k-1}^{r} - T_{J,k}^{r} \right) - l_{J} C_{J,k+1/2} \left(T_{J,k}^{r} - T_{J,k+1}^{r} \right).$$
(3-144)

The linearized form of the matrix coefficients at the top of the shell mesh, k=K, are found from Eq. 3-67 as

$$O_{j,k}^{r} = \frac{\rho_{j,K}^{r} V_{j,K}}{\delta t} + l_{K} \left(C_{j-1/2,K}^{r} + C_{j+1/2,K}^{r} \right) W_{j,k}^{r} + l_{j} C_{j,K-1/2} W_{j,K} , \qquad (3-145)$$

$$P_{j,K}^r = l_K C_{j+1/2,K}^r W_{j+1,K}^r , \qquad (3-146)$$

$$Q_{j,K}^r = l_K C_{j-1/2,k}^r W_{j-1,K} , \qquad (3-147)$$

$$R_{j,k}^{r} = -\frac{\rho_{j,K}^{r} V_{j,K}}{\delta t} \left(e_{j,k}^{r} - e_{j,k}^{n} \right) + l_{K} C_{j-1/2,K}^{r} \left(T_{j-1,k}^{r} - T_{j,k}^{r} \right) + l_{K} C_{j+1/2,K}^{r} \left(T_{j,k}^{r} - T_{j+1,K}^{r} \right) - l_{j} C_{j,k-1/2}^{r} \left(T_{j,K-1}^{r} - T_{j,k}^{r} \right).$$
(3-148)

The linearized form of the coefficients at the bottom of the mesh, k=1, are found from Eq. 3-66 as,

$$O_{j,1} = \frac{\rho_{j,1}^r V_{j,1}}{\delta t} + l_1 \left(C_{j-1/2,1}^r + C_{j+1/2,1}^r \right) W_{j,1}^r + l_j W_{j,1}^r , \qquad (3-149)$$

$$P_{j,1}^r = l_1 C_{j+1/2,1}^r W_{j+1/2,1}^r , \qquad (3-150)$$

$$Q_{j,1}^r = l_1 C_{j-1/2}^r W_{j-1,1}^r , \qquad (3-151)$$

$$R_{j,1}^{r} = -\rho_{j,1}^{r} V_{j,1} \left(e_{j,1}^{r} - e_{j,1}^{n} \right) + l_{1} C_{j-1/2,1}^{r} \left(T_{j-1,1}^{r} - T_{j,1}^{r} \right) + l_{1} C_{j+1/2,1}^{r} \left(T_{j,1}^{r} - T_{j+1,1}^{r} \right) - l_{j} C_{j,1+1/2}^{r} \left(T_{j,1}^{r} - T_{j,2}^{r} \right).$$
(3-152)

The specific form of the matrix coefficients for grid cells on the interior surface of the shell is dependent on whether solidified corium, molten corium, or overlying medium is locally adjacent to the shell. For grid cells locally adjacent to molten corium, the form of the coefficients is further dependent upon whether or not crust growth on the shell surface is specified as a user option. Linearization of the nodal energy balances for the nodes on the interior surface of the shell, Eqs. 3-68 and 3-69, results in the expression

$$O_{1,k}^r \,\delta e_{1,k} = P_{1,k}^r \,\delta e_{2,k} + R_{1,k}^r + S_k \,\delta e_{melt}^{adj} \,, \tag{3-153}$$

where

 δe_{melt}^{adj} = melt specific enthalpy increment adjacent to shell,

$$O_{1,k}^{r} = \begin{cases} \frac{\rho_{1,k}^{r} V_{1,k}}{\delta t} + l_{k} (h_{adj,k}^{r} + C_{1+1/2,k}^{r}) W_{1,k} + \\ + l_{1} (C_{1,k+1/2}^{r} + C_{1,k+1/2}^{r}); melt \ present, no \ crust, or \ melt \ absent \\ \frac{\rho_{1,k}^{r} V_{1,k}}{\delta t} + l_{k} \left[C_{1+1/2,k}^{r} + \frac{k_{cr}(T_{sol,cr} - T_{1,k}^{r})}{(\delta_{cr,k}^{r})^{2}} (d_{1}^{cr})_{k}^{r} + \frac{k_{cr}(T_{sol,cr} - T_{1,k}^{r})}{\delta_{cr,k}^{r}} + \\ + l_{1} (C_{1,k-1/2}^{r} + C_{1,k+1/2}); melt \ present \ with \ crust. \end{cases}$$
(3-154)

$$P_{1,k}^r = l_k C_{1+1/2,k}^r W_{2,k}^r , \qquad (3-155)$$

$$Q_{1,k}^r = 0 , (3-156)$$

$$R_{1,k}^{r} = \begin{cases} \frac{\rho_{1,k}^{r} V_{1,k}}{\delta t} \left(e_{1,k}^{r} - e_{1,k}^{n} \right) + l_{k} h_{adj,k}^{r} \left(T_{adj,k}^{r} - T_{1,k}^{r} \right) \\ -l_{k} C_{1+\frac{1}{2},k}^{r} \left(T_{1,k}^{r} - T_{2,k}^{r} \right) + l_{1} C_{1,k-\frac{1}{2}}^{r} \left(T_{1,k-1}^{r} - T_{1,k}^{r} \right) \\ -l_{1} C_{1,k+1/2} \left(T_{1,k}^{r} - T_{1,k+1}^{r} \right); melt \ present, \ no \ crust, or \ melt \ absent, \\ -\frac{\rho_{1,k}^{r} V_{1,k}}{\delta t} \left(e_{1,k}^{r} - e_{1,k}^{n} \right) + l_{k} k_{cr} \frac{\left(T_{sol,cr}^{r} - T_{1,k}^{r} \right)}{\delta_{cr,k}^{r}} \\ -l_{k} C_{1+\frac{1}{2},k}^{r} \left(T_{1,k}^{r} - T_{2,k}^{r} \right) + l_{1} C_{1,k-\frac{1}{2}}^{r} \left(T_{1,k-1}^{r} - T_{1,k}^{r} \right) \\ -l_{1} C_{1,k+\frac{1}{2}}^{r} \left(T_{1,k}^{r} - T_{1,k+1}^{r} \right); melt \ present \ with \ crust \ growth, \end{cases}$$
(3-157)

$$S_{k}^{r} = \begin{cases} 0; \ melt \ absent \\ l_{k} \ h_{adj,k}^{r} \ W_{melt,adj}^{r}; \ melt \ present, no \ crust \\ -l_{k} \ k_{cr} \ \frac{(T_{sol,cr} - T_{1,k}^{r})}{(\delta_{cr,k}^{r})^{2}} (d_{melt}^{cr})_{k}^{r}; \ melt \ present \ with \ crust \ growth. \end{cases}$$
(3-158)

and $(d_1^{cr})_k$ and $(d_{melt}^{cr})_k$ are the local shell crust forward elimination derivative functions which are found from Eqs. 3-70 and 3-72 as (cf. Eqs. 3-106 and 3-109 for definitions),

$$(d_1^{cr})_k^r = -\frac{k_{cr}}{\zeta_{cr}\Gamma_{cr,k}^r}$$
(3-159)

$$(d_{melt}^{cr})_{k}^{r} = \frac{h_{shell}^{r}}{2\zeta_{cr}} \left[h_{shell}^{r} \frac{(T_{1,k}^{r} - T_{sol,cr})}{\zeta_{cr} \Gamma_{cr,k}^{r}} - 1 \right]$$
(3-160)

In the region of the shell covered by melt (i.e., $S_k^r \neq 0$), the shell specific enthalpy increments are forward-eliminated through an expansion of the form,

$$\delta e_{j,k} = \theta_{j,k}^0 + \theta_{j,k}^1 \, \delta e_{melt,adj} \, . \tag{3-161}$$

For k>1, the forward elimination coefficients satisfy the equations

$$O_{j,k}^{r} \theta_{j,k}^{l} = P_{j,k}^{r} \theta_{j+1,k}^{l} + Q_{j,k}^{r} \theta_{j-l,k}^{l} + {\binom{R_{j,k}^{r};l=0}{0;\,l=1}}; l = 0,1 .$$
(3-162)

For k=1, the coefficients satisfy the equations,

$$O_{1,k}^r \,\theta_{1,k}^l = P_{1,k}^r \,\theta_{2,k}^l + \binom{R_{1,k}^r;l=0}{S_k^r;l=1}, l = 0,1 \ . \tag{3-163}$$

Given the shell forward elimination coefficients defined in Eqs. 3-162 and 3-163, the term characterizing the shell thermal loading due to interaction with melt in Eq. 3-9,

$$\dot{q}_{shell}^{n+1} = S_{j+1/2} \sum_{k=1}^{N_{sub}} l_k h_{shell}^{n+1} \left(T_j^{n+1} - (T_{shell})_k^{n+1} \right) ,$$

may be forward-eliminated. The results of the linearization yield,

$$\dot{q}_{shell}^{n+1} = \varphi_0^r + \varphi_1^r \,\delta e_{melt}^{adj} \,, \qquad (3-164)$$

where, for the case of no crust growth on the shell,

$$\varphi_0^r = S_{j+1/2} \sum_{k+1}^{N_{sub}} l_k h_{shell}^r \left(T_{adj}^r - T_{1,k}^r - W_{1,k}^r \,\theta_{1,k}^o \right) \tag{3-165}$$

$$\varphi_1^r = S_{j+1/2} \sum_{k=1}^{N_{sub}} l_k h_{shell}^r \left(W_{melt}^{adj} - W_{1,k}^r \,\theta_{1,k}^o \right) \tag{3-166}$$

For the case of crust growth on the shell, the coefficients are found as,

$$\varphi_0^r = S_{j+1/2} \sum_{k=1}^{N_{sub}} l_k h_{shell}^r (T_{adj}^r - T_{sol})$$
(3-167)

$$\varphi_0^r = S_{j+1/2} \sum_{k=1}^{N_{sub}} l_k h_{shell}^r W_{melt}^{adj} .$$
(3-168)

Given the forward elimination for the incremental changes in substrate specific enthalpy, concrete degassing rate, crust and ablation rates, and shell thermal loading, the detailed melt conservation of mass and energy equations are then solved for the local melt constituent height increments and the local melt specific enthalpy increments. The local melt constituent heights are linearized as,

$$(h_j^i)^{r+1} = (h_j^i)^r + \delta h_j^i ,$$
 (3-169)

and therefore,

$$h_j^{r+1} = h_j^r + \delta h_j , \qquad (3-170)$$

where

$$\delta h_j = \sum_{i=1}^{16} \delta h_j^i . \tag{3-171}$$

Linearization of the general conservation of mass equation, Eq. 3-7, yields

$$0_{j}^{r} \,\delta h_{j}^{i} + P_{j}^{r} \,\delta h_{j+1}^{i} + Q_{j}^{r} \,\delta h_{j-1}^{i} + R_{j}^{r} + S_{j}^{r} \,\delta e_{j} = 0 \,\,, \qquad (3-172)$$

where

$$0_{j}^{r} = \frac{A_{j}}{\delta t} + S_{j-1/2}^{r} \langle -U_{j-1/2}^{n+1}, 0 \rangle + S_{j+1/2} \langle U_{j+1/2}^{n+1}, 0 \rangle , \qquad (3-173)$$

$$P_j^r = -S_{j+1/2} \langle -U_{j+1/2}^{n+1}, 0 \rangle , \qquad (3-174)$$

$$Q_j^r = -S_{j-1/2} \langle U_{j-1/2}^{n+1}, 0 \rangle , \qquad (3-175)$$

$$R_{j}^{r} = \frac{A_{j}}{\delta t} [(h_{j}^{i})^{r} - (h_{j}^{i})^{n}] + S_{j-1/2} [(h_{j}^{i})^{r} \langle -U_{j-1/2}^{n+1}, 0 \rangle - (h_{j}^{i})^{r} \langle U_{j-1/2}^{n+1}, 0 \rangle] + S_{j+1/2} [(h_{j}^{i})^{r} \langle -U_{j+1/2}^{n+1}, 0 \rangle - (h_{j}^{i})^{r} \langle U_{j-1/2}^{n+1}, 0 \rangle] \frac{\beta^{i} A_{j}}{\rho_{l}^{i}} [(F_{H_{2}O})_{j}^{r} \gamma_{H_{2}O}^{i}] ((m_{H_{2}O})_{j}^{r} + (\Omega_{O}^{H_{2}O})_{j}^{r}) + (F_{CO_{2}})_{j}^{r} \gamma_{CO_{2}}^{i} ((m_{CO_{2}})_{j}^{r} + (\Omega_{O}^{CO_{2}})_{j}^{r}) - A_{j} \frac{\rho_{s}^{i}}{\rho_{l}^{i}} [X_{sf}^{i} ((\frac{d\eta}{dt})_{j}^{r} + (\tau^{O})_{j}^{r}) + X_{melt}^{i} ((\frac{d\delta_{cr}}{dt})_{j}^{r} + (\sigma^{O})_{j}^{r})] - A_{j} X_{vessel}^{i} \frac{(m_{vessel})_{j}^{n+1}}{\rho_{l}^{i}} (3-176) S_{j}^{r} = -\beta^{i} A_{j} [(F_{H_{2}O})_{j}^{r} \gamma_{H_{2}O}^{i} (\Omega_{O}^{H_{2}O})_{j}^{r} + (F_{CO_{2}})_{j}^{r} \gamma_{CO_{2}}^{i} (\Omega_{O}^{CO_{2}})_{j}^{r}] + A_{j} \frac{\rho_{s}^{i}}{\rho_{l}^{i}} [X_{sf}^{i} (\tau^{1})_{j}^{r} + X_{melt}^{i} (\sigma^{1})_{j}^{r}] .$$
(3-177)

Linearization of the melt conservation of energy equation, Eq. 3-9, yields

$$O_{j}^{r} \,\delta e_{j} + P_{j}^{r} \,\delta e_{j+1} + Q_{j}^{r} \,\delta e_{j-1} + R_{j}^{r}$$
$$+ T_{j}^{r} \,\delta h_{j} + W_{j}^{r} \,\delta h_{j-1} + X_{j}^{r} \,\delta h_{j+1} = 0 , \qquad (3-178)$$

$$O_{j}^{r} = \left[\frac{A_{j}}{\delta t} + S_{j-1/2} \langle -U_{j-1/2}^{n+1}, 0 \rangle + S_{j+1/2} \langle U_{j+1/2}^{n+1}, 0 \rangle \right] (\rho h)_{j}^{r} + A_{j} \left[(h_{bot})_{j}^{r} (W_{j}^{r} - (W_{1} \theta_{1}^{1})_{j}^{r}) + (h_{top})_{j}^{r} W_{j}^{r} \right] + A_{j} \rho \left[e_{ablation} (\tau^{1})_{j}^{r} + e_{crust} (\sigma^{1})_{j}^{r} \right] + D \left(j - J_{adj} \right) \varphi_{1}^{r} - A_{j} \left[\left(F_{H_{2}O} \right)_{j}^{r} \left(\Omega_{1}^{H_{2}O} \right)_{j}^{r} \sum_{i} \gamma_{H_{2}O}^{i} q_{ox,H_{2}O}^{i} + \left(F_{CO_{2}} \right)_{j}^{r} \left(\Omega_{1}^{CO_{2}} \right)_{j}^{r} \sum_{i} \gamma_{CO_{2}}^{i} q_{ox,CO_{2}}^{i} \right], \quad (3-179) P_{j}^{r} = -S_{j+1/2} \langle -U_{j+1/2}^{n+1}, 0 \rangle \left(\rho h \right)_{j+1}^{r}, \qquad (3-180)$$

$$Q_j^r = S_{j-1/2} \langle U_{j-1/2}^{n+1}, 0 \rangle (\rho h)_{j-1}^r , \qquad (3-181)$$

$$\begin{aligned} R_{j}^{r} &= \frac{A_{j}}{\delta t} \Big[(\rho h e)_{j}^{r} - (\rho h e)_{j}^{n} \Big] - S_{j-1/2} \langle U_{j-1/2}^{n+1}, 0 \rangle (\rho h e)_{j-1}^{r} \\ &- S_{j+1/2} \langle -U_{j+1/2}^{n+1}, 0 \rangle (\rho h e)_{j+1}^{r} + \Big[S_{j-1/2} \langle -U_{j-1/2}^{n+1}, 0 \rangle \\ &+ S_{j+1/2} \langle U_{j+1/2}^{n+1}, 0 \rangle \Big] (\rho h e)_{j}^{r} + A_{j} \Big[(h_{bot})_{j}^{r} (T_{j}^{r} - (T_{bot})_{j}^{r} \Big) \\ &- (W_{1} \theta_{1}^{0})_{j}^{r} \Big) + (h_{top})_{j}^{r} \Big(T_{j}^{r} - (T_{top})_{j}^{r} \Big) \Big] \\ &+ A_{j} \rho_{j} \Big[e_{ablation} (\tau^{o})_{j}^{r} + e_{crust} (\sigma^{o})_{j}^{r} \Big] + D (j - J_{adj}) \varphi_{o}^{r} \\ &- A_{j} \Big[(F_{H_{2}O})_{j}^{r} \left((\dot{m}_{H_{2}O})_{j}^{r} + (\Omega_{0}^{CO_{2}})_{j}^{r} \right) \sum_{i} \gamma_{L_{2}O}^{i} q_{ox,H_{2}O} \\ &+ (F_{CO_{2}})_{j}^{r} \left((\dot{m}_{cO_{2}})_{j}^{r} + (\Omega_{0}^{CO_{2}})_{j}^{r} \right) \sum_{i} \gamma_{CO_{2}}^{i} q_{ox,CO_{2}}^{i} \\ &- A_{j} \rho_{j} h_{j}^{r} (X_{melt}^{UO_{2}})_{j}^{r} (\dot{q}_{decay})^{n+1} - A_{j} (\dot{m}_{vessel})_{j}^{n+1} e_{vessel}^{n+1} , \end{aligned}$$
(3-182)
$$T_{j}^{r} = \Big[\frac{A_{j}}{\delta t} + S_{j-1/2} \langle -U_{j-1/2}^{n+1}, 0 \rangle + S_{j+1/2} \langle U_{j+1/2}^{n+1}, 0 \rangle \Big] (\rho e)_{j}^{r} \\ &- A_{j} \rho_{j}^{r} (\dot{q}_{decay})^{n+1} (X_{melt}^{UO_{2}})_{j}^{r} \end{cases}$$
(3-183)

$$W_j^r = -S_{j-1/2} \langle U_{j-1/2}^{n+1}, 0 \rangle (\rho e)_{j-1}^r , \qquad (3-184)$$

$$X_j^r = -S_{j+1/2} \langle -U_{j+1/2}^{n+1}, 0 \rangle (\rho e)_{j+1}^r , \qquad (3-185)$$

Note that Eqs. 3-166 and 3-172 form a coupled set of equations for the melt height and melt specific increments. The solution technique employed here is to first solve Eq. 3-172 with the coefficient S_j^r set equal to zero in this equation. This assumption reduces Eq. 3-172 to a simple tri-diagonal matrix which is readily solved for the melt height increments. Given the height increments, Eq.

3-178 is then solved for the specific enthalpy increments. Given the enthalpy increments, the height increments are then updated through the solution of Eq. 3-172 with S_i^r calculated through Eq. 3-177.

Given the height and enthalpy increments through the solution of Eqs. 3-172 and 3-178, the melt constituent heights and enthalpies are updated through Eqs. 3-110 and 3-169. The substrate enthalpies are then updated through Eq. 3-121. The shell enthalpies are then updated through Eq. 3-161. The crust and ablation depths and rates are then updated through Eqs. 3-16 through 3-53. Finally, the concrete degassing rate is updated through Eqs. 3-60 and 3-61. The solution is then checked for overall convergence against the user-specified convergence criteria (see Section 4).

FORWARD ELIMINATION SOLUTION SCHEME: WATER INVENTORY EQUATIONS For situations in which the detailed water inventory model is invoked, then the local variables to be determined from the difference equations developed above are the water specific enthalpy, height, and velocity. Given the converged solutions for the melt spreading equations, then the cell edge velocities and water depths are first determined through the simultaneous solution of Eqs. 3-73 to 3-77 by performing an iterative calculation on the linearized form of these equations. To this end, the cell edge velocities are expanded as,

$$U_{w,j-1/2}^{r+1} = U_{w,j-1/2}^r + \delta U_{w,j-1/2}$$
(3-186)

where:

 $\delta U_{w,i-1/2}$ = incremental change in water cell edge velocity

Similar expressions apply at the j+1/2 and j-3/2 cell edges. The end of timestep water depths in Eq. 3-73 are forward eliminated in terms of the incremental changes in cell edge velocities. Substitution of Eq. 3-186 into Eq. 3-73 and linearizing the resultant expression yields,

$$H_{w,j}^{r+1} = H_{w,j}^r + F_j^r + G_j^r \delta U_{w,j-1/2} + I_j^r \delta U_{w,j+1/2}$$
(3-187)

where:

$$F_{j} = \frac{\delta t}{A_{j}} \left\{ \frac{(\dot{m}_{w})_{j}^{r}}{\rho_{l}} + S_{j-1/2} < U_{w,j+1/2}^{r}, 0 > H_{w,j-1}^{r} + S_{j+1/2} < -U_{w,j+1/2}^{r}, 0 > H_{w,j+1}^{r} - S_{j-1/2} < -U_{w,j-1/2}^{r}, 0 > H_{w,j}^{r} - S_{j+1/2} < U_{j+1/2}^{r}, 0 > H_{w,j}^{r} \right\},$$
(3-188)

$$G_{j} = \frac{\delta t S_{j-1/2}}{A_{j}} \{ H_{w,j-1}^{r} < sgn(U_{w,j-1/2}^{r}), 0 > -H_{w,j}^{r} < -sgn(U_{w,j-1/2}^{r}), 0 > \},$$
(3-189)

$$I_{j} = \frac{\delta t S_{j+1/2}}{A_{j}} \{ H_{w,j+1}^{r} < sgn(U_{w,j+1/2}^{r}), 0 > -H_{w,j}^{r} < -sgn(U_{w,j+1/2}^{r}), 0 > \}.$$
(3-190)
The forward elimination for $H_{w,j-1}^{r+1}$ in Eq. 3-73 is obtained by setting j=j-1 in Eqs. 3-187 through 3-190. Substitution of Eqs. 3-186 through 3-190 into the momentum equation, Eq. 3-73 and linearizing the resulting expression yields, for j=2,..,J,

$$O_j^r \,\delta U_{w,j-1/2} + P_j^r \,\delta U_{w,j+1/2} + Q_j^r \delta U_{w,j-3/2} + R_j = 0, \qquad (3-191)$$

where:

$$+\frac{sgn(U'_{w,j-1/2})}{H^n_{w,j}}f^r_{j-1/2}U^r_{w,j-1/2} + \frac{g}{(\delta z_j + \delta z_{j-1})}(G^r_j - I^r_{j-1})$$
(3-192)

$$P_{j}^{r} = \delta z_{j-1} \frac{\left(1 - sgn(U_{w,j-1/2}^{r})\right)}{2\delta z_{j}\delta z_{T}} U_{w,j-1/2}^{r} + \frac{g I_{j}^{r}}{(\delta z_{j} + \delta z_{j-1})}$$
(3-193)

$$Q_{j}^{r} = -\delta z_{j} \frac{\left(1 + sgn\left(U_{w,j-\frac{1}{2}}^{r}\right)\right)}{2\delta z_{j-1}\delta z_{T}} U_{j-\frac{1}{2}}^{r} - \frac{g \, G_{j-1}^{r}}{(\delta z_{j} + \delta z_{j-1})}, \qquad (3-194)$$

$$R_{j}^{r} = \frac{U_{w,j-1/2}^{r} - U_{w,j-1/2}^{n}}{\delta t} + \frac{\delta z_{j} \left(1 + sgn(U_{w,j-1/2}^{r})\right)}{2\delta z_{T} \delta z_{j-1}} U_{j-1/2}^{r} \left(U_{w,j-1/2}^{r} - U_{w,j-3/2}^{r}\right)$$

$$+\frac{\delta z_{j-1} \left(1-sgn\left(U_{w,j-1/2}^{r}\right)\right)}{2\delta z_{j}\delta z_{T}}U_{w,j-1/2}^{r}\left(U_{w,j+1/2}^{r}-U_{w,j-3/2}^{r}\right)+\frac{1}{2}\frac{f_{j-1/2}^{r}}{H_{w,j}^{n}}U_{w,j-1/2}^{r}\left|U_{w,j-1/2}^{r}\right|$$
$$+\frac{g}{\left(\delta z_{j}+\delta z_{j-1}\right)}\left(H_{w,j}^{r}+F_{j}^{r}+E_{j}^{n}-H_{w,j-1}^{r}+F_{j-1}^{r}-E_{j-1}^{n}\right)$$
(3-195)

For j=1, the coefficients for the no flow boundary condition are

$$O_1^r = 1,$$

 $P_1^r = 0,$ (3-196)
 $Q_1^r = 0,$
 $R_1^r = 0.$

Similarly, for j=J+1, the coefficients are of the form

$$O_{j+1}^r = 1$$
,
 $P_{J+1}^r = 0$, (3-197)
 $Q_{J+1}^r = 0$,
 $R_{J+1}^r = 0$.

Equation 3-191 constitutes a linear set of equations, in the form of a tridiagonal matrix, for the incremental changes in the cell edge velocities. Given the current estimate of the edge velocities and water heights, Eq. 3-191 is solved to obtain the incremental velocity changes. The end of timestep velocities are then updated through Eq. 3-186. Given the updated velocities, Eq. 3-76 is then solved to obtain the updated water heights. This procedure is then repeated until the incremental velocity changes decrease below userspecified convergence criteria (See Section 4).

Given the end of timestep velocities and heights, the water conservation of energy equation, Eq. 2-325, is then solved. Similar to the approach used to solve for the water flow velocities, the water specific enthalpy and temperature are expanded as,

$$e_{w,j}^{r+1} = e_{w,j}^r + \delta e_{w,j} \tag{3-198}$$

$$T_{w,j}^{r+1} = T_{w,j}^r + \frac{dT}{de_w} \delta e_{w,j} = T_{w,j}^r + \delta e_{w,j}/c_l$$
(3-199)

Linearization of the water conservation of energy equation, Eq. 3-78, then yields:

$$S_{j}^{r} \,\delta e_{w,j} + T_{j}^{r} \,\delta e_{w,j+1} + V_{j}^{r} \,\delta e_{w,j-1} + W_{j}^{r} = 0 \tag{3-200}$$

where:

$$S_{j}^{r} = \left[\frac{A_{j}}{\delta t} + S_{j-1/2} \langle -U_{w,j-1/2}^{n+1}, 0 \rangle + S_{j+1/2} \langle U_{w,j+1/2}^{n+1}, 0 \rangle \right] \left(\rho_{l} H_{w}\right)_{j}^{r} + \frac{A_{j} (h_{wat})_{j}^{r}}{c_{l}} + (\dot{m}_{dc})_{j}^{n+1}$$
(3-201)

$$T_{j}^{r} = -S_{j+1/2} \langle -U_{w,j+1/2}^{n+1}, 0 \rangle \left(\rho_{l} H_{w}\right)_{j+1}^{r}$$
(3-202)

$$V_j^r = S_{j-1/2} \langle U_{w,j-1/2}^{n+1}, 0 \rangle \left(\rho_l H_w \right)_{j-1}^r$$
(3-203)

$$W_{j}^{r} = \frac{A_{j}}{\delta t} \Big[\left(\rho_{l} H_{w} e_{w} \right)_{j}^{r} - \left(\rho_{l} H_{w} e_{w} \right)_{j}^{n} \Big] - S_{j-1/2} \langle U_{w,j-1/2}^{n+1}, 0 \rangle \left(\rho_{l} H_{w} e_{w} \right)_{j-1}^{r} \\ -S_{j+1/2} \langle -U_{w,j+1/2}^{n+1}, 0 \rangle \left(\rho_{l} H_{w} e_{w} \right)_{j+1}^{r} + \Big[S_{j-1/2} \langle -U_{w,j-1/2}^{n+1}, 0 \rangle \\ + S_{j+1/2} \langle U_{w,j+1/2}^{n+1}, 0 \rangle \Big] \big(\rho_{l} H_{w} e_{w} \big)_{j}^{r} - A_{j} \big(q_{wat}^{"} \big)_{j}^{r} - \left(\dot{m}_{inj} e_{inj} \right)_{j}^{n+1} \\ + \left(\dot{m}_{dc} \right)_{j}^{n+1} e_{w,j}^{r} \Big]$$
(3-204)

Equation 3-200 constitutes a linear set of equations, in the form of a tridiagonal matrix, for the incremental changes in water specific enthalpy. Given the current enthalpy estimates, Eq. 3-200 is solved to obtain the incremental enthalpy changes. The end of timestep enthalpies are then updated through Eq. 3-198. This procedure is repeated until the incremental enthalpy changes decrease below user-specified convergence criteria (See Section 4). Within the iteration, a specific check on the local coolant specific enthalpy is made to determine if it has reached the saturation point. If this case is encountered, then the tri-diagonal matrix coefficients are set to yield a null change in local coolant enthalpy; i.e.,

$$S_{j}^{r} = 1$$
,
 $T_{J}^{r} = 0$, (3-205)
 $V_{J}^{r} = 0$,
 $W_{I}^{r} = 0$.

Section 4

DESCRIPTION OF MELTSPREAD3 FILE INPUT

The input requirements to set up and execute a simulation with MELTSPREAD3 are described in this section. For reactor cases, the input may be categorized as follows:

- (1) Plant-specific information regarding the composition and geometry of the containment floor area over which the corium may spread.
- (2) Time-dependent corium pour rate, composition, temperature, and decay heat level obtained from in-vessel calculations for a particular severe accident sequence.
- (3) Cavity conditions: wet versus dry; time-dependent flooding location, temperature, and flowrate, as well as the location and size of spillover point(s).
- (4) User-supplied operational parameters which control the physical modeling assumptions used in the calculations.

To implement the above information, a variety of user options have been incorporated to provide flexibility in the modeling of corium spreading processes. The major user-specified modeling options include:

- (1) General spreading nodalization scheme,
- (2) General concrete composition,
- (3) Spreading over steel and/or concrete surfaces,
- (4) Melt dispersion from the RPV over dispersed as well as localized areas,
- (5) The potential for modeling melt jet breakup in a water pool underlying the RPV if the cavity is wet,
- (6) Wet versus dry cavity conditions, and
- (7) Forced convection and/or bubble agitation downward heat transfer models.

The required code input to invoke these options is described in detail below.

DESCRIPTION OF INPUT FILE

Definitions of the input parameter names and functions, as well as the format for the MELTSPREAD3 input file, are provided in Table 4-1. Unless otherwise indicated in the table, the input data must be in the form of SI units (kilograms, meters, seconds, degrees Kelvin).

Table 4-1 MELTSPREAD3 INPUT FILE DESCRIPTION

Line	Variable	Notes
No.	Name	
0	TITLE	Arbitrary, user-defined text descriptor for calculation that is written as a header to text output file spreadout.dat; 72 character limit
1	TCONI, RSAND	Initial concrete temperature and substrate equivalent sand roughness
2	ICTC	 This line defines the substrate type. Set ICTC = 1, 2, or 3 for default limestone common sand, siliceous, or limestone-limestone concrete types, respectively; see Table 4-2 for the composition of these default concretes. Set ICTC = 5 if substrate is entirely steel. Finally, set ICTC=4 for user-specific concrete composition, defined in Lines 3-4. <i>Notes:</i> 1) If ICTC ≠ 4, Lines 3-4 are omitted. 2) If ICTC=5, Line 5 is omitted; also see next two notes. 3) If the basemat is a composite mixture of concrete and steel (or some other material that is not concrete), then set the concrete properties here (i.e. ICTC=1-4). Identification of region(s) in the substrate where materials other than concrete are located is handled at Line 30. 4) If the substrate consists entirely of some alternate material that is neither concrete nor steel (e.g. ceramic insulator), then set ICTC = 5 and define the alternate material properties at Lines 42-47.
3	XWTC (1)-XWTC (7)	Weight % CO ₂ , H ₂ O, K ₂ O, Na ₂ O, TiO ₂ , SiO ₂ and CaO, respectively, in concrete
4	XWTC (8)-XWTC (14)	Weight % Mg0, Al_2O_3 , Fe0, Fe_2O_3 , Fe_3O_4 Fe, and Cr in concrete
5	TCS, TCL, TDC	Concrete solidus, liquidus, and erosion temperatures
6	TFWS, TFWL	Concrete free water dryout temperature range
7	TBWS, TBWL	Concrete bound water [Ca(OH) ₂] decomposition temperature range
8	TMCAS, TMCAL	Concrete dolomite [MgCa(CO ₃) ₂] decomposition temperature range
9	TCAS, TCAL	Concrete calcium carbonate [CaCO ₃] decomposition temperature range
10	TFOS, TFOL	Melt oxide solidus-liquidus temperature range
11	TFMS, TFML	Melt metal phase solidus-liquidus temperature range
12	NPOURS	Number of melt pour time intervals; Lines 13-15 are repeated NPOURS times

		Pour time interval, TST to TSTOP
	TST (I), TSTOP (I) AINTP (I), BINTP (I)	• AINTP and BINTP are coefficients for linear curve fit to melt pour temperature over the
13		time interval (i.e. MELT=AINTP+BINTP*TIME).
	ADEC (I), BDEC (I)	• Similarly, ADEC and BDEC are coefficients for linear fit to melt decay heat level
		(expressed as $W/kg UO_2$) over the time interval.
14	NISTP	Number of melt constituents draining over pour interval
15	IT, APOUR (IT,I), BPOUR(IT,I)	Coefficients for linear curve fit to melt pour rate (i.e. APOUR+BPOUR*TIME) for IT-th melt constituent over time interval in Line 13. This line is repeated NISTP times.
16	NJET, NJETD, NJETND, ERPV, POROSBED	 Melt jet fragmentation model control parameters. Set NJET=0 to bypass this option; <i>in this case Lines 17-18 are omitted</i> and the setting of other parameters on this line are irrelevant. Set NJET=1 for the case in which jet fragmentation occurs, with the fragmented & quenched material assumed to be subsumed into the melt, effectively lowering the melt pour temperature. Set NJET=2 for the case in which the fragmented material is assumed to be retained as a discrete particle bed on top the spreading melt. If NJET=1 or 2, Line 17 is repeated NJETD times (minimum of two) for RPV hole diameter time vs. diameter table. If NJET=2, Line 17 is repeated NJETND times, with each line defining a node that is a receptor for particulate formed from jet fragmentation. ERPV is the elevation of the RPV lower head over the basemat POROSBED is the porosity of the bed formed from fragmentation. If NJET=2, this
17		parameter should be set between 0 and 1. RPV hole diameter vs. time table (Line is repeated NIETD times: minimum is two)
17		When NJET=2, these are nodes that are identified as recentors for particulate from jet
18	IJ	fragmentation: this line is repeated NJETND times.
		The following 5 lines allow the user to over-write code-computed melt/solidified debris
		thermo-physical properties and use user-specified values if desired.
10	NOVHT, COVS, COVL, DHSOV,	• Set NOVHT=0 to use code-calculated melt molecular weight (g/mole), solid/liquid
19	XMOLOV, ROVS, ROVL	specific heat, latent heat of fusion, and solid/liquid density, respectively. Values are
		irrelevant if NOVHT=0.
ļ		• If NOVHT=0, data on this line must be provided, but the values do not matter.
		Set NOVTK=0 to use calculated core debris solid and liquid phase thermal conductivities,
20	NOVTK, TKOVS, TKOVL	respectively, or set NOVTK=1 to overwrite with user specified values TKOVS and TKOVL
01	NOVILIM VISOV	(W/III-K). Values IITELEVANT II NUVIK=U.
		specified value VISOV (log/m sec). Value irrelevant if NOVUM=0
		1 specificul value visto v (kg/m ⁻ see). Value metevalue move om -0.

22	NOVEM, EMOV	Set NOVEM=0 to use calculated melt radiation emissivity, or set NOVEM=1 to overwrite with user specified value EMOV. Value irrelevant if NOVEM=0.
23	NOVSIG, SIGOV	Set NOVSIG=0 to use calculated melt surface tension, or set NOVSIG=1 to overwrite with
		user specified value SIGOV (N/m). Value irrelevant if NOVSIG=0.
	NGEOM	• Parameter controlling spreading area meshing options. Set NGEOM=1 for automated
24		Mark I input, or set NGEOM=2 for user-specified meshing option.
		• Note: If NGEOM=1, Lines 33-34 are omitted. If NGEOM=2, Lines 25-32 are omitted.
		 NSMP = Number of spreading nodes in sump pit
		• NPED = Number of spreading nodes between edge of sump pit and pedestal wall
25	NSMP, NPED, NDOR, NDOOR,	 NDOR = Number of spreading nodes in doorway
23	NSHL, NANULS	 NDOOR = Number of doorways in pedestal wall
		 NSHL = Number of spreading nodes outside pedestal doorway to liner
		• NANULS = Number of spreading nodes in the balance of the drywell annulus
		• RSUMP = Average hydraulic radius of sump pit
		• ELSMP = Sump pit depth
06	RSUMP, ELSMP, RPED, TPED, WDOOR, RLINER	• RPED = Inner radius of pedestal wall
26		• TPED = Thickness of pedestal wall
		• WDOOR = Width of doorway opening(s) in pedestal wall
		• RLINER = Drywell liner radius at floor level
07	DOOND	Melt pour dispersion radius beneath RPV (<rped). if="" njet="" note:="">0, then RCOMP should</rped).>
27	RCOMP	be set \leq RSUMP so that the jet breakup analysis is conducted in the sump region.
0.0	NONDON THOUGH	NSMPCV = $0/1$ if the sump cover plates are absent/present at pour inception
28	NSMPCV, THCKCV	Thickness of sump cover plate; value is irrelevant if NSMPCV = 1
		NBOIL controls the Mark I sump spillover calculation option:
		• If NBOIL=0, melt spreading over sump cover plates is calculated according to the setting
		of NSMPCV.
		• If NBOIL=1, sump is assumed to spillover under the user-specified conditions defined
		below. The settings of these parameters do not matter if NBOIL=0.
00	NDOU TMDOU TEDOU VEINT	• TMBOIL = Time at which sump spillover occurs
29	NBOIL, IMBOIL, IEBOIL, VEINI	 TEBOIL = Temperature of melt in sump at time of spillover
		 VFINT = Melt void fraction in sump at time of spillover
		• Notes:
		1) If NBOIL=0, Line 30 is omitted. If NBOIL=1, set NSMPCV=1 in Line 28.
		2) This is a legacy option that is rarely used as the code is fully capable of calculating
		sump filling and spillover using a mechanistic approach based on pour conditions.

30	XBLT (I)	Vector defining user-specified melt constituents in sump at spillover (wt%) for I=1-15; nomenclature is provided in Table 4-3. Line 30 is repeated 15 times (I=1-15).
31	NSWALL	 Parameter controlling calculation of heat losses from the melt to the sidewalls in the drywell annulus of the Mark I containment. Set NSWALL=0 to neglect sidewall heat losses, or set NSWALL=1 to include sidewall losses as evaluated through Eq. 4-5.
32	ANGFAN	Spreading angle outside doorway (setting can range from 0 to 180°).
33	NUMNOD	Number of spreading node cells for the case NGEOM=2; see Line 24. Note : this line and line 34 are omitted if NGEOM=1.
34	IFLGA (I), DXNODE (I), RAD (I), ARC (I+1), AREA (I), ELEVAT (I), HCAP(I)	 Input data for user-defined spreading area mesh. <i>Note</i>: this line is repeated NUMNOD times. AREA(I) = Node spreading area ARC(I) = Spreading arc length, or perimeter, at I-1/2 interface for node RAD(I) = Radial position of cell along spreading length DXNODE(I) = Overall node length ELEVAT(I) = Initial substrate elevation of node IFLGA(I) = 0 or 1 if corium is or is not a receptor for corium draining from the RPV into this node. <i>Note:</i> If NJET> 0, this should only be set equal to one in a single node that is defined as the receptor for the melt jet. HCAP(I) = node elevation limitation for cases in which the upper surface elevation in the flow channel is locally limited in height (e.g., flow through a constriction). <i>Note:</i> if a constriction does not exist, set this number to a large value well above the plausible spreading height.
35	NVTPE, NSOLTP, NSOLF, ALPMAX, CRAMCON	 This line sets the melt viscosity modeling assumptions (<i>Note:</i> settings are irrelevant if NOVUM=1 in Line 22). Set NVTPE=1 to use the Ishii-Zuber correlation to account for solids buildup in the melt, or set NVTPE=2 to use the Ramacciotti correlation. Set NSOLTP=1 for the case in which the oxide phase solid fraction is assumed to vary linearly between the solidus-liquidus, or set NSOLTP=2 to input a table of solid fraction versus normalized temperature difference between the liquid and solid. For cases in which NVTPE=1, set ALPMAX to the oxide phase solid fraction at which the viscosity of the melt becomes infinite (i.e., it is a solid). If NVTPE=2, the setting of this parameter is irrelevant. CRAMCON = constant in the Ramacciotti viscosity correlation. If NVTPE = 1, the setting of this parameter is irrelevant.

36	TNORM, FRCSOL	 For the case in which NSOLTP = 2, this is the user-defined input table for normalized melt temperature [i.e. (TFOL-TMELT)/(TFOL-TFOS); see Line 10 for variable definitions] vs. oxide phase solid fraction. If NSOLTP = 1 this line is omitted from the input file.
37	NMVER	• If NSOLTP = 2, this line is repeated NSOLF times. The next 10 lines define the basemat axial mesh at each lateral spreading node location, and also allow alternative basemat materials (i.e., other than concrete) to be treated. NMVER = the total number of vertical node cells in the underlying substrate at each spreading node location.
38	XBCN (I), XDCN (I)	 XDCN(I) = Substrate inter-nodal spacing between the I th and I+1 st substrate node cells. XBCN(I) = Location of the interface between the Ith and I+1 st substrate node cells (XBCN(I) < XDCN(I)). Note: Line 29 is repeated NMVER times
39	NSTEEL, NSIMST	 This line allows selected nodes within the substrate to be treated as steel, or as some other material with user-defined input properties. NSTEEL = total number of substrate nodes which are composed of steel. NSIMST is the control variable providing the ability to overwrite steel property data with user-defined information. Set NSIMST = 0 to retain steel properties, or NSIMST = 1 to overwrite. Notes: When NSTEEL = 0 or ICTC = 5 (see Line 2), Line 40 is omitted. If NSTEEL > 0 or ICTC = 5 and the non-concrete material is something other than steel, then set NSIMST = 1 and define material properties in Lines 41-46. If NSIMST = 1, then the substrate composition vector XCSI(I) is used under ablation conditions to assign the ablation products to the melt according to the composition of the ablating material. If NSIMST = 0, Lines 41-46 are omitted.
40	IX, IY	Indices specifying the x-y locations within the substrate mesh where non-concrete nodes are located. Note: Line 40 is repeated NSTEEL times.
41	TSIS, TSIL, CSIS, CSIL, DHSIL	TSIS, TSIL = alternative substrate solidus and liquidus temperatures CSIS, CSIL = alternative substrate solid and liquid phase specific heats DHSIL = alternative substrate latent heat of fusion
42	RSIS, RSIL, TKSIS, TKSIL, ESIL	RSIS, RSIL = alternative substrate solid and liquid phase densities TKSIS, TKSIL = alternative substrate solid and liquid phase thermal conductivities ESIL = alternative substrate radiation emissivity

43	XCSI(1) - XCSI (4)	Weight fractions of Zr, Fe, Cr, and Ni in alternative substrate, respectively
44	XCSI(5) - XCSI (8)	Weight fractions of B, U, B ₄ C, ZrO ₂ in alternative substrate, respectively
45	XCSI(8) - XCSI (12)	Weight fractions of FeO, Fe_2O_3 , Fe_3O_4 , and Cr_2O_3 in alternative substrate, respectively
46	XCSI(13) - XCSI (16)	Weight fractions of NiO, B ₂ O ₃ , UO ₂ , and concrete slag in alternative substrate, respectively.
47	NSKIPE	 This parameter controls the structural heatup calculation for melt contacting a structural element (assumed to be steel) located at a user-defined location (node) in the spreading mesh. This option was specifically developed to analyze heatup of the Mark I liner under conditions in which the melt is calculated to contact the liner. Set NSKIPE=0 to bypass this option, <i>in which case Lines 48-49 are omitted</i>. Set NSKIPE = 1 to invoke this option, in which case control parameters are defined in Lines 48-49.
48	NBMADJ, NUMSHH, NUMSHV, NBFZOE, NCRTEM, NLOGSH	 These parameters control the structural heatup calculation if that option is selected (i.e. NSKIPE=1). NBMADJ = Melt spreading node that is adjacent to structural element/liner; melt thermal hydraulic conditions in this node (i.e., velocity and depth) are used to calculate impingement heat transfer to element. NUMSHH = Number of node cells into which the lateral thickness of the element/liner, THSHL, is subdivided. NUMSHV = Number of node cells into which the vertical height of the element/liner, HNDOT, is subdivided. NBFZOE = 1 if crust growth is not permitted on the liner, or NBFZOE=2 if crust growth is permitted. NCRTEM = 0 to specify the melt solidus as the freezing temperature used in the crust growth calculation on the liner, or set NCRTEM=1 to specify the melt temperature at initial contact with the liner as the crust freezing temperature. NLOGSH = 0 to use Martin's slot jet impingement heat transfer coefficient between the melt and the liner; set NLOGSH=1 to use the Theofanous bubble-driven recirculation heat transfer coefficient; or set NLOGSH=2 to use the sum of the slot jet impingement and bubble-driven recirculation heat transfer coefficients.

		These are additional parameters controlling the structural element/liner heatup calculation if that option is selected
49	TSHELI, HNODT, THSHL, ANGSHL, BWIDTH	• TSHELI = Initial liner temperature (assumed to be uniform)
		• HNODT = Total vertical height of the liner (parallel to the liner surface) to be nodalized
		• THSHL = Liner thickness (assumed to be uniform)
		• ANGSHL = Liner angle with respect to vertical (degrees).
		• BWIDTH = Assumed width of the slot jet impinging on the liner, typically taken to be the
		doorway width in Mark I applications
		Note: Line 49 is omitted if NSKIPE=0.
		• TBOUND = Temperature of overlying structure (assumed constant); employed for
		radiation heat transfer calculation from the melt surface when water is not present, or
50	TBOUND EMISCN PDRVWI	the melt height exceeds the downcomer height if water is present.
50	Iboond, Emisch, Ibriwe	• EMISCN = Radiation emissivity of overlying structure, used for radiation heat transfer
		evaluation from melt surface if water is not locally present.
		• PDRYWL = Drywell absolute pressure (MPa).
		Parameters that control the heat transfer modeling assumptions at the melt upper surface.
		• Set NWAT = 0 if the cavity remains dry
		• Set NWAT = 1 if the cavity is maintained at saturation temperature corresponding to the
		containment pressure, PDRYWL, and at a constant water level of HDOWNC
	NWAT, HDOWNC, TWATI,	• Set NWAT=2 if the detailed water inventory model is invoked; specifications are provided
- 1		in Lines 52-57.
51	EWATI	• HDOWNC = constant water level over basemat surface for the case NWAT =1. If NWAT =
		0 or 2, the setting of HDOWNC is irrelevant.
		• I WAII = initial water temperature in the cavity for the case NWAI = 2 (assumed
		Unitorial. $EWATE = initial water upper surface elevation in the parity for the case NWAT = 0$
		• EWATI- Initial water upper surface elevation in the cavity for the case NWAT - 2 (occurred uniform)
		Note: If NWAT<2 Lines 52-57 are omitted
		For detailed water inventory model (NWAT = 2), this parameter allows water to be injected
		at user-defined points and times over the calculation $Set NIN I = 0$ if there are no injection
	NINJ	points. If there are injection points, set NINJ = number of spreading nodes into which
52		water is injected at any time over the calculation.
		Notes: If NINJ = 0, Lines 53-54 are omitted. If NINJ > 0, then lines 53-54 are repeated
		NINJ times.

		For the I-th injection point:
53	NINJP(I), NPTINJ(I)	• NINJP(I) = the node in the spreading mesh into which the water is injected, and
		• NPTINJ(I) = number of points in the interpolation table for water injection flowrate
		(XDTINJ(I)) and temperature (TDTINJ(I)) over the calculation.
	TIMINJ(I), XDTINJ(I), TDTINJ(I)	Input table with NPTINJ(I) line entries defining:
		• TIMINJ(I) = time
		• XDTINJ(I) = water injection flowrate (kg/sec)
34		• TDTINJ(I) = water injection temperature
		Notes: at least two points are required (i.e. NPTINJ(I) ≥ 2 on Line 53), and the time
		interval(s) TIMINJ(I) should cover the full time domain of the calculation.
		For detailed water inventory model (NWAT = 2), this parameter allows water spillover at
		user-defined locations in the mesh if the local water height reaches the spillover inlet
		elevation(s). An example are the downcomers into the Torus of the Mark I containment. If
55	NDOWNC	there are spillover points, set NDOWNC = number of nodes in the spreading mesh where
		spillover can occur.
		Notes: If NDOWNC = 0, Lines 56-57 are omitted. If NDOWNC > 0, then Lines 56-57 are
		repeated NDOWNC times.
		L Fon the L the anillower mainte
		For the 1-th spinover point:
		 NDC(I) = the node in the spreading mesh where spillover can occur,
56	NDC(I), ELDCO(I), NPTDC(I)	 NDC(I) = the node in the spreading mesh where spillover can occur, ELDCO(I) = elevation above substrate at which spillover can begin, and
56	NDC(I), ELDCO(I), NPTDC(I)	 NDC(I) = the node in the spreading mesh where spillover can occur, ELDCO(I) = elevation above substrate at which spillover can begin, and NPTDC(I) = number of points in the interpolation table that provides the spillover arc
56	NDC(I), ELDCO(I), NPTDC(I)	 NDC(I) = the node in the spreading mesh where spillover can occur, ELDCO(I) = elevation above substrate at which spillover can begin, and NPTDC(I) = number of points in the interpolation table that provides the spillover arc length as a function of elevation above the spillover inlet.
56	NDC(I), ELDCO(I), NPTDC(I)	 NDC(I) = the node in the spreading mesh where spillover can occur, ELDCO(I) = elevation above substrate at which spillover can begin, and NPTDC(I) = number of points in the interpolation table that provides the spillover arc length as a function of elevation above the spillover inlet. Input table with NPTDC(I) line entries defining:
56	NDC(I), ELDCO(I), NPTDC(I)	 NDC(I) = the node in the spreading mesh where spillover can occur, ELDCO(I) = elevation above substrate at which spillover can begin, and NPTDC(I) = number of points in the interpolation table that provides the spillover arc length as a function of elevation above the spillover inlet. Input table with NPTDC(I) line entries defining: ELDCX(I) = elevation above the spillover inlet height (<i>i.e., local water depth minus the</i>
56	NDC(I), ELDCO(I), NPTDC(I)	 NDC(I) = the node in the spreading mesh where spillover can occur, ELDCO(I) = elevation above substrate at which spillover can begin, and NPTDC(I) = number of points in the interpolation table that provides the spillover arc length as a function of elevation above the spillover inlet. Input table with NPTDC(I) line entries defining: ELDCX(I) = elevation above the spillover inlet height (<i>i.e., local water depth minus the inlet elevation</i>), and
56	NDC(I), ELDCO(I), NPTDC(I)	 For the I-th spinover point: NDC(I) = the node in the spreading mesh where spillover can occur, ELDCO(I) = elevation above substrate at which spillover can begin, and NPTDC(I) = number of points in the interpolation table that provides the spillover arc length as a function of elevation above the spillover inlet. Input table with NPTDC(I) line entries defining: ELDCX(I) = elevation above the spillover inlet height (<i>i.e., local water depth minus the inlet elevation</i>), and CRDCX(I) = cord length
56	NDC(I), ELDCO(I), NPTDC(I)	 NDC(I) = the node in the spreading mesh where spillover can occur, ELDCO(I) = elevation above substrate at which spillover can begin, and NPTDC(I) = number of points in the interpolation table that provides the spillover arc length as a function of elevation above the spillover inlet. Input table with NPTDC(I) line entries defining: ELDCX(I) = elevation above the spillover inlet height (<i>i.e., local water depth minus the inlet elevation</i>), and CRDCX(I) = cord length <i>Notes:</i>
56	NDC(I), ELDCO(I), NPTDC(I)	 For the I-th spinover point: NDC(I) = the node in the spreading mesh where spillover can occur, ELDCO(I) = elevation above substrate at which spillover can begin, and NPTDC(I) = number of points in the interpolation table that provides the spillover arc length as a function of elevation above the spillover inlet. Input table with NPTDC(I) line entries defining: ELDCX(I) = elevation above the spillover inlet height (<i>i.e., local water depth minus the inlet elevation</i>), and CRDCX(I) = cord length Notes: At least two points are required [i.e., NPTDC(I) > 2 on Line 56]
56	NDC(I), ELDCO(I), NPTDC(I) ELDCX(I), CRDCX(I)	 For the I-th spinover point: NDC(I) = the node in the spreading mesh where spillover can occur, ELDCO(I) = elevation above substrate at which spillover can begin, and NPTDC(I) = number of points in the interpolation table that provides the spillover arc length as a function of elevation above the spillover inlet. Input table with NPTDC(I) line entries defining: ELDCX(I) = elevation above the spillover inlet height (<i>i.e., local water depth minus the inlet elevation</i>), and CRDCX(I) = cord length Notes: At least two points are required [i.e., NPTDC(I) > 2 on Line 56] The elevation range ELDCX(I) should fully span plausible water depths that may be
56	NDC(I), ELDCO(I), NPTDC(I) ELDCX(I), CRDCX(I)	 For the I-th spinover point: NDC(I) = the node in the spreading mesh where spillover can occur, ELDCO(I) = elevation above substrate at which spillover can begin, and NPTDC(I) = number of points in the interpolation table that provides the spillover arc length as a function of elevation above the spillover inlet. Input table with NPTDC(I) line entries defining: ELDCX(I) = elevation above the spillover inlet height (<i>i.e., local water depth minus the inlet elevation</i>), and CRDCX(I) = cord length Notes: At least two points are required [i.e., NPTDC(I)≥2 on Line 56] The elevation range ELDCX(I) should fully span plausible water depths that may be encountered, from 0 to a maximum height.
56	NDC(I), ELDCO(I), NPTDC(I) ELDCX(I), CRDCX(I)	 For the I-th spinover point: NDC(I) = the node in the spreading mesh where spillover can occur, ELDCO(I) = elevation above substrate at which spillover can begin, and NPTDC(I) = number of points in the interpolation table that provides the spillover arc length as a function of elevation above the spillover inlet. Input table with NPTDC(I) line entries defining: ELDCX(I) = elevation above the spillover inlet height (<i>i.e., local water depth minus the inlet elevation</i>), and CRDCX(I) = cord length Notes: At least two points are required [i.e., NPTDC(I) > 2 on Line 56] The elevation range ELDCX(I) should fully span plausible water depths that may be encountered, from 0 to a maximum height. The 'cord length' CRDCX(I) is defined such that the water height above the spillover
56	NDC(I), ELDCO(I), NPTDC(I) ELDCX(I), CRDCX(I)	 For the I-th spinover point: NDC(I) = the node in the spreading mesh where spillover can occur, ELDCO(I) = elevation above substrate at which spillover can begin, and NPTDC(I) = number of points in the interpolation table that provides the spillover arc length as a function of elevation above the spillover inlet. Input table with NPTDC(I) line entries defining: ELDCX(I) = elevation above the spillover inlet height (<i>i.e., local water depth minus the inlet elevation</i>), and CRDCX(I) = cord length Notes: At least two points are required [i.e., NPTDC(I)≥2 on Line 56] The elevation range ELDCX(I) should fully span plausible water depths that may be encountered, from 0 to a maximum height. The 'cord length' CRDCX(I) is defined such that the water height above the spillover inlet multiplied by the interpolated cord length equals the water flow area into the
56	NDC(I), ELDCO(I), NPTDC(I) ELDCX(I), CRDCX(I)	 For the I-th spinover point: NDC(I) = the node in the spreading mesh where spillover can occur, ELDCO(I) = elevation above substrate at which spillover can begin, and NPTDC(I) = number of points in the interpolation table that provides the spillover arc length as a function of elevation above the spillover inlet. Input table with NPTDC(I) line entries defining: ELDCX(I) = elevation above the spillover inlet height (<i>i.e., local water depth minus the inlet elevation</i>), and CRDCX(I) = cord length Notes: At least two points are required [i.e., NPTDC(I)≥2 on Line 56] The elevation range ELDCX(I) should fully span plausible water depths that may be encountered, from 0 to a maximum height. The 'cord length' CRDCX(I) is defined such that the water height above the spillover inlet multiplied by the interpolated cord length equals the water flow area into the downcomer. For instance, if the downcomer is a circular pipe with a horizontal

58	NBFRZO, NTHINC, NABLFM, NDRNFM, NBCBOT, NCRTOP, NADAB	 NBFZRO is the primary input variable controlling freezing behavior in the melt. Set NBFRZO = 1 for bulk solidification (i.e., no crust formation at melt/crust interface), or set NBFRZO = 2 for crust growth/remelting calculation on the substrate surface. Note that regardless of the setting of NBFRZO, the corium is immobilized if the melt temperature falls below the solidus temperature. <i>User Guidance:</i> Set NBFRZO = 1; this is the freezing assumption made in all code validation calculations and is the most numerically stable assumption. With this setting, the settings of NTHINC, NABLFM, and NDRNFM do not matter. NTHINC controls crust modeling at the melt/substrate interface if NBFROZ = 2 (bottom crust modeled). Set NTHINC = 0 for crust growth modeling, or set NTHINC = 1 for heat transfer limited by thin crust segments. NABLFM controls the disposition of ablated substrate material when crust growth is not specified (NBFRZO = 1). Set NABLFM = 1 if the ablated substrate material remains on the surface as a molten film, or set NABLFM = 2 if the ablated material is continuously mixed into the melt. NDRNFM controls the disposition of ablated substrate material when crust growth is specified (NBFRZO = 2). Set NDRNFM = 1 for porous crust allowing ablated material to continuously drain through the crust, or NDRNFM = 2 for the case in which the crust is non-porous and the ablated material is trapped beneath the crust. <i>User Guidance:</i> Set NDRNFM = 1; other studies (i.e. with CORQUENCH) have shown that NDRNFM = 2 is an unrealistic boundary condition (i.e., the crust rapidly remelts and disappears). NCRTOP controls the thin top crust is assumed to exist regardless of gas flux. <i>User Guidance:</i> For best estimate analyses, set NCRTOP = 0 as this assumption was made in all MELTSPREAD validation
		 calculations. NBCBOT controls the heat transfer coefficient modeling assumption used at the melt/substrate interface. Set NBCBOT = 1 to use Bradley's bubble agitation downward heat transfer coefficient model; set NBCBOT = 2 to use Kao and Kazimi's revised periodic contact model; set NBCBOT = 3 to use forced convection (i.e. Dittus-Boelter) model; set NBCBOT = 4 to use sum of bubble agitation and forced convection models; or set NBCBOT = 5 to use sum of periodic contact and forced convection models. <i>User Guidance</i>: Use NBCBOT = 3 if the basemat is not made of concrete (i.e. does not produce gas upon decomposition), or set NBCBOT=4 if it is made of concrete. These are the assumptions made in all MELTSPREAD validation calculations that focused on evaluating maximum melt penetration distance. NADAB controls the ability to perform an adiabatic spreading calculation. This parameter was implemented so that the code fluid mechanics algorithms could be validated against isothermal spreading tests with simulant materials. Set NADAB = 0 to bypass this option, or set NADAB = 1 to perform an adiabatic

59	NINTF, HINTF	 This line allows an additional interfacial heat transfer resistance to be added at the melt/substrate interface and was motivated by the fact that metal spreading data indicates that an additional resistance forms due to a lack of surface wetting. Set NINTF = 0 if this option is bypassed, or NINTF = 1 if an interfacial resistance exists. HINTF = user-specified interface resistance (i.e., heat transfer coefficient, W/m²-K) at interface. The setting of this parameter is arbitrary if NINTF = 0.
60	XFCABL, XNDMIN	 Basemat ablation and debris solidification control parameters: XFCABL = Mapping criteria for substrate ablation calculation. This is the fractional amount that a node can be ablated from the thickness before the local basemat array is remeshed by incorporating the residual material into the next node down into the basemat. <i>User Guidance:</i> Set XFACBL = 0.01 based on experience. XNDMIN = Minimum node size for freezing and immobilized corium. At the melt leading edge, material can sequentially freeze causing a layered buildup of material. This parameter sets the minimum node thickness that the accumulating material is allowed to grow to until a new node is started on top of the existing material. <i>User Guidance:</i> XNDMIN is typically set to 2 cm.
61	NVELP, NITMAX, DAVMX, DVMX, NINVIS	 Integration control parameters for <i>melt</i> fluid mechanics calculation: NVELP = Number of subintervals into which DTIME is subdivided for the fluid mechanics calculation (a finer time step is needed for this algorithm). NITMAX = Maximum allowable iterations to meet DAVMX and DVMX. DAVMX, DVMX = Average and maximum allowable incremental changes in cell edge velocities before the fluid mechanics calculation is deemed to be converged. Set NINVIS = 0 to evaluate frictional pressure losses during melt relocation, or set NINVIS = 1 to perform an inviscid flow calculation. User Guidance: Typical settings for these parameters are 5, 20, 0.001 m/s and 0.005 m/s.
62	NENMAX, DEAVMX, DEMX	 Integration control parameters for <i>melt</i> conservation of energy equation: NENMAX = Maximum allowable iterations to meet DEAVMX and DEMX. DEAVMX, DEMX = Average and maximum allowable incremental changes in melt specific enthalpy before the conservation of energy equation is deemed to be converged. User Guidance: Typical values for these parameters are 20, 300 J/kg, and 600 J/kg.

NVELPW, NITMAXW, DAVMXW, DVMXW	Integration control parameters for <i>water</i> fluid mechanics calculation:
	• NVELPW = Number of subintervals into which DTIME is subdivided for the fluid
	mechanics calculation (a finer time step is needed for this algorithm).
	• NITMAXW = Maximum allowable iterations to meet DAVMX and DVMX.
	• DAVMXW, DVMXW = Average and maximum allowable incremental changes in cell edge
	velocities before the fluid mechanics calculation is deemed to be converged.
	Note : Settings for these parameters are irrelevant if NWAT ≤ 1 ; see Line 51.
	User Guidance : Typical settings for these parameters are 2, 5, 0.001 m/s and 0.005 m/s.
	Integration control parameters for <i>water</i> conservation of energy equation:
	 NENMXW = Maximum allowable iterations to meet DEAVMXW and DEMXW.
NENMXW, DEAVMXW, DEMXW	• DEAVMXW, DEMXW = Average and maximum allowable incremental changes in water
	specific enthalpy before the conservation of energy equation is deemed to be converged.
	User Guidance: Typical values for these parameters are 20, 300 J/kg, and 600 J/kg.
	Parameters controlling output file characteristics:
	• NPRINT controls the amount of data printed to the text output file 'spreadout.dat'. Set
	NPRINT=1 for abbreviated output, or set NPRINT=2 for verbose output that also includes
	the basemat nodal temperature arrays.
	• NPFREQ = frequency at which output data are written to the text output file; data are
	printed every DTIME NPFREQ seconds.
	• NPEND = Number of vertical temperature node arrays within the liner that are printed to
NPRINT, NPFREO, NPEND,	the text output file. This option if bypassed if the liner heatup calculation is not enabled
NBEDCQ	(i.e. NSKIPE = 0; see Line 47), or the liner has not been contacted by melt.
-	• NBEDCO controls the nature of the output data that is written to the COROUENCH
	initiation file 'comput.dat'. Set NBEDCO = 0 if particulate formed from jet erosion
	(NJET=2; see Line 16) is to be retained as a separate debris bed in comput. dat, or set
	NBEDCO = 1 if it is to be integrated with the underlying melt and thermally equilibrated
	with that material.
	Note: If NIET < 2, or a follow on coloritation with COPOLIENCH is not going to be
1] 1] 1]	VELPW, NITMAXW, DAVMXW, VMXW ENMXW, DEAVMXW, DEMXW PRINT, NPFREQ, NPEND, BEDCQ

66	NTIMSPC	 NTIMSPC sets the number of specific times (defined in Line 67) over the course of the calculation that an output file 'fort.<i>number</i>' is generated, with 'number' starting at 10 the first file that is produced, and increasing by 1 for each sequential file produced thereafter. The specific parameters written to the output file are defined in Table 5-2. The file outputs can be copied into the excel spreadsheet 'plotfort.1x' that generates selected graphs of the data for review and evaluation. Note: The maximum setting for NTIMSPC is 10. Example: The user desires spatial plots of the information in Table 5-2 at 10, 20, and 30 seconds. To accomplish this set NTIMSPC = 3, and input 10, 20, and 30 on the next three
		lines of the input file (see Line 67). This will produce the files fort.10, fort.11, and fort.12 that provide the data in Table 5-2 at 10, 20, and 30 seconds, respectively.
67	TIMSPC(I)	 TIMSPC(I) are the specific times at which output files are to be generated with the spatially dependent data defined in Table 5-2. Note: This line is repeated NTIMSPC times. If NTIMSPC = 0, this line is omitted.
68	NPLFREQ, NPLTOT	 NPLFREQ = frequency that data are periodically written to various additional plotting files, as described below and for Lines 69-71. Data are printed every DTIME·NPFREQ seconds. NPLTOT sets the total number of nodes (specifically defined in Line 69) for which an individual output file 'fort.number' is generated, with 'number' starting at 20 for the first node, and increasing by 1 for each sequential node thereafter. The specific parameters at the node site that are written to the output file are defined in Table 5-3. The file outputs can be copied into the excel spreadsheet 'plotfort.2x' that generates selected graphs of the data for review and evaluation. Note: The maximum setting for NPLTOT is 10. Example: The user desires time-dependent plots of the information in Table 5-3 at nodes 10, 20, and 30. To accomplish this set NPLTOT = 3, and input 10, 20, and 30 on the next three lines of the input file (see Line 69). This will produce plot the files fort.20, fort.21, and fort.22 that provide the data in Table 5-3 every DTIME·NPFREQ seconds.
69	NPLLOC(I)	 NPPLOC(I) are the specific nodes at which output files are to be generated with the time-dependent melt property data defined in Table 5-3. Note: This line is repeated NPLTOT times. If NPLTOT = 0, this line is omitted.
70	NBPL	NBPL sets the number of basemat nodes at which the temperatures are to be written to the output file 'fort.30'. Note: Line 71 is repeated NBPL times. If NBPL=0, Line 71 is omitted.
71	IXP(I), IYP(I)	IXP(I) and IYP(I) are the x-y nodal indices within the basemat at which temperatures are written out to the output file 'fort.30.'

		• TIMEO = Starting time for the calculation
72	TIMEO, DTIME, TMAX	• DTIME = Integration time step
		 TMAX = Maximum time to which the calculation is to be performed

The chronological order of the input file can be summarized as follows:

- (1) Concrete initial temperature, composition, roughness, and decomposition (dryout) temperatures,
- (2) Assumed solidus/liquidus temperatures for the oxide and metal phases of the corium issuing form the RPV,
- (3) Corium pour rate, composition, temperature, and decay heat level,
- (4) Spreading nodalization scheme and melt dispersion area beneath the RPV,
- (5) Substrate nodalization scheme,
- (6) Drywell liner nodalization scheme and crust growth modeling assumptions,
- (7) Cavity atmospheric conditions (wet versus dry),
- (8) Spreading modeling assumptions regarding the presence or absence of crust growth, disposition of ablated substrate material, and assumed downward heat transfer coefficients,
- (9) Integration control parameters,
- (10) Frequency and detail of the printing of computed information.

As indicated in Table 4-1, the opening line of the input file is a place holder for text input that the user can utilize for labeling the input file as desired. This line is also written to the text output file 'spreadout.dat' for continuity.

The first data input of line of the input file defines the initial substrate temperature, TCONI, and equivalent sand roughness, RSAND. The initial substrate temperature is assumed to be uniform.

For regions of the substrate composed of concrete, the second line of the input (Line 2) defines the concrete type, ICTC. Referring to Table 4-2, set ICTC=1 for the default limestone-common sand composition; set ICTC=2 for the default siliceous composition; set ICTC=3 for the default limestone-limestone composition; or set ICTC=4 for user-specified concrete composition. Finally, set ICTC=5 if the substrate is composed entirely of steel.

If ICTC=4, the next three lines of the input file (Lines 3-5) define the weight **percents** of the concrete constituents, and the concrete solidus/liquidus and erosion (ablation) temperatures. Line 3 defines the weight percents of CO_2 , H_2O , K_2O , Na_2O , TiO_2 , SiO_2 and CaO, respectively, while Line 4 defines the weight of percents of MgO, Al_2O_3 , FeO, Fe_2O_3 , Fe_3O_4 , Fe, and Cr, respectively. Line 5 defines the solidus/liquidus and erosion (ablation) temperatures for the user-

specified composition. Note that if ICTC \leq 3 (i.e., default composition chosen), then Lines 3-5 are omitted from the input file.

For both the default and user-specified concrete compositions, Lines 6-9 define the assumed concrete dryout temperature ranges. The decomposition temperatures for dryout of free water, calcium hydroxide $(Ca(OH)_2)$, dolomite $(MgCa(CO_3)_2)$, and calcium carbonate $(CaCO_3)$ are provided in Table 4-3 below. Line 6 defines the decomposition solidus/liquidus temperatures for dryout of free water. Line 7 defines the solidus/liquidus temperatures for dryout of $Ca(OH)_2$. Line 8 defines the solidus/liquidus temperatures for dryout of $MgCa(CO_3)_2$. Line 9 defines the solidus/liquidus temperatures for dryout of $CaCO_3$.

Constituent	Limestone/Common Sand Concrete (ICTC=1)		Siliceous Concrete (ICTC=2)		Limestone/Limestone Concrete (ICTC=3)	
	Weight	Mole	Weight	Mole	Weight	Mole
	Percent	Percent	Percent	Percent	Percent	Percent
SiO_2	28.8	22.8	69.7	60.7	7.0	5.2
MgO	9.8	11.6	0.7	0.9	7.3	8.2
CaO	26.4	22.4	13.7	12.8	42.4	34.0
Fe_2O_3	1.6	0.5	1.0	0.3	0.8	0.2
Al_2O_3	3.6	1.7	4.0	2.1	1.9	0.8
Na_2O	1.1	0.8	0.7	0.6	-	-
K ₂ O	0.6	0.3	1.4	0.8	0.4	0.2
TiO_2	0.1	0.1	0.8	0.5	0.1	0.1
CO_2	21.8	23.4	1.00	1.2	33.2	34.0
H_2O	6.2	16.4	6.91	20.0	6.9	17.3

		_	
Table 4-2	COMPOSITION	OF DEFAULT	CONCRETES

Table 4-3 SUMMARY OF DECOMPOSITION REACTIONS TREATED IN MELTSPREAD3 COMPOSITION OF DEFAULT CONCRETES

Compound	Formula	Decomposition Reaction	Decomposition Temperature (K)
Free Water	H ₂ 0		Saturation
			Temperature
Dolomite	$CaMg(CO_3)_2$	$CaMg(CO_3)_2 \rightarrow$	1033
		$CaO + MgO + 2CO_2$	
Calcite (Calcium	CaCO ₃	$CaCO_3 \rightarrow$	1172
Carbonate)		$CaO + CO_2$	
Calcium Hydroxide	<i>Ca</i> (<i>OH</i>) ₂	$Ca(OH_2) \rightarrow$	853
-		$CaO + H_2O$	

Lines 10 through 15 define the corium freezing temperatures and time dependent corium pour conditions. Line 10 defines the corium oxide phase solidus and liquidus temperatures, while Line 11 defines the metallic phase solidus and liquidus temperatures. Lines 12-15 are then define the time-dependent corium pour rate, composition, temperatures, and decay heat level. Line 12 defines the number of time intervals into which the pour conditions may be conveniently divided. For instance, a pour with a constant discharge rate, temperature, composition, and decay heat level which lasts t_{pour} seconds would be divided into NPOURS=2 intervals. The first interval defines the time-dependent pour conditions, while the second interval sets the pour rate equal to zero beginning at t_{pour} seconds. For pours of higher complexity, this approach may be easily generalized.

For the I th pour interval, I=1..., NPOURS, the interval start and stop times are defined through the vectors TST(I) and TSTOP(I), where TST(I) \leq t < TSTOP(I). Over the I th pour interval, the corium discharge temperature is calculated through the equation,

$$T_{corium} = AINTP(I) + BINTP(I) * (t - TST(I)) , \qquad (4-1)$$

where the units on AINTP(I) are degrees Kelvin and the units on BINTP(I) are degrees Kelvin per second. As in evident from Eq. 4-1, a linear variation in corium discharge temperature over the I th pour interval is allowed. The corium decay heat level is similarly calculated through the equation

$$\dot{q}_{decay} = ADEC(I) + BDEC(I) * (t - TST(I))$$
(4-2)

where the units on ADEC(I) are Watts per kilogram UO_2 , and the units on BDEC(I) are Watts per kilogram UO_2 per second. Over the I th pour interval, the discharge rate for the IMP-th corium constituent is calculated through the equation,

$$\dot{m}(IMP) = APOUR(IMP, I) + BPOUR(IMP, I) * (t - TST(I))$$
(4-3)

where the units on APOUR(IMP,I) are kilograms per second, and the units of BPOUR (IMP,I) are kilograms per second squared. MELTSPREAD3 currently accepts input from up to 16 melt constituents. The nomenclature for the melt constituents, which must be adhered to in the input file, is provided in Table 4-4.

Line 12 defines the number of pour intervals, NPOUR. Lines 13-15, which are repeated NPOURS times, then define the specific pour conditions over each

interval. Line 13 defines the pour interval start and stop times (TST(I) and TSTOP (I)), the corium discharge temperature coefficients (AINTP(I) and BINTP(I)), and the decay heat level coefficients (ADEC(I) AND BDEC(I)). Line 14 defines the total number of corium constituents draining from the RPV over the current interval, NISTP. Line Group 15 then defines the pour rate coefficients, APOUR(IMP,I), and BPOUR (IMP,I). Note that there will be NISTP Lines in Line Group 15. If a given corium constituent is not draining from the RPV over the I-th interval, there is no need to input zero coefficients for APOUR(ITP,I) and BPOUR(ITP,I) as these arrays are zeroed out prior to reading from the input file. If the corium discharge rate over the I-th interval is zero, then set NISTP=0, in which case Line Group 15 should be omitted from the input file for the I-th pour interval. **Note carefully, however**, that if NISTP=0, the decay heat level coefficients, ADEC(I) and BDEC(I), must still be defined correctly since the decay heat level calculated through Eq. 4-2 is used to evaluate the internal heating in molten or solidified corium already on the drywell floor.

Index, IT	Corium
	Constituent
1	Zr
2	Fe
3	Cr
4	Ni
5	В
6	U
7	B ₄ C
8	ZrO ₂
9	Fe0
10	Fe_2O_3
11	Fe_3O_4
12	Cr_2O_3
13	NiO
14	
15	<i>U0</i> ₂
16	Concrete ¹

Table 4-4 NOMENCLATURE FOR CORIUM CONSTITUENTS

Lines 16 to 18 are the melt jet fragmentation model control parameters that can be implemented under flooded cavity conditions (alternatively, the code automatically bypasses this option if water is absent in the jet impact zone).

¹ Concrete composition assumed to equal that specified in Line Nos. 2-4 (See Table 4-2).

Set NJET=0 to bypass this option; in this case Lines 17-18 are omitted and the setting of other parameters on this line are irrelevant. Set NJET=1 for the case in which jet fragmentation occurs, with the fragmented and quenched material assumed to be subsumed into the melt, effectively lowering the melt pour temperature. Conversely, set NJET=2 for the case in which the fragmented material is assumed to be retained as a discrete particle bed on top the spreading melt. In this case, Line 18 is repeated NJETND times, with each line defining a node that is a receptor for particulate formed from jet fragmentation. POROSBED is the porosity of the bed formed from fragmentation; this parameter should be set *between* 0 and 1. If NJET > 0, then Line 17 is a table used to specify the RPV hole opening diameter vs. time (minimum of two lines). Finally, ERPV to the elevation of the RPV lower head over the basemat and is used (in conjunction with local concrete erosion, melt, and water depths) to calculate the total jet fall height that affects diameter and velocity of the jet at impact with the water pool.

Lines 19 to 23 allow the user to over-write code-computed melt/solidified debris thermo-physical properties and use user-specified values as desired. These options can be used to explore material property parametric effects or to examine spreading of simulant materials (see Appendix C). On Line 19, set NOVHT=1 to overwrite code-calculated melt/solidified debris molecular weight (g/mole), solid/liquid phase specific heat, latent heat of fusion, and solid/liquid densities, respectively. Input values for these parameters are irrelevant if NOVHT=0, but numbers still need to be supplied.

Similarly, Lines 20 through 23 allow the user to overwrite the melt/solidified debris thermal conductivity, viscosity, emissivity, and surface tension, respectively, with the leading integer used to determine if that option is selected, and the following number is the specified value if chosen. If the control parameter is set to zero, a value still needs to be provided for the physical property even though it is not used in the calculation.

Lines 24-34 are used to set up the spreading nodalization scheme. There are currently two user alternatives. The first alternative is suitable for Mark I containments similar to that illustrated previously in Figures 1-1 and 1-2; i.e., a pedestal region with or without sumps and a specified number of personnel access doorways, and a drywell annulus. The second alternative allows the user to specify an arbitrary 1-D flow geometry. The choice between these two alternatives is determined by the parameter NGEOM which is defined in Line 24. Set NGEOM=1 for the automated Mark I nodalization scheme, or set NGEOM=2 for the arbitrary 1-D flow channel nodalization scheme. For the automated scheme, the containment pedestal and drywell annulus floor areas are divided into five regions: (1) pedestal sump, (2) balance of pedestal floor between sump edge and pedestal wall, (3) doorway opening(s), (4) flow sector between outside the doorway(s) and drywell liner, and (5) the balance of the drywell annulus. In the pedestal region, the flow is assumed to occur in a 360° sector. Within the doorway opening(s), 1-D channel flow is calculated. Between the doorway opening(s) and containment liner, sector flow is assumed (the user supplies the flow angle). In the balance of the drywell annulus, the flow is assumed to occur in a 1-D channel of width equal to twice the distance between the liner and outside of the pedestal wall, i.e., symmetrical turning of the corium issuing from the doorway(s) into the annulus is assumed. If more than one doorway is specified, symmetrical flow out of each doorway is assumed. An illustration of a typical Mark I spreading nodalization scheme is provided in Figure 4-1.



Figure 4-22 Illustration of basic characteristics of a Mark I nodalization scheme produced by the automated option NGEOM=1

If NGEOM=1, Line 25 defines the number of spreading nodes in the sump, NSMP, the number of nodes in the balance of the pedestal, NPED, the number of nodes in the pedestal doorway opening(s), NDOR, the number of doorway

openings, NDOOR, the number of nodes in the flow sector outside the doorway, NSHL, and the number of nodes in the balance of the drywell annulus, NANULS. Line 26 defines the floor area dimensions; namely, the sump hydraulic diameter, RSUMP, the average sump depth below the pedestal floor, ELSMP (may be input as a positive or negative quantity, but the elevation is taken as negative internal to the code), the inner radius of the pedestal wall, RPED, the thickness of the pedestal wall, TPED, the width of the doorway openings, WDOOR, and the liner radius, RLINER.

Given the floor area dimensions and the number of spreading nodes in each of the above described regions, a uniform-mesh nodalization scheme is constructed in each of the regions. Line 27 defines the assumed corium pour dispersion radius in the pedestal region beneath the RPV. For instance, if the pour is assumed to issue from the RPV in a coherent jet and is unattenuated by below vessel structure, then RCOMP should be set equal to the jet radius. Conversely, corium interaction with below vessel structure may cause the melt to be splattered over a distributed area in which case RCOMP should be set equal to the expected melt dispersion radius. MELTSPREAD3 checks the dispersion radius against the radial location of the in-pedestal nodes. If the radial location of a given node lies within RCOMP, then this node is flagged as a receptor for corium issuing from the RPV. The user is cautioned that the inpedestal nodalization scheme should be constructed such that the code is able to spatially resolve the flow characteristics from the RPV. For instance, if it is desired to examine spreading characteristics for the case of a coherent jet, then the node cell dimension in the impingement region should be set equal to, or less than, the jet radius. If the node size is chosen larger than the jet radius, then the flow is smeared over the larger area thereby artificially reducing the impingement heat transfer.

Lines 28-30 control the modeling assumptions regarding the flow of corium over the sump cover plates in the Mark I containment. Line 28 defines whether or not the sump cover plates are initially in place at the start of the pour. Set NSMPCV=0 if the cover plates are initially absent, or set NSMPCV=1 if the plates are initially present. If NSMPCV=1, then THCKCV should be set equal to the sump cover plate thickness. If NSMPCV=0, corium initially accumulates in the sumps until the melt height exceeds the sump depth at which point the corium will begin to flow out of the sumps. If NSMPCV=1, the corium will flow over the cover plates until the plates are ablated through. At this point, any corium over the top of the plate is relocated to the bottom of the sump, the cell velocity at the edge of the sump is set equal to zero, and the calculation carries on from this point.

Line group 29-30 provides the user with the option of specifying the time and the melt thermal hydraulic conditions when spillover of melt from the Mark I sumps occurs. For instance, this option may be used to mock up situations² in which melt simultaneously collects both over and under the sump cover plates for a period of time. If NBOIL=0, then this option is bypassed. If NBOIL=1, then the sump is assumed to spillover (i.e., fill with voided melt to the bottom of the cover plates) at time t=TMBOIL. For t<TMBOIL, melt issuing from the RPV (Line groups 13-15) is assumed to flow over the cover plates.³ At t=TMBOIL, the melt inventory in the sump is initialized according to the userspecified composition XBLT(I), with the voided melt height at each spreading node site set equal to the sump pit depth, ELSMP. The steel cover plates, plus any melt/solidified debris over the plates, is added to the initial melt inventory within the sump. The melt temperature is then uniformly set equal to TEBOIL, and the cell velocity at the edge of the sump is set equal to zero. The calculation then continues on from this point under the assumption that melt issuing from the RPV drains directly into the sump. Note that this is a legacy option that was implemented early in the code development phase to look at some specific issues, but this option is rarely used as the code is fully capable of calculating sump filling and spillover using a mechanistic approach based on melt pours conditions.

Line 31 controls the assumption of corium heat transfer to the sidewalls in the balance of the annulus beyond the sector region(s) outside the pedestal doorway(s). Set NSWALL=0 for no sidewall heat transfer, or set NSWALL=1 if heat transfer to the sidewalls is allowed. If NSWALL=1, the sidewall heat transfer is currently modeled based on the downward heat flux with an effective area enhancement,

$$q_{down})_j = F_j A_j \left(T_j - T_{bot,j} \right). \tag{4-4}$$

where F_i is the cell area enhancement factor which is defined as

 $^{^2}$ e.g., rapid formation of a localized perforation through the cover plates due to an impinging melt jet, in conjunction with the dispersal of lower-temperature melt around the impingement zone, may lead to such a situation.

³ During this stage, an erosion calculation of the cover plates is <u>not</u> initiated if the local plate surface temperature reaches the steel melting temperature (as would be done for the case in which NSMPCV=1 and NBOIL=0). In this case, a convective boundary condition is locally maintained until t = TMBOIL.

$$F_j = 1 + \frac{4\,\delta x_j h_j}{A_j} \tag{4-5}$$

Line 32 defines the assumed flow angle outside the pedestal doorways (in degrees), ANGFAN. Note that ANGFAN should be set in the range of 0-180°.

If NGEOM=2, Line Groups 33-34 define the user-specified spreading nodalization scheme. Line 33 defines the number of spreading nodes, NUMNOD. Line Group 34 then defines the cell size, radial location, spreading perimeter, area, initial lower surface elevation, and upper surface elevation limit for each node. The nomenclature for the input is illustrated in Figure 4-2. The integer IFLGA specifies the node as a receptor of corium draining from the RPV. Set IFLGA(I)=1 if the node is a receptor, or set IFLGA(I)=0 if the node is not a receptor. There should be NUMNOD Lines in Line Group 34. Note that for this input option, the code does not perform a detailed check on the elevation gradient (as for the case of the Mark I sump calculation which is described in Section 3). Thus, if an initial elevation gradient exists, the gradient must be gradual or else artificial back flow will be calculated. Further note that if the melt upper surface elevation is unrestricted, set HCAP to an arbitrary but large number. If the melt height locally rises to the level of HCAP, the depth is limited by HCAP at this point. However, heat transfer to overlying atmosphere (wet or dry) at this location is still calculated using the normal code heat transfer subroutines, and no heatup or ablation of this overlying structure is calculated.



Figure 4-23 Illustration of nomenclature for spreading nodalization scheme

Line 35 sets the melt viscosity modeling assumptions if the code property routines are to be used (i.e. NOVUM = 0 in Line 22). Set NVTPE=1 to use the Ishii-Zuber correlation to account for solids buildup in the melt, or set NVTPE=2 to use the Ramacciotti correlation. In addition, set NSOLTP=1 for the case in which the oxide phase solid fraction is assumed to vary linearly between the solidus-liquidus, or set NSOLTP=2 to input a table of solid fraction versus normalized temperature difference between the liquid and solid. When NSOLTP=2, input the user-defined input table for normalized melt temperature [i.e. (TFOL-TMELT)/(TFOL-TFOS); see Line 10 for variable definitions] vs. oxide phase solid fraction on Line 36. If NSOLTP = 1 this line is omitted from the input file.

For cases in which NVTPE=1, set ALPMAX in Line 35 to the oxide phase solid fraction at which the viscosity of the melt becomes infinite (i.e., it behaves as a solid). If NVTPE=2, the setting of this parameter is irrelevant. Similarly, if NVTPE = 2, set CRAMCON equal to the constant in the Ramacciotti viscosity correlation. If NVTPE = 1, the setting of this parameter is irrelevant.

Lines 37-47 define the basemat **axial** mesh at each lateral spreading node location, and also allows alternative basemat materials (i.e., other than concrete) to be treated. Line 37 defines the number of nodes in each substrate nodal array. Line Group 38 defines the cell interface location, XBCN, and the total distance between nodes, XDCN, for each substrate node. The nomenclature is illustrated in Figure 4-3. Line Group 38 should have NMVER entries. An illustration of a typical substrate nodalization scheme for a Mark I containment type is shown in Figure 4-4.

The default composition of all substrate node cells is concrete. However, the user has the option of designating as many steel nodes as desired in the substrate. Alternatively, for nodes selected to be steel, the steel properties can be overwritten with user-defined input properties to look at spreading on non-steel or non-concrete surfaces. This is accomplished through Lines 39 and 40. In Line 39, NSTEEL defines the total number of substrate nodes which are designated to be steel. Line Group 40 then defines the index location of each steel node, IX and IY, where IX = horizontal index location and IY = vertical index location. The indexing nomenclature is illustrated in Figure 4-5. Line Group 40 should have NSTEEL entries. The index locations may be input in any order. If no steel nodes are present in the substrate, then set NSTEEL=0. If NSTEEL=0, or if the basemat is declared to be entirely made of steel by setting ICTC = 5 in Line 2, then Line Group 40 is omitted from the input file entirely. Further note that for the case NGEOM=1 and NSMPCV=1 (i.e.,

automated Mark I spreading nodalization with sump covers in place), it is not required to flag the sump cover plates as steel, as this is done automatically by the code.



Figure 4-24 Illustration of nomenclature for substrate nodalization scheme



Figure 4-25 Illustration of a typical Mark I nodalization scheme

As noted, steel properties can be overwritten to examine spreading over basemats not composed of steel or concrete. NSIMST is the control variable providing this ability; set NSIMST = 0 to retain steel properties, or NSIMST = 1 to overwrite steel properties with data provided in Lines 41 to 46. For situations in which NSIMST = 1, then the substrate composition vector XCSI(I) defined in Lines 43-46 is used under ablation conditions to assign the ablation products to the melt according to the composition of the ablating material. Lines 41-42 define the alternate material properties with TSIS/TSIL denoting the solidus/liquidus temperatures; CSIS/CSIL the solid/liquid phase specific heats; DHSIL the latent heat of fusion; RSIS/RSIL the solid/liquid phase densities; TKSIS/TKSIL solid/liquid phase thermal conductivities; and finally ESIL is the material radiation emissivity.



Figure 4-26 Illustration of substrate indexing nomenclature

Lines 47-49 control the Mark I liner heatup calculation. This option can also be used to examine heatup of some other steel element at some point in the spreading domain. Line 47 defines the parameter NSKIPE, which is set equal to 0 if the liner heatup calculation is to be bypassed, or set NSKIPE equal to 1 to perform the heatup calculation if the corium propagates to the liner. If NSKIPE=0, Lines 48-49 are omitted from the input file. If NSKIPE=1, Line 48 defines the liner location, number of liner nodes, liner crust growth options, and the heat transfer coefficient between the melt and the liner. For flow from left to right, set NBMADJ equal to the spreading node to the right of which the liner lies. (For the Mark I automated nodalization scheme, set NBMADJ = NSMP + NPED + NDOR + NANULS to perform the liner heatup calculation immediately across from the pedestal doorway). Currently the input processor constructs a uniform cell mesh in the liner. Set NUMSHH equal to the number of uniformly spaced node cells into which the liner thickness is to be discretized. Set NUMSHV equal to the number of uniformly spaced node cells into which the desired length of the liner is to be nodalized. (Recall that the node size along the length of the liner is subject to the Courant numerical stability criterion; see Eq. 3-134). Set NBFZOE=2 if crust growth on the liner is to be calculated, or set NBFZOE=1 if crust growth is not permitted. If crust growth on the liner is to be calculated (NBFZOE=2), then set NCRTEM=0 to use the melt solidus⁴ as the crust freezing temperature, or set NCRTEM=1 to use the melt temperature at initial contact with liner as the crust freezing temperature. The parameter NLOGSH controls the choice of the heat transfer coefficient between the melt and the liner. Set NLOGSH=0 to use the Theofanous bubble-driven recirculation heat transfer correlation; or set NLOGSH=2 to use the sum of the slot jet impingement and bubble-driven recirculation heat transfer correlations (See Section 2 for a description of these correlations).

Line 49 defines the initial liner temperature, dimensions, inclination angle with respect to vertical, and the slot jet width impinging on liner. Set TSHELI equal to the initial liner temperature. Set HNODT equal to the total length of the liner to be nodalized. Set THSHL equal to the liner thickness. Set ANGSHL equal to the liner inclination angle with respect to the vertical. Set BWIDTH equal to the width of the melt jet impinging on the liner, which is used to evaluate Martin's slot jet impingement heat transfer correlation if that option is chosen (See definition of NLOGSH in Table 4-1).

Line 50 defines the atmospheric conditions in the drywell cavity. Set TBOUND equal to the temperature of the structure above the pedestal and drywell floors, and set EMISCN equal to the radiation emissivity of this structure. If water is absent atop the melt, then radiation heat transfer to the overlying structure is calculated. Set PDRYWL equal to the drywell absolute pressure in the *units of Megapascals*.

Lines 51-57 control the heat transfer modeling assumptions at the melt upper surface. Set NWAT as follows:

- 1) NWAT=0 if the cavity remains dry
- 2) NWAT=1 if the cavity is maintained at saturation temperature corresponding to the containment pressure, PDRYWL, and at a constant water level of HDOWNC

⁴ If the melt temperature adjacent to the shell is above the oxide phase solidus and the melt contains oxide, then the crust freezing temperature is set equal to the oxide phase solidus. Otherwise, the freezing temperature is set equal to the metal phase solidus.

3) NWAT=2 if the detailed water inventory model is invoked; specifications are provided in Lines 52-57.

Note that if NWAT=0 or 2, the setting of HDOWNC in Line 51 is irrelevant. When NWAT=2, TWATI and EWATI are the initial water temperature and level in the cavity, respectively.

When NWAT=2, Lines 52 - 57 allow water injection and spillover points within the mesh to be defined. Water injection is controlled in Line 52; set NINJ=0 if there is no water injection, or set NINJ equal to the number of spreading nodes into which water is injected at any time over the calculation. Note that if NINJ=0, Lines 53-54 are omitted. If NINJ>0, then lines 53-54 are used to define water injection data as follows. For the I-th injection point, NINJP(I) is the node in the spreading mesh into which the water is injected, and NPTINJ(I) is the number of points in the interpolation table for water injection flowrate (XDTINJ(I)) and temperature (TDTINJ(I)) over the calculation. The requirements for the injection input tables are provided in Table 4-1.

Similarly, the parameter NDOWNC provides the capability to model water spillover at user-defined locations in the mesh if the local water height reaches the spillover inlet elevation(s). An example are the downcomers into the Torus of the Mark I containment. If there are spillover points set NDOWNC equal to the number of nodes in the spreading mesh where spillover can occur. Note that if NDOWNC=0, Lines 56-57 are omitted in the input file. If NDOWNC > 0, then Lines 56-57 are used to define water spillover points as follows. For the Ith spillover point, NDC(I) is the node in the spreading mesh where spillover can occur. ELDCO(I) is the elevation above the substrate at which spillover can begin, and NPTDC(I) is the number of points in the interpolation table that provides the spillover 'cord' or arc length as a function of elevation above the spillover inlet. The input table with NPTDC(I) line entries defines the elevation above the spillover inlet height (i.e., local water depth minus the inlet elevation), and the equivalent 'cord length' at that elevation available for spillover. The 'cord length' is defined such that the water height above the spillover inlet multiplied by the interpolated cord length equals the water flow area into the downcomer. For instance, if the downcomer is a circular pipe with a horizontal opening, then the cord length is simply the pipe circumference.

Line 60 defines the heat transfer coefficient and boundary condition options currently available in the code. User guidance on appropriate settings for these parameters based on the current level of model development and validation are also provided in the table. Set NBFRZO equal to 1 for bulk freezing of the corium or set NBFRZO equal to 2 for freezing through crust formation at the melt lower surface. If NBFRZO=2, set NTHINC=0 for crust growth/remelting calculation, or set NTHINC=1 for downward heat transfer limited by thin crust segments.

If the substrate is ablating, the parameters NABLFM and NDRNFM specify the disposition of the ablated substrate material. The parameter NABLFM controls the disposition of ablated material when crust growth is not specified (NBFRZO=1). Set NABFLM=1 if the ablated material is assumed to remain on the surface as a molten film, or set NABFLM=2 if the ablated material is assumed to be continuously mixed into the melt. The parameter NDRNFM controls the disposition of ablated substrate when crust growth is specified (NBFRZO=2). Set NDRNFM=1 for a porous overlying crust, such that the ablated material continuously drains through the crust, or set NDRNFM=2 for the case in which the crust is non-porous and the ablated material is trapped beneath the crust.

The parameter NBCBOT controls the choice of the downward heat transfer coefficient. Set NBCBOT=1 to use Bradley's model; set NBCBOT=2 to use Kao and Kazimi's revised periodic contact model; set NBCBOT=3 to use the Dittus-Boltler forced convection heat transfer correlation; set NBCBOT=4 to use the sum of Bradley's model and the force convection correlation; or set NBCBOT=5 to use the sum of Kao and Kazimi's model and the forced convection correlation.

The parameter NCRTOP defines the thin crust boundary condition at the melt upper surface. Set NCRTOP=0 for the cases in which sparging decomposition gases are assumed to preclude crust formation at the melt upper surface. Set NCRTOP=1 to override the check on the gas velocity in which case a thin top crust is assumed to always exist at the melt upper surface.

Line 59 allows the user to specify an additional interfacial heat transfer resistance to be added at the melt/substrate interface and was motivated by the fact that metal spreading data indicates that an additional resistance forms due to a lack of surface wetting for steel spreading tests. Set NINTF=0 if this option is bypassed, or NINTF=1 if an interfacial resistance HINTF exists. The setting of HINTF is arbitrary if NINTF=0.

Line 60 defines the substrate ablation mapping factor, XFCABL, and the bulk freezing node size, XNDMIN. XFACBL is the fractional amount that a node can be ablated from the initial thickness before the local basemat array is remeshed by incorporating the residual material into the underlying node. The recommended value for XFCABL is 0.01 although computed results (thankfully) seem to be rather insensitive to the setting of this parameter. The additional parameter XNDMIN specifies the node cell size assigned to solidified corium upon incorporation into the substrate nodal array. If the local depth of solidified corium is less than XNDMIN, then the corium is incorporated into the substrate as a distinct node. If the depth is greater than XNDMIN, then the corium is divided into as many cells of length XNDMIN as possible, with the residual amount incorporated as a distinct node atop the solidified melt. This approach allows the user the ability to control the node spatial resolution in solidified corium, where the effects of decay heat are of interest. The user is cautioned, however, not to specify XNDMIN too small such that the node accumulation of solidified material causes the substrate nodal vector dimension to exceed the vector dimension in the code (currently 999). This will not cause the code to abnormally terminate, as a local check on the number of substrate nodes is performed at each time step. If the number of nodes has reached the vector dimension, then nodes at the bottom of the nodal array are truncated in order to incorporate the solidified corium. (This may lead to an eventual loss of concrete beneath the solidified corium and, as a result, the concrete decomposition gas flux becomes zero). Thus, XNDMIN should be chosen to reflect the anticipated depth of solidified corium, in addition to however many nodes are initially allotted to concrete (NMVER). Typically, this minimum node size has been set to 2 cm.

Line 61 defines the integration control parameters for the gravity-driven melt spreading fluid mechanics calculation. Due to the non-linearity in the advection term in the momentum equation, the fluid mechanics calculation may not be numerically stable at time steps suitable for the solution of the conservation of energy equation. Thus, the time step for the fluid mechanics calculation is taken as an integer multiple of the time step for the conservation of energy equation; i.e.

$$\delta t_{fluid} = \delta t_{energy} / NVELP. \tag{4-6}$$

The-end-of-time step cell-edge velocities for the solution of the conservation of energy equation are then calculated by taking NVELP smaller time steps. For a conservative approach, set NVELP equal to 5. DAVMX and DVMX are the iteration convergence tolerances on the average and maximum incremental changes in melt cell edge velocities that are defined as

$$DAVMX \le \frac{1}{N_s} \sum_i |\delta u_i| \tag{4-7}$$

$$DVMX \le max(|\delta u_i|) \tag{4-8}$$

where N_s is the number of spreading nodes containing corium (h>0), and max (\cdot) denotes the largest element of the vector. NITMAX is the maximum number of iterations allowed to meet the convergence criteria defined in Eqs. 4-7 and 4-8. Recommended values are NITMAX=20, DAVMX= .005 m/s, and DVMX=.01 m/s. If convergence is not achieved, an error message is written to the diagnostics file 'diag.dat,' but the calculation is not terminated.

Line 62 similarly defines the integration convergence criteria for the solution of the melt conservation of energy equation. DEAVMX and DEMX are the iteration convergence tolerances on the average and maximum incremental changes in corium specific enthalpy which are defines as,

$$DEAVMX \leq \frac{1}{N_s} \sum_i |\delta e_i| \tag{4-9}$$

$$DEMX \le max(|\delta e_i|) \tag{4-10}$$

NENMX is the maximum number of iterations allowed to meet the convergence criteria defined in Eqs. 4-9 and 4-10. Recommended values are NENMAX=20, DEAVMX 300 J/kg and DEMX= 600 J/kg. If convergence is not achieved, an error message is written to the diagnostics file 'diag.dat,' but the calculation is not terminated.

Similar convergence checks are applied to the water conservation of momentum and energy equation solutions when the detailed water inventory model is used (NWAT=2). The analogous convergence control parameters are defined in Lines 63-64. These lines are included even if NWAT<2; however, settings are arbitrary under this condition.

Line 64 controls the frequency and amount of printed data. Set NPFREQ equal to the number of time steps between calling the output processor, PRINTS (i.e., data are printed every NPFREQ· δ t seconds). Set NPEND equal to the number of liner nodes along the length of the liner to be printed when the output processor is called. This option is included to suppress writing out nodal temperatures far up on the liner where the temperatures are not expected to change significantly or are not of interest. To print all of the liner nodal temperatures, set NPEND=NUMSHV. When the output processor is called, the parameter NPRINT controls the volume of printed output. Set NPRINT=2 to print the bulk of the computed information, including the entire inventory of substrate nodal temperatures are printed when the output processor is called, the

called, but underlying node temperatures are not. Set NPRINT=1 to suppress printing of the remaining nodal temperatures. Finally, NBEDCQ controls the nature of the output data that is written to the CORQUENCH initiation file 'cqinput.dat'. Set NBEDCQ = 0 if particulate formed from jet erosion (NJET=2; see Line 16) is to be retained as a separate debris bed in cqinput.dat, or set NBEDCQ = 1 if it is to be integrated with the underlying melt and thermally equilibrated with that material. Note that if NJET<2, or a follow-on calculation with CORQUENCH is not going to be performed, then the setting for NBEDCQ is irrelevant. Note that supporting software that can be used to automate the development of a CORQUENCH input file from the MELTPSREAD output is described in Appendix D.

NTIMSPC in Line 66 sets the number of times over the course of the calculation that an output file 'fort.number' is generated, with 'number' starting at 10 for the first file that is produced, and increasing by 1 for each sequential file produced thereafter. These files contain data on spatially dependent variables (e.g., melt temperature, depth, heat flux to underlying concrete, ...) that can be copied into the supplied excel spreadsheet 'plotfort.1x' for graphical evaluation. Note that the maximum setting for NTIMSPC is 10. TIMSPC(I) on Line Group 67 are the specific times at which output files are to be generated with the spatially dependent data; this line is repeated NTIMSPC times. If NTIMSPC=0, this line is omitted. Additional information on the data contained in these files is provided in the section on code output.

NPLFREQ on line 68 sets the frequency that data are written to various additional plotting files (i.e., the data are printed every DTIME·NPFREQ seconds; see Line 72 for DTIME definition) that are described below.

The first time-dependent data files produced are defined by the variable NPLTOT on Line 68, which sets the number of nodes for which an output file 'fort.number' is generated, with 'number' starting at 20 for the first file that is produced, and increasing by 1 for each sequential file produced thereafter. These files contain information on time dependent data at specified node sites (e.g., melt temperature, depth, heat flux to underlying concrete, ...) that can be copied into the supplied excel spreadsheet 'plotfort.2x' for graphical evaluation. Note that the maximum setting for NPLTOT is 10. NPLLOC(I) on Line Group 69 are the specific nodes for which output files are to be generated with time dependent data; this line is repeated NPLTOT times. If NPLTOT=0, this line is omitted. Additional information on the data contained in these files is provided in the section on code output.

NBPL on Line 70 sets the number of basemat nodes at which the temperatures are to be written to the output file 'fort.30', with IXP(I) and IYP(I) on Line Group 71 defined as the x-y nodal indices within the basemat for which temperatures are to be written out. Note that Line 71 is repeated NBPL times, and that this line is omitted if NBPL=0. Additional information on the data contained in these files is provided in the section on code output.

Line 72 defines the integration time step and the start and stop times for the calculation. Set TIMEO equal to the initial time, DTIME is the integration time step, and TMAX is the total time to which the calculation is to be performed. The integration time step should be chosen carefully. The fundamental limitation on the time step size is that the corium should not be convected across more than one spreading cell over a given time step. If this limitation is not met, then the heat transfer calculations will not be able to resolve whether or not the corium should have been frozen and immobilized in upstream cells. For a given spreading cell size, δx , the limitation on the time step is therefore of the form

$$\delta t \le \frac{\delta x}{U_{max}} \tag{4-11}$$

where U_{max} is the maximum anticipated spreading velocity over the flow field. For Mark I containments, an upper bound on U_{max} may be obtained by considering the limiting case in which the entire volumetric flowrate from the RPV is diverted out the doorway(s). Neglecting buildup and retention of corium in the pedestal region, the flow velocity out of the pedestal doorway may be approximated using open channel flow theory⁵,

$$U_{max} = \left(\frac{g \, \dot{Q}_{door}}{W_{door}}\right)^{1/3} \tag{4-12}$$

where

 W_{door} = doorway width,

 \dot{Q}_{door} = volumetric flowrate out of the pedestal doorway.

The flowrate out of the doorway is related to the volumetric flowrate from the RPV through the expression,

$$\dot{Q}_{door} = \frac{\dot{Q}_{RPV}}{N_{door}} \tag{4-13}$$

⁵ For example, see F. M. White, <u>Fluid Mechanics</u>, McGraw-Hill (1986).
where N_{door} = number of pedestal doorway openings.

Equation 4-11 defines the maximum allowable time step to ensure a physically realistic solution. However, the practical time step (i.e., the time step which ensures convergence of the conservation of energy equation) may be lower. Due to the highly nonlinear form of the equations, it is difficult to develop a simple criterion for the time step which would ensure convergence of the conservation of energy equation. Thus, it is recommended try a few different time steps to check on the variations of the results with time step size. Extensive experience indicates that a time step of 10 ms is more than adequate for most applications involving both MAAP and MELCOR-type pours.

Section 5

DESCRIPTION OF MELTSPREAD3 FILE OUTPUT

MELTSPREAD3 produces up to 9 file output types that document the results of the spreading analysis carried out on the basis of user-specified modeling assumptions, melt pour and cavity conditions, and the cavity geometry. A high level summary of these files is provided in Table 5-1.

TEXT OUTPUT FILE DESCRIPTION

The text output file 'spreadout.dat' contains text and data produced from each run. Prior to initiating the numerical integration, the code first echo-prints the input file, and then writes out a summary of the user-specified input data and computational options. Printed data regarding the corium and underlying substrate includes corium oxide and metal phase solidus and liquidus temperatures, concrete type and composition, concrete dryout and ablation temperatures, and concrete and slag densities. The corium freezing and substrate ablation options are printed. The cavity conditions, including presence or absence of water, overlying structure temperature and emissivity, water saturation temperature and subcooling, and maximum water height, are printed. Regarding heat transfer boundary conditions, the choice of downward heat transfer coefficient is printed, as well as assumptions regarding melt stream jet breakup behavior if that option is invoked.

A summary of the spreading nodalization scheme is then printed. The printed data includes radial location, channel width normal to flow, area, and elevation for each spreading node cell. If the shell heatup calculation is to be performed, a summary of the shell nodalization scheme and crust growth options are printed. A banner is then written to the output file indicating that the end of the summary of user-input data has been reached, and the calculation is starting.

Each time the PRINTS subroutine is called, MELTSPREAD writes to the output file up to nine blocks of calculated information. At each spreading node location, the first block of printed information summarizes the boundary condition flag, NBCINT, substrate elevation, surface temperature, cumulative substrate ablation depth, crust depth, molten film depth, and corium spreading velocity at the j-1/2 cell edge. The water spreading velocity is also printed if the detailed water inventory model is invoked.

Table 5-1 SUMMARY OF MELTSPREAD3 DATA OUTPUT FILES

No.	File Name	Summary Description
1	spreadout.dat	ASCII text file summarizing: i) input data and modeling assumptions, and ii) computed information at user-specified time intervals.
2	fort.1x	Plotting file providing spatially dependent melt spreading data at user-specified times; see Table 5-2 for contents description. Up to 10 files can be generated by this option, with 'x' in fort.1x ranging from 0 to 9, accordingly.
3	fort.2x	Plotting file providing time dependent melt spreading data at user-specified node locations; see Table 5-3 for contents description. Up to 10 files can be generated by this option, with 'x' in fort.2x ranging from 0 to 9, accordingly.
4	fort.10x	Plotting file providing spatially dependent crust thickness and temperatures on the shell if that modeling option has been selected and the melt has contacted the shell; see Table 5-4 for contents description. Up to 10 files can be generated by this option, with 'x' in fort.2x ranging from 0 to 9, accordingly. In this application, the file descriptor 'x' corresponds to the same times as those specified for No. 2 above.
5	jetdata.dat	Plotting file providing time dependent melt jet breakup data if the jet breakup model is invoked (i.e. NJET > 0, see Table 4-1 in code input description); see Table 5-5 for contents description.
6	waterdata.dat	Plotting file providing time dependent water inventory data if the water inventory model is invoked (i.e. NWAT=2; see Table 4-1 in code input description); see Table 5-6 for contents description.
7	meltloc.dat	Quick-look plotting file providing time-dependent extent-of- spreading data and peak shell surface temperature; see Table 5- 7 for contents description.
8	diag.dat	Output diagnostics file. Aside from the output file header 'Diagnostics file output:' this file should be empty following a successful run. If problems with convergence or other issues arise during the run, an error message is written providing a few details. Convergence issues can be addressed either by reducing the integration time step or by increasing the number of iterations as needed in lines 63 through 66 of the input file (see Table 4-1 in code input description).
9	cqinput.dat	Data file tabulating melt, crust, and particle bed compositions, at each node at the end of the calculation. This file is written out in a format that is compatible with the CORQUENCH4 input file requirements to automate preparation of the input file for that code.

The second block of printed information includes the local corium enthalpy, temperature, collapsed metal phase depth, collapsed oxide phase depth, total

collapsed depth, corium-to-overlying medium heat flux, corium-to-substrate heat flux, and oxidation energy flux within the corium layer due to reaction of metallic melt constituents with sparging concrete decomposition gases. Note that if no molten corium currently exists at a given node, the data at this location are set equal to zero. Data regarding corium which has been solidified and incorporated into the substrate is printed out in a block described later. If the water inventory model is invoked, water temperature and depth at each node are also printed.

The third block of computed information summarized the local concrete dryout information. The local decomposition gas mass fluxes for dryout of free water, $Ca(OH)_{2,} MgCa(CO_3)_{2,} and CaCO_3$ are printed, as well as the local superficial gas velocity and corium void fraction. Note that if no molten corium exists at a given node site, the void fraction is set equal to zero.

The fourth block of printed information summarizes the local melt thermophysical properties. The thermal conductivity, density, molten phase specific heat, surface tension, emissivity, and derivative of temperature with respect to specific enthalpy at each node cell are printed.

The fifth and sixth blocks of printed information summarize the current overall corium mass balances. The fifth block summarizes the cumulative mass of each corium constituent ejected from the RPV up to the current time. The sixth block of printed information summarizes the corium constituent masses remaining in a molten state on the pedestal and drywell floors, including concrete slag. If the melt jet fragmentation model is invoked and the fragmented material is assumed to be rendered into a particle bed, the cumulative mass of each constituent in the debris bed is also printed, as well as the distribution of that material at the various spreading node locations.

The seventh block of printed information summarized area-averaged quantities and total cumulative quantities. The total corium mass ejected from the RPV is printed, as well as the total corium mass remaining in a molten state on the pedestal and drywell floors (both metal and oxide phases). The average top and bottom heat fluxes from the melt are printed, as is the average oxidation energy flux within the melt. The average concrete decomposition gas mass flux and corresponding average superficial gas velocity are printed. Additionally, the average melt void fraction is printed. If jet fragmentation is modeled, then the total mass of fragmented material is also printed, as well as the amount of steam produced from jet fragmentation. If the detailed water inventory model is invoked, then the total mass of water remaining on the floor, mass of steam produced, water spillover into downcomer(s), injected water mass, integrated heat transfer to water, and water mass balance (should remain a small fraction of the total water mass involved in the calculation) are also printed.

The eight block of computed information, which may be omitted from the output file by setting NPRINT=1, summarizes the current substrate node temperatures and distance between cell centers. The index location of each cell is printed (NX, NY), as well as the cell "type" of material, TP. Note that TP=0 corresponds to solidified corium, TP=1 corresponds to concrete, and TP=2 corresponds to steel.

If corium propagates to the containment shell and the shell heatup calculation is to be performed, the ninth block of printed information summarizes shell node temperatures and local crust depths.

In addition to the above information, banners are written to the output file when significant events occur. For the Mark I calculation with sump covers in place, a banner is written to the output file when the cover plates have been ablated through and the overlying corium is relocated to the bottom of the sump. The time at which this event occurs is also printed. If the shell heatup calculation is to be performed and the corium propagates to the shell, a banner is written to the output file indicating the time at which this event occurs.

In order to minimize the volume of printed information, the output processor only prints information through and including the cell corresponding to the leading edge of the spreading layer. This capability suppresses redundant printing of initial condition information where corium has not yet spread. However, this feature is disabled if the water inventory model is invoked as water can (and in most cases is) present over nodes that have not been covered by core debris.

PLOTTING FILE OUTPUT DESCRIPTIONS

As shown in Table 5-1, MELTSPREAD3 produces six data files that can be imported into Excel spread sheets provided along with the code that graphically display the computed information. These plots cover most key information that is utilized for assessing the extent and impact of core debris spreading in accident analyses. Definitions of the information written out to the six plotting files listed in Table 5-1 are detailed in Tables 5-2 to 5-7. The corresponding supplied Excel spread sheet names for plotting the data are also noted.

Column	Output Variable	Units
А	Distance Along Spreading Length	m
В	Solid Surface Elevation	cm
С	Remaining Substrate Elevation	cm
D	Collapsed Melt Upper Surface Elevation	cm
Е	Water Upper Surface Elevation	cm
F	Melt Temperature	K
G	Melt Metal Layer Depth	cm
Н	Melt Oxide Layer Depth	cm
Ι	Total Melt Depth	cm
J	Voided Melt Depth	cm
K	Voided Melt Upper Surface Elevation	cm
L	Melt Void Fraction	-
М	Melt Sparging Rate	cm/s
Ν	Surface Temperature of Solid Surface	K
0	Spreading Melt Velocity	cm/s
Р	Heat Flux at Melt Upper Surface	kW/m^2
Q	Heat Flux at Melt Lower Surface	kW/m^2
R	Heat Flux in Melt Due to Oxidation Reactions	kW/m^2
S	Melt Bottom Crust Thickness	cm
Т	Thickness of Slag Film at Melt Bottom Surface	cm
U	Melt Viscosity	kg/m-s
V	Integrated Mass of Frozen Metal Along Spreading Length	kg
W	Integrated Mass of Frozen Oxide Along Spreading Length	kg
Х	Integrated Mass of Particle Bed Along Spreading Length	kg
Х	Integrated Total Frozen Mass Along Spreading Length	kg
Y	Integrated Mass of Molten Metal Along Spreading Length	kg
Z	Integrated Mass of Molten Oxide Along Spreading Length	kg
AA	Integrated Total Molten Mass Along Spreading Length	kg
AB	Integrated Total Debris Mass Along Spreading Length	kg

Table 5-2 SUMMARY OF OUTPUT VARIABLES WRITTEN TO 'fort.1x' FILES THAT CAN BE IMPORTED AND PLOTTED IN THE EXCEL SPREADSHEET 'plotfort.1x'.

Column	Output Variable	Units
А	Spreading Node Number	_
В	Time	(sec)
С	Solid Surface Elevation	cm
D	Remaining Substrate Elevation	cm
E	Collapsed Melt Upper Surface Elevation	cm
F	Water Upper Surface Elevation	cm
G	Melt Temperature	K
Н	Melt Metal Layer Depth	cm
Ι	Melt Oxide Layer Depth	cm
J	Total Melt Depth	cm
Κ	Voided Melt Depth	cm
L	Voided Melt Upper Surface Elevation	cm
М	Melt Void Fraction	-
Ν	Melt Sparging Rate	cm/s
0	Surface Temperature of Solid Surface	K
Р	Spreading Melt Velocity	cm/s
Q	Heat Flux at Melt Upper Surface	kW/m^2
R	Heat Flux at Melt Lower Surface	kW/m^2
S	Heat Flux in Melt Due to Oxidation Reactions	kW/m^2
Т	Melt Bottom Crust Thickness	cm
U	Thickness of Slag Film at Melt Bottom Surface	cm
V	Melt Viscosity	kg/m-s
W	Melt Solid Fraction	-

Table 5-3 SUMMARY OF OUTPUT VARIABLES WRITTEN TO 'fort.2x' FILES THAT CAN BE IMPORTED AND PLOTTED IN THE EXCEL SPREADSHEET 'plotfort.2x'

Table 5-4 SUMMARY OF OUTPUT VARIABLES WRITTEN TO 'fort.10x' FILES THAT CAN BE IMPORTED AND PLOTTED IN THE EXCEL SPREADSHEET 'plotfort.10x'

Column	Output Variable	Units
А	Distance Along Shell	m
В	Crust Thickness	mm
С	Surface Temperature	Κ
D	Temperature at 2nd Node into Shell	Κ
Е	Temperature at 3rd Node into Shell	Κ
F	Temperature at 4th Node into Shell	Κ
G	Temperature at 5th Node into Shell	Κ

Table 5-5 SUMMARY OF OUTPUT VARIABLES WRITTEN TO THE FILE 'jetdata.dat' THAT CAN BE IMPORTED AND PLOTTED IN THE EXCEL SPREADSHEET 'plotjet'

Column	Output Variable	Units
А	Time	sec
В	Fall Height RPV to water	m
С	RPV Hole Diameter	m
D	Jet Diameter at Water Surface	m
E	Jet Velocity at RPV Exit	m/sec
F	Jet velocity at Water Surface	m/sec
G	Jet Weber Number at Water Surface	-
Н	Jet Froude Number at Water Surface	-
Ι	Jet Penetration Distance: Saito Correlation	m
J	Jet Penetration Distance: Epstein Correlation	m
K	Theoretical Jet Penetration Distance	m
L	Actual Penetration Distance	m
М	Water Depth in Jet Receptor Node	m
Ν	Fraction Jet Fragmented	-
0	Fragmented Particle Bed Mass	kg
Р	Total Pour Mass	kg
Q	Melt Temperature at RPV Exit	K
R	Coherent Melt Jet Temperature	K
S	Melt Specific Enthalpy at RPV Exit	MJ/kg
Т	Coherent Melt Specific Enthalpy	MJ/kg
U	Vapor Density	kg/m ³
V	Water Pool Density	kg/m ³
W	Melt Pour Rate from RPV	kg/s

Table 5-6	SUMMARY O	FOUTPUT	VARIABLES	WRITTEN	TO THE FILE	'waterdata.dat'	THAT CAN BI	E IMPORTED /	AND PLOTTED
IN THE EXCEL SPREADSHEET 'plotwat'									

Column	Output Variable	Units
А	Time	sec
В	Water Injection Rate	kg/sec
С	Flowrate into Downcomers	kg/sec
D	Total Steam Production Rate	kg/sec
E	Total Injection	kg
F	Total Flow into Downcomers	kg
G	Total Steam Production	kg
Н	Remaining Water on Floor	kg
Ι	Water Mass Balance	kg
J	Steam from Jet Fragmentation	kg/sec
K	Total from Jet Fragmentation	kg

Table 5-7 SUMMARY OF OUTPUT VARIABLES WRITTEN TO THE FILE 'meltloc.dat' THAT CAN BE IMPORTED AND PLOTTED IN THE EXCEL SPREADSHEET 'plotmeltloc'

Column	Output Variable	Units
А	Time	sec
В	Spreading Distance	m
С	Spreading Area	m^2
D	Peak Shell Surface Temperature	K

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Appendix A

TABULATION OF FUNCTIONS FOR FORWARD ELIMINATION NUMERICAL SCHEME

The purpose of this appendix is to document functions that arise in the development of the forward elimination numerical scheme described in Section 3. The nomenclature employed here is identical to that used in Section 3. For purposes of brevity, the superscript r (denoting current value) is omitted in the following equations.

CRUST AND ABLATION FORWARD ELIMINATION DERIVATIVE FUNCTIONS

The crust and ablation depth derivative functions are defined as

$$d_1^{Cr} = \frac{d\delta_{Cr}}{dT_1},\tag{A-1}$$

$$d_{melt}^{cr} = \frac{d\delta_{cr}}{dT_1},\tag{A-2}$$

$$d_2^{st} = \frac{d\eta}{dT_2},\tag{A-3}$$

$$d_{melt}^{st} = \frac{d\eta}{dT},$$
 A-4)

The crust and ablation rate derivative functions are defined as,

$$f_1^{cr} = \frac{d}{dT_1} \left[\frac{d\delta_{cr}}{dt} \right],\tag{A-5}$$

$$f_{melt}^{cr} = \frac{d}{dT} \left[\frac{d\delta_{cr}}{dt} \right],\tag{A-6}$$

$$f_2^{st} = \frac{d}{dT_2} \left[\frac{d\eta}{dt} \right],\tag{A-7}$$

$$f_{melt}^{st} = \frac{d}{dT} \left[\frac{d\eta}{dt} \right], \tag{A-8}$$

The specific forms of the derivative functions for the various melt/substrate boundary conditions are provided below.

<u>NBCINT=1</u>: For this case, all derivative functions equal zero.

<u>NBCINT=2</u>:

$$d_1^{cr} = -\frac{k_{cr}}{\zeta_{cr}\Gamma_{cr}} \tag{A-9}$$

$$d_{melt}^{cr} = \frac{h_{bot}}{2\zeta_{cr}} \left[\frac{h_{bot}(T - T_{sol,cr})}{\zeta_{cr}\Gamma_{cr}} - 1 \right]$$
(A-10)

$$f_1^{cr} = -\frac{k_{cr}}{2\delta t \zeta_{cr} \delta_{cr}} \left[1 + \frac{(T_{sol,cr} - T_1)}{\delta_{cr}} d_1^{cr} \right]$$
(A-11)

$$f_{melt}^{cr} = -\frac{h_{bot}}{2\delta t \zeta_{cr}} \left[1 + \frac{k_{cr}(T_{sol,cr} - T_1)}{h_{bot}\delta_{cr}^2} d_{melt}^{cr} \right]$$
(A-12)

All derivative functions for the ablation depth and ablation rate equal zero. <u>NBCINT=3</u>: For this case, all derivative functions equal zero. <u>NBCINT=4</u>:

$$d_2^{st} = -\frac{\bar{k}}{\Gamma_{st}\zeta_{st}} \tag{A-13}$$

$$d_{melt}^{st} = \frac{h_{bot}}{2\zeta_{st}} \left[\frac{h_{bot}(T - T_{sol,st})}{\zeta_{st}\Gamma_{st}} - 1 \right]$$
(A-14)

$$f_2^{st} = -\frac{\bar{k}}{2\delta t \,\zeta_{st} \,\eta} \Big[1 + \frac{(T_{sol,st} - T_2)}{\eta} d_2^{st} \Big] \tag{A-15}$$

$$f_{melt}^{st} = -\frac{h_{bot}}{2\delta t \,\zeta_{st}} \left[1 + \bar{k} \frac{(T_{sol,st} - T_2)}{h_{bot} \eta^2} d_{melt}^{st} \right] \tag{A-16}$$

All derivative functions for the crust depth and crust rate equal zero.

<u>NBCINT=5</u>: This case is identical to case 4, with the exception that the bottom heat transfer coefficient, h_{bot} , is replaced by the effective heat transfer coefficient across the molten film, \bar{h} , as defined in Eq. 3-31.

<u>NBCINT=6</u>:

$$d_1^{cr} = 0 \tag{A-17}$$

$$d_{melt}^{cr} = \frac{h_{bot}}{2\zeta_{cr}} \left[\frac{h_{bot}(T - T_{sol,cr})}{\zeta_{cr}\Gamma_{cr}} - 1 \right]$$
(A-18)

$$d_2^{st} = -\frac{\bar{k}}{\zeta_{st}\Gamma_{st}} \tag{A-19}$$

$$d_{melt}^{st} = \frac{k_{cr}(T_{sol,cr} - T_{sol,st})}{2 \zeta_{st} \delta_{cr}^2} \left[1 - \frac{k_{cr}(T_{sol,cr} - T_{sol,st})}{\zeta_{cr} \Gamma_{cr}} \right]$$
(A-20)

$$f_1^{cr} = 0 \tag{A-21}$$

$$f_{melt}^{cr} = -\frac{h_{bot}}{2\zeta_{cr}\,\delta t} \left[1 + \frac{k_{cr}(T_{sol,cr} - T_{sol,st})}{\delta_{cr}^2 h_{bot}} d_{melt}^{cr} \right] \tag{A-22}$$

$$f_2^{st} = -\frac{\bar{k}}{2\zeta_{st}\,\delta t\eta} \left[1 + \frac{(T_{sol,st} - T_2)}{\eta} d_2^{st} \right] \tag{A-23}$$

$$f_{melt}^{st} = -\frac{\bar{k}(T_{sol,st} - T_2)}{2 \zeta_{st} \,\delta t \,\eta^2} \, d_{melt}^{st} + \frac{k_{cr}(T_{sol,cr} - T_{sol,st})}{2 \zeta_{st} \,\delta t \,\delta_{cr}^2} d_{melt}^{cr} \tag{A-24}$$

NBCINT=7:

$$d_2^{st} = -\frac{\bar{k}}{\zeta_{st}\,\Gamma_{st}}\tag{A-25}$$

$$d_{melt}^{st} = \frac{h_{bot}}{2\zeta_{st}} \left[\frac{h_{bot}(T - T_{sol,cr})}{\zeta_{st} \Gamma_{st}} - 1 \right]$$
(A-26)

$$f_2^{st} = -\frac{\bar{k}}{2\zeta_{st}\,\delta t\,\eta} \Big[1 + \frac{(T_{sol,st} - T_2)}{\eta} d_2^{st} \Big] \tag{A-27}$$

$$f_{melt}^{st} = -\frac{h_{bot}}{2\zeta_{st}\,\delta t} \left[1 + \frac{\bar{k}(T_{sol,st} - T_2)}{\eta} d_{melt}^{st} \right] \tag{A-28}$$

All derivative functions for the crust depth and crust growth rate equal zero. <u>NBCINT=8</u>:

$$d_1^{cr} = 0 \tag{A-29}$$

$$d_{melt}^{cr} = \frac{h_{bot}}{2\zeta_{cr}} \left[\frac{h_{bot}(T - T_{sol,cr})}{2\zeta_{cr}\Gamma_{cr}} - 1 \right]$$
(A-30)

$$d_2^{st} = -\frac{\bar{k}}{\zeta_{st}\Gamma_{st}} \tag{A-31}$$

$$d_{melt}^{st} = \frac{k_{eff}(T_{sol,cr} - T_{sol,st})}{2\zeta_{st}\delta_{cr}^2} \left[1 - \frac{k_{eff}(T_{sol,cr} - T_{sol,st})}{\zeta_{st}\Gamma_{st}\delta_{cr}} \right] d_{melt}^{cr}$$
(A-32)

$$f_1^{cr} = 0 \tag{A-33}$$

$$f_{melt}^{cr} = -\frac{h_{bot}}{2\zeta_{cr}\,\delta t} \left[1 + \frac{k_{eff}(T_{sol,cr} - T_{sol,st})d_{melt}^{cr}}{\delta_{cr}^2 \, h_{bot}} \right] \tag{A-34}$$

$$f_2^{st} = -\frac{k_{eff}}{2\,\delta t\,\zeta_{st}\,\eta} \Big[1 + \frac{(T_{sol,st} - T_2)d_2^{st}}{\eta} \Big] \tag{A-35}$$

$$f_{melt}^{st} = \frac{k_{eff}}{2\,\delta t\,\zeta_{st}}\,\frac{(T_{sol,cr} - T_{sol,st})}{\delta_{cr}^2}d_{melt}^{cr} \tag{A-36}$$

<u>NBCINT=9</u>:

$$d_2^{st} = -\frac{\bar{k}}{\zeta_{st}\Gamma_{st}} \tag{A-37}$$

$$d_{melt}^{st} = \frac{h_{bot}}{2\zeta_{st}} \left[\frac{h_{bot}(T - T_{sol,cr})}{2\zeta_{st}\Gamma_{st}} - 1 \right]$$
(A-38)

$$f_2^{st} = -\frac{\bar{k}}{2 \,\delta t \,\zeta_{st} \,\eta} \Big[1 + \frac{(T_{sol,st} - T_2)}{\eta} d_2^{st} \Big] \tag{A-39}$$

$$f_{melt}^{st} = -\frac{h_{bot}}{2\,\delta t\,\zeta_{st}} \Big[1 + \frac{\bar{k}(T_{sol,st} - T_2)}{h_{bot}\,\eta^2} d_{melt}^{st} \Big] \tag{A-40}$$

CONCRETE DECOMPOSITION FORWARD ELIMINATION COEFFICIENTS

Assume that the dryout front is currently located between the j-th and j+1 st substrate nodes. Except when the substrate is ablating and the dryout

isotherm lies between the first two nodes at the substrate surface, the functional form of the dryout front propagation velocity is determined from Eq. 3-60 as

$$\dot{x}_{dc}^{i} = function (T_{j}, T_{j+1}, \dot{e}_{j}[T_{j-1}, T_{j}, T_{j+1}], \dot{e}_{j+1}[T_{j}, T_{j+1}, T_{j+2}])$$
 (A-41)

where ($\dot{}$) denotes differentiation with respect to time. The forward elimination coefficients are determined from Eq. A-41 by taking the total differential of this equation, yielding:

$$(\dot{x}_{dc}^{i})^{r+1} = (\dot{x}_{dc}^{i})^{r} + \frac{\partial \dot{x}_{dc}^{i}}{\partial T_{j}} W_{j} \delta e_{j} + \frac{\partial x_{dc}^{i}}{\partial T_{j+1}} W_{j+1} \delta e_{j+1}$$

$$+ \frac{\partial \dot{x}_{dc}^{i}}{\partial \dot{e}_{j}} \left[\frac{\partial \dot{e}_{j}}{\partial T_{j}} W_{j} \delta e_{j} + \frac{\partial \dot{e}_{j}}{\partial T_{j+1}} W_{j+1} \delta e_{j+1} + \frac{\partial \dot{e}_{j}}{\partial T_{j-1}} W_{j-1} \delta e_{j-1} \right]$$

$$+ \frac{\partial x_{dc}^{i}}{\partial \dot{e}_{j+1}} \left[\frac{\partial \dot{e}_{j+1}}{\partial T_{j+1}} W_{j+1} \delta e_{j+1} + \frac{\partial \dot{e}_{j+1}}{\partial T_{j}} W_{j} \delta e_{j} + \frac{\partial \dot{e}_{j+1}}{\partial T_{j+2}} W_{j+2} \delta e_{j+2} \right].$$

$$(A-42)$$

Evaluation of the partial derivatives given Eqs. 3-56 and 3-57 and then substituting the resultant expressions into Eq. A-42 yields,

$$\dot{x}_{dc}^i)^{r+1} = \dot{x}_{dc}^i)^r + \Omega_o^i + \Omega_1^i \delta e_{melt}$$
(A-43)

where the dryout front forward elimination coefficients are defined as,

$$\Omega_{o}^{i} = (\zeta_{j} + \zeta_{g})\theta_{j}^{o} + \zeta_{j+1}\theta_{j+1}^{o} + \zeta_{j-1}\theta_{j-1}^{o} + \zeta_{j+2}\theta_{j+2}^{o}$$
(A-44)

$$\Omega_{1}^{i} = (\zeta_{j} + \zeta_{g})\theta_{j}^{1} + \zeta_{j+1}\theta_{j+1}^{1} + \zeta_{j-1}\theta_{j-1}^{1} + \zeta_{j+2}\theta_{j+2}^{1} + \zeta_{melt}, \qquad (A-45)$$

and,

$$\zeta_{j} = \frac{W_{j}}{\left(T_{j+1} - T_{j}\right)} \left[2\dot{x}_{dc}^{i} + \frac{l_{j,j+1}W_{j+1}\dot{e}_{j+1}}{T_{j+1} - T_{j}} \right] - \frac{l_{j,j+1}W_{j}^{2}}{\rho_{j}V_{j}} \frac{\left(T_{dc}^{i} - T_{j+1}\right)\left(\beta + C_{j,j+1/2}\right)}{\left(T_{j+1} - T_{j}\right)^{2}} + \frac{l_{j,j+1}W_{j}W_{j+1}}{\rho_{j+1}V_{j-1}} \frac{\left(T_{j} - T_{dc}^{i}\right)}{\left(T_{j+1} - T_{j}\right)^{2}} C_{j+1,j-1/2}$$

$$\zeta_{j+1} = -\frac{W_{j+1}}{\left(T_{j+1} - T_{j}\right)} \left[2\dot{x}_{dc}^{i} + \frac{l_{j,j+1}W_{j}\dot{e}_{j}}{\left(T_{j+1} - T_{j}\right)} \right] + \frac{l_{j,j+1}W_{j}W_{j+1}}{\rho_{j}V_{j}} \frac{\left(T_{dc}^{i} - T_{j+1}\right)C_{j,j+1/2}}{\left(T_{j+1} - T_{j}\right)^{2}}$$
(A-46)

$$-\frac{l_{j,j+1}W_{j+1}^2}{\rho_{j+1}V_{j+1}} \frac{\left(T_j - T_{dc}^i\right)}{\left(T_{j+1} - T_j\right)^2} \left(C_{j+1,j-1/2} + C_{j+1,j+1/2}\right)$$
(A-47)

$$\zeta_{j-1} = \begin{cases} 0; & j = 1\\ 0; & j = 2 \text{ and } NBCINT \ge 4\\ \frac{l_{j,j+1}W_jW_{j-1}}{\rho_jV_j} \frac{(T_{dc}^i - T_{j+1})}{(T_{j+1} - T_j)^2} C_{j,j-\frac{1}{2}}; otherwise \end{cases}$$
(A-48)

$$\zeta_{j+2} = \frac{l_{j,j+1}W_{j+1}W_{j+2}}{\rho_{j+1}V_{j+1}} \frac{\left(T_j - T_{dc}^i\right)}{\left(T_{j+1} - T_j\right)^2} C_{j+1,j+1/2}$$
(A-49)

$$\beta = \begin{cases} h_{bot} \quad ; \ j = 1 \ and \ NBCINT = 1 \\ k_{cr}/\delta_{cr}; \ j = 1 \ and \ NBCINT = 2 \\ 0 \quad ; \ j = 1 \ and \ NBCINT = 3 \\ \bar{k}/n \quad ; \ j = 2 \ and \ NBCINT \ge 4 \\ C_{j,j-1/2} \quad ; \qquad otherwise \end{cases}$$
(A-50)

$$\zeta_{g} = \begin{cases} -\frac{l_{j,j+1}W_{j}^{2}}{\rho_{j}V_{j}} \frac{\left(T_{dc}^{i} - T_{j+1}\right)}{\left(T_{j+1} - T_{j}\right)^{2}} \frac{k_{cr}(T_{sol,cr} - T_{j})}{\delta_{cr}^{2}} d_{1}^{cr}; j = 1 \text{ and } NBCINT = 2\\ -\frac{l_{j,j+1}W_{j}^{2}}{\rho_{j}V_{j}} \frac{\left(T_{dc}^{i} - T_{j+1}\right)}{\left(T_{j+1} - T_{j}\right)^{2}} \frac{\bar{k}(T_{sol,st} - T_{j})}{\eta^{2}} d_{1}^{st}; j = 2 \text{ and } NBCINT \ge 4\\ 0; \qquad otherwise \end{cases}$$
(A-51)

$$\zeta_{melt} = \begin{cases} \frac{l_{j,j+1}W_j}{\rho_j V_j} (T_{dc}^i - T_{j+1}) h_{bot} W_{melt}; & j = 1 \text{ and } NBCINT = 1\\ -\frac{l_{j,j+1}W_j}{\rho_j V_j} \frac{(T_{dc}^i - T_{j+1})}{(T_{j+1} - T_j)^2} \frac{k_{cr}(T_{sol,cr} - T_j)}{\delta_{cr}^2} W_{melt} d_{melt}^{cr}; j = 1 \text{ and } NBCINT = 2\\ \frac{l_{j,j+1}W_j}{\rho_j V_j} \frac{(T_{dc}^i - T_{j+1})}{(T_{j+1} - T_j)^2} h_{bot} W_{melt}; & j = 1 \text{ and } NBCINT = 3\\ -\frac{l_{j,j+1}W_j}{\rho_j V_j} \frac{(T_{dc} - T_{j+1})}{(T_{j+1} - T_j)^2} \frac{(T_{sol,st} - T_j)}{\eta^2} W_{melt} d_{melt}^{st}; & j = 2 \text{ and } NBCINT \ge 4\\ 0; & otherwise \end{cases}$$

For the case in which the substrate is ablating and the dryout front lies between the first two nodes (j=1 and NBCINT \geq 4), the functional form of the dryout front velocity equation is found from Eq. 3-61 as

$$\dot{x}_{dc}^{i} = function(T_{2}, \eta[T_{2}, T], \dot{\eta}[\eta, T_{2}, T], \dot{e}_{2}[\eta, T_{2}, T_{3}])$$
(A-53)

The forward elimination coefficients are determined from this equation by taking the total derivative, which yields

$$\dot{x}_{dc})^{r+1} = \dot{x}_{dc}^{r} + \frac{\partial \dot{x}_{dc}}{\partial T_{2}} W_{2} \delta e_{2} + \frac{\partial \dot{x}_{dc}}{\partial \eta} \left(\frac{\partial \eta}{\partial T_{2}} W_{2} \delta e_{2} + \frac{\partial \eta}{\partial T} W_{melt} \delta e_{melt} \right) + \frac{\partial \dot{x}_{dc}}{\partial \dot{\eta}} \left(\frac{\partial \dot{\eta}}{\partial \eta} \frac{\partial \eta}{\partial T_{2}} W_{2} \delta e_{2} + \frac{\partial \dot{\eta}}{\partial \eta} \frac{\partial \eta}{\partial T} W_{melt} \delta e_{melt} + \frac{\partial \dot{\eta}}{\partial T_{2}} W_{2} \delta e_{2} + \frac{\partial \dot{\eta}}{\partial T} W_{melt} \delta e_{melt} \right)$$
(A-54)
$$+ \frac{\partial \dot{x}_{dc}}{\partial \dot{e}_{2}} \left(\frac{\partial \dot{e}_{2}}{\partial \eta} \frac{\partial \eta}{\partial T_{2}} W_{2} \delta e_{2} + \frac{\partial \dot{e}_{2}}{\partial \eta} \frac{\partial \eta}{\partial T} W_{melt} \delta e_{melt} + \frac{\partial \dot{e}_{2}}{\partial T_{2}} W_{2} \delta e_{2} + \frac{\partial \dot{e}_{2}}{\partial T_{3}} W_{3} \delta e_{3} \right)$$

Evaluation of the partial derivatives given in Eqs. 3-56 and 3-57 and substituting the resultant expressions into the above equation yields the following expressions for the forward elimination coefficients

$$\Omega_o = \zeta_2 \theta_2^0 + \zeta_3 \theta_3^0 \tag{A-55}$$

$$\Omega_1 = \zeta_2 \theta_2^1 + \zeta_3 \theta_3^1 + \zeta_{melt} \tag{A-56}$$

where

$$\zeta_{2} = \frac{\dot{x}_{dc}W_{2}}{\left(T_{sol,st} - T_{2}\right)} + \frac{W_{2}}{\left(T_{sol,st} - T_{2}\right)} \left[\dot{\eta} + \eta W_{2}\dot{e}_{2}\frac{\left(T_{sol,st} - T_{dc}^{i}\right)}{\left(T_{sol,st} - T_{2}\right)^{2}}\right] - \frac{1}{\rho_{2}V_{2}}\left(\frac{\bar{k}}{\eta} + C_{2,2+1/2}\right) \left(\frac{T_{sol,st} - T_{dc}^{i}}{T_{sol,st} - T_{2}}\right) \eta W_{2}^{2} + \left(\frac{T_{sol,st} - T_{dc}^{i}}{T_{sol,st} - T_{2}}\right) \left(\dot{e}_{2} - \frac{1}{\rho_{2}V_{2}}\frac{\bar{k}(T_{sol,st} - T_{2})}{\eta}\right) W_{2}^{2}d_{2}^{st} \quad (A-57) - \left(\frac{T_{dc}^{i} - T_{2}}{T_{sol,st} - T_{2}}\right) W_{2}f_{2}^{st} - \left(\frac{T_{dc}^{i} - T_{2}}{T_{sol,st} - T_{2}}\right) W_{2}f_{2}^{st} - \left(\frac{T_{sol,st} - T_{dc}^{i}}{T_{sol,st} - T_{2}}\right) W_{2}g_{2}^{st} - \left(\frac{T_{sol,st} - T_{dc}^{i}}{T_{sol,st} - T_{dc}^{i}}\right) W_{2}g_{2}^{st} - \left(\frac{T_{sol,st} - T_{dc}^{i}}{T_{sol,st} - T_{dc}^{i}}}\right) W_{2}g_{2}^{st} - \left(\frac{T_{sol,st} - T_{dc}^{i}}{T$$

$$\zeta_{melt} = W_2 W_{melt} \left(\frac{T_{sol,st} - T_{dc}^l}{T_{sol,st} - T_2} \right) \left(\dot{e}_2 - \bar{k} \frac{(T_{sol,st} - T_2)}{\eta \rho_2 V_2} \right) d_{melt}^{st} - \left(\frac{T_{dc}^l - T_2}{T_{sol,st} - T_2} \right) W_{melt} f_{melt}^{st}$$
(A-59)

Appendix B

DOCUMENTATION OF THERMOPHYSICAL PROPERTY SUBROUTINES

The objective of this Appendix is to document the thermophysical property subroutines that are incorporated into MELTSPREAD3. The subroutines that evaluate the melt properties are described first, followed by a description of the subroutines that evaluate the properties of concrete and steel. Finally, the subroutines that evaluate the properties of the water coolant/vapor and concrete decomposition gases are described. Except where otherwise noted, SI units (kilograms, meters, seconds, degrees Kelvin) are used in all of the subroutines.

MELT PROPERTY SUBROUTINES

Given the collapsed melt constituent heights and the bulk melt temperature, subroutine ETF within the code evaluates the melt specific enthalpy and derivative of temperature with respect to specific enthalpy. Conversely, given the melt specific enthalpy and the collapsed melt constituent heights, subroutine ETF evaluates the melt temperature and the derivative of temperature with respect to specific enthalpy. In these subroutines, the melt is assumed to consist of distinct oxide and metal phases, each of which is characterized by a solidus and liquidus temperature. The solidus and liquidus temperatures are required to be distinct, and the enthalpy of each phase is assumed to vary linearly between the solidus/liquidus values. The metal and oxide melt constituents currently modeled in MELTSPREAD3 were shown previously in Table 2-2.

For a given melt constituent below the solidus, a parabolic relationship between specific enthalpy and temperature is assumed,

$$e_i(T) = a_{sol,i} T^2 + b_{sol,i} T + c_{sol,i},$$
 (B-1)

where $a_{sol,i}$, $b_{sol,i}$, and $c_{sol,i}$ are the solid phase specific enthalpy coefficients. Above the liquidus, a linear relationship between melt specific enthalpy and temperature is assumed,

$$e_i(T) = b_{lia,i}T + c_{lia,i},\tag{B-2}$$

where $b_{liq,i}$ and $c_{liq,i}$ are the liquid phase specific enthalpy coefficients. The solid and liquid phase coefficients are summarized in Table B-1 for the various melt/concrete constituents currently modeled in MELTSPREAD3. These

coefficients are initialized in subroutine CPROPI. The constituents with indices 1-18 in Table B-1 are treated as components of concrete, while constituents with indices 8-28 are treated as components of melt and solidified debris. The overlap of constituents with indices 8-18 accounts for the fact that concrete decomposition products are incorporated into the melt during concrete ablation. The coefficients in Table B-1 have been defined such that specific enthalpy of the solid phase is equal to zero at a reference temperature of 298 K, with the exception of the decomposable concrete constituents $Ca(OH)_2$, $CaCO_3$, $CaMg(CO_3)_2$, Fe_2O_3 , and K_2O_2 . The solid phase coefficients for these constituents have been defined such that the molar specific enthalpy evaluated from Eq. B-1 equals the heat of formation from the oxides at the reference temperature of 298 K. The assumed heats of formation for the decomposable concrete constituents are shown in Table B-2. Condensed water in the concrete also undergoes evaporation at the saturation temperature corresponding to the system pressure. However, the condensed ("solid") phase coefficients for this constituent have been defined such that the molar specific enthalpy at 298 K equals zero, while the vapor ("liquid") phase coefficients have been defined such that the molar enthalpy at the saturation temperature (T_{lig,H_20}) equals the liquid phase enthalpy plus the latent heat of vaporization.

With the exception of the decomposable and evaporable concrete constituents, the liquid phase coefficients in Table B-1 have been defined such that the latent heat of fusion for a given melt constituent is given through the relationship,

$$\Delta e_{freeze,i} = e_i(T_{liq,i}) - e_i(T_{sol,i}) \tag{B-3}$$

where $T_{sol,i}$ and $T_{liq,i}$ are the constituent solidus/liquidus temperatures, which are taken equal to the solidus/liquidus for the particular (metal or oxide) phase of which the i-th melt constituent is a member.

Within the freezing temperature range, a linear relationship between the melt specific enthalpy and temperature is assumed,

$$e_i(T)c_{freeze,i} + b_{freeze,i} T, \tag{B-4}$$

where

$$c_{freeze,i} = e_i (T_{sol,i}) - T_{sol,i} \frac{\Delta e_{freeze,i}}{T_{liq,i} - T_{sol,i}},$$
(B-5)

$$b_{freeze,i} = \frac{\Delta e_{freeze,i}}{T_{liq,i} - T_{sol,i}} \,. \tag{B-6}$$

Index	Constituent	$a_{sol} \cdot 10^3$	b _{sol}	$c_{sol} \cdot 10^{-4}$	b _{liq}	c _{lia} 10 ⁻⁴	Reference
		$(J/mol \cdot K^2)$	(J/mol·K)	(J/mol)	(J/mol·K)	(J/mol)	No.
1	Ca(0H) ₂	12.37	90.61	-13.75	0.00	0.00	81
2	CaCO ₃	16.79	88.73	-20.57	0.00	0.00	81
3	$MgCa(CO_3)_2$	45.31	142.5	-74.38	0.00	0.00	81
4	H ₂ O,liq	18.56	62.80	-2.051	0.00	0.00	82
5	H ₂ O, vap	0.00	0.00	footnote ¹	0.00	footnote1	82
6	K ₂ O,sol	20.94	72.14	-38.65	0.00	0.00	81
7	К ₂ 0, vap	0.00	0.00	0.00	0.00	footnote ²	81
8	Na ₂ O	-2.452	106.5	-3.152	104.6	1.402	81
9	TiO ₂	2.717	67.5	-2.041	100.4	-1.093	83
10	SiO ₂	5.312	57.92	-1.773	85.77	-4.225	81
11	CaO	2.843	47.11	-1.429	62.76	4.331	81
12	MgO	2.533	44.85	-1.359	60.67	3.807	81
13	Al_2O_3	6.587	108.3	-3.287	192.5	-8.202	83
14	FeO	4.719	49.32	-1.512	68.20	0.939	81
15	Fe_2O_3	1.444	140.4	-12.19	142.3	3.915	81
16	Fe_3O_4	0.0	203.4	-6.060	213.4	5.872	81
17	Fe	2.481	33.58	-1.023	46.02	-1.082	84
18	Cr	7.696	17.84	-0.600	39.33	0.075	84
19	Ni	2.036	29.16	-0.888	43.10	-0.938	84
20	Zr	0.00	33.07	-0.989	33.47	0.618	84
21	U	0.00	44.34	-1.322	47.91	-0.971	84
22	B_4C	13.28	84.74	-2.645	136.0	3.749	83
23	В	3.409	17.08	-0.539	31.38	2.995	84
24	Cr_2O_3	5.467	115.1	-3.480	156.9	2.312	83
25	NiO	3.922	48.15	-1.469	59.87	2.948	81, 85, 86
26	<i>U0</i> ₂	18.17	40.90	-0.808	130.9	-3.091	87
27	ZrO_2	0.00	85.48	-2.549	100.4	1.713	88
28	B_2O_3	42.89	44.68	-1.713	129.7	-3.212	83

Table B-1 SUMMARY OF SOLIDUS/LIQUIDUS SPECIFIC ENTHALPY COEFFICIENTS FOR THE MELT/CONCRETE CONSTITUENTS TREATED IN MELTSPREAD3

 $\frac{1}{c} = a_{sol,H_20,liq} (T_{liq,H_20})^2 + b_{sol,H_20,liq} T_{liq,H_20} + c_{sol,H_20,liq} + 8.534 \cdot 10^{-2} (T_{liq,H_20})^2 + 13.645 T_{liq,H_20} + 4.752 \cdot 10^4$ $\frac{1}{c} c = a_{sol,K_20,liq} (T_{caco_3,liq})^2 + b_{sol,K_20,sol} T_{caco_3,liq} + c_{sol,K_20,sol}$

Decomposition Reaction	Heat of Formation from the Oxides (kJ/mole)	Reference
$CaMg(CO_3)_2 \rightarrow CaO + MgO = 2 CO_2$	-697.26	81
$CoCO_3 \rightarrow CaO + CO_2$	-177.82	71
$Ca(OH)_2 \rightarrow CaO + H_2O$	-109.45	81
$K_2O, sol \rightarrow K_2 + 1/2 O_2$	-363.17	81
$Fe_2O_3 \rightarrow 2/3 \ Fe_3O_4 + 1/6 \ O_2$	-79.7	81

 Table B-2
 HEAT OF FORMATION FROM THE OXIDES FOR THE VARIOUS CONCRETE DECOMPOSITION REACTION TREATED IN MELTSPREAD3

Given the melt temperature, the melt specific enthalpy is then evaluated in subroutine ETF through the following expression:

$$e(T) = AT^2 + BT + C$$
, (B-7)

where

$$A = \frac{1}{\bar{M}} \sum_{i} x_i \ a_i, \tag{B-8}$$

$$B = \frac{1}{\bar{M}} \sum_{i} x_i \ b, \tag{B-9}$$

$$C = \frac{1}{\overline{M}} \sum_{i} x_i \ c_i, \tag{B-10}$$

$$x_i = \frac{\frac{h_i \rho_i}{M_i}}{\sum i \frac{h_i \rho_i}{M_i}}, \qquad (B-11)$$

$$\overline{M} = \sum X_i M_i, \tag{B-12}$$

and

 x_i = mole fraction of i-th melt constituent,

 ρ_i = density of i-th melt constituent,

 h_i = collapsed height of i-th melt constituent,

 M_i = molecular weight of i-th melt constituent,

And finally a_i , b_i and c_i are the melt specific enthalpy coefficients that are defined relative to the melt freezing temperature ranges as

$$a_{i} = \begin{cases} a_{sol,i}; & T \leq T_{sol,i} \\ 0; & T_{sol,i} < T < T_{liq,i} \\ a_{liq,i}; & T \geq T_{liq,i} \end{cases}$$
(B-13)

$$b_{i} = \begin{cases} b_{sol,i}; & T \leq T_{sol,i} \\ b_{freeze,i}; & T_{sol,i} < T < T_{liq,i} \\ b_{liq,i}; & T \geq T_{liq,i} \end{cases}$$
(B-14)

$$c_{i} = \begin{cases} c_{sol,i}; & T \leq T_{sol,i} \\ c_{freeze,i}; & T_{sol,i} < T < T_{liq,i} \\ c_{liq,i}; & T \geq T_{liq,i} \end{cases}$$
(B-15)

The derivative of melt temperature with respect to specific enthalpy is then evaluated through the differentiated form of Eq. B-7, viz.,

$$\frac{dT}{de} = \frac{1}{2AT+B}.$$
(B-16)

Given the specific enthalpy, subroutine TEF evaluates the melt temperature. This is accomplished by first calculating the specific enthalpy at the solidus and liquidus for both the metal and oxide phases of the melt with Eqs. B-7 through B-15 (i.e., four enthalpy temperature points are determined). Given the enthalpies at the solidus and liquidus, the coefficients in Eq. B-7 are evaluated with Eqs. B-8 through B-12, in conjunction with the following expressions which are revised forms of Eqs. B-13 through B-15,

$$a_{i} = \begin{cases} a_{sol,i}; & e \le e_{sol,i} \\ 0; e_{sol,i} < e < e_{liq,i} \\ a_{liq,i}; & e \ge e_{liq,i} \end{cases}$$
(B-17)

$$b_{i} = \begin{cases} b_{sol,i}; & e \le e_{sol,i} \\ b_{freeze,i}; e_{sol,i} < e < e_{liq,i} \\ b_{liq,i}; & e \ge e_{liq,i} \end{cases}$$
(B-18)

$$c_{i} = \begin{cases} c_{sol,i}; & e \leq e_{sol,i} \\ c_{freeze,i}; e_{sol,i} < e < e_{liq,i} \\ c_{liq,i}; & e \geq e_{liq,i} \end{cases}$$
(B-19)

With the coefficients of Eq. B-7 determined, the melt temperature as a function of enthalpy is found by inverting Eq. B-7 to obtain, for the case in which A=0,

$$T = \frac{e-C}{B}, \qquad (B-20)$$

and for the case in which $A \neq 0$,

$$T = \frac{1}{2} \frac{B}{A} + \sqrt{\frac{B^2}{4A^2} - \frac{(C-E)}{A}} .$$
 (B-21)

Given the melt temperature from Eq. B-20 or B-21, the derivative of temperature with respect to specific enthalpy is then found from Eq. B-16.

Given the collapsed melt constituent heights and the melt temperature, the melt thermal conductivity is evaluated through subroutine CONDF. In this subroutine, the melt is assumed to consist of distinct oxide and metal phases, each of which is characterized by a solidus and liquidus temperature. The metal and oxide phase thermal conductivities are evaluated through the support subroutines CONDM and CONDO, respectively, which are called by subroutine CONDF. For a given melt constituent, the thermal conductivity is evaluated through an expression of the form,

$$k_{i} = \sum_{j=0}^{6} C_{j}^{i} (T_{R}^{i})^{j}, \qquad (B-22)$$

where C_j^i , j=0,..., 6, are the thermal conductivity coefficients for the i-th melt constituent and T_R^i is the normalized melt temperature. The normalized temperature and conductivity coefficients are defined in Tables B-3 and B-4 for the melt metal and oxide phase constituents, respectively. For the metal phase below the solidus temperature, the effective thermal conductivity is evaluated through a volume weighting based on the conductivities of the individual melt constituents,

$$k_m = \sum_{metals} V_i k_i, \tag{B-23}$$

where

$$V_i = \frac{h_i}{\sum_{metals} h_i}, \qquad (B-24)$$

and k_i is given through Eq. B-22. Note that the sum on i in Eqs. B-23 and B-24 is over the metal phase constituents of the melt. Above the metal phase liquidus, the effective thermal conductivity is approximated as a constant, and is evaluated through the expression,

$$k_{liq,m} = \frac{k_{sol,m}}{\beta_m},\tag{B-25}$$

where $k_{sol,m} = k_m(T_{sol,m})$ denotes the metal phase conductivity evaluated at the metal solidus temperature through Eq. B-23, and β_m is a constant which is currently taken equal to 1.6. As discussed in Reference [89], this ratio is appropriate for metals such as iron which immediately below the solidus has a crystalline structure in which each atom has eight nearest neighbors. When the melt temperature lies between the metal phase solidus and liquidus, the thermal conductivity is evaluated using the parallel conductance model proposed by Weiner,^[90] assuming a linear relationship between melt temperature and liquid fraction within the freezing transition,

$$k_m = \frac{1}{\frac{1-\emptyset_m}{k_{Sol,m}} + \frac{\emptyset_m}{k_{liq,m}}},\tag{B-26}$$

where

$$\phi_m = \frac{T - T_{sol,m}}{T_{liq,m} - T_{sol,m}}; T_{sol,m} \le T \le T_{liq,m}, \tag{B-27}$$

Metal Phase Constituent	Definition of T _R	Co	<i>C</i> ₁	<i>C</i> ₂	<i>C</i> 3	C4	C 5	C 6	Reference
Stainless (Fe, Cr, Ni)	$\frac{1700 \cdot T}{T_{sol,m}}$	8.116	$1.618 \cdot 10^{-2}$						91
Zr	$\frac{2098 \cdot T}{T_{sol,m}}$	7.510	$2.090 \cdot 10^{-2}$	$1.450 \cdot 10^{-5}$	$7.670 \cdot 10^{-9}$				92
U	$\frac{1405 \cdot T}{T_{sol,m}}$	21.64	$1.859 \cdot 10^{-2}$	3.539·10 ⁻⁶					92
B ₄ C	$\frac{2743 \cdot T}{T_{sol,m}}$	65.51	$1.625 \cdot 10^{-1}$	$2.289 \cdot 10^{-4}$	$1.786 \cdot 10^{-7}$	7.892·10 ⁻¹¹	$1.833 \cdot 10^{-14}$	$1.736 \cdot 10^{-18}$	92

Table B-3 METAL PHASE CONSTITUENTS FOR THERMAL CONDUCTIVITY BELOW THE SOLIDUS

Table B-4 OXIDE PHASE CONSTITUENTS FOR THERMAL CONDUCTIVITY BELOW THE SOLIDUS

Oxide Phase Constituent	Definition of T _R	Co	<i>C</i> ₁	<i>C</i> ₂	C ₃	C4	C 5	<i>C</i> ₆	Reference
UO ₂	$\frac{3120 \cdot T}{T_{sol,o}}$	14.04	$2.315 \cdot 10^{-2}$	$2.076 \cdot 10^{-5}$	9.661·10 ⁻⁹	$1.797 \cdot 10^{-12}$	$1.101 \cdot 10^{-16}$	5.381.10 ⁻²⁰	931
Zr0 ₂	$\frac{2973 \cdot T}{T_{sol,o}}$	0.835	$1.810 \cdot 10^{-4}$						88
СаО	$\frac{2289 \cdot T}{T_{sol,o}}$	$2.619 \cdot 10^{-2}$	$2.209 \cdot 10^{-1}$	$1.108 \cdot 10^{-3}$	$2.433 \cdot 10^{-6}$	-2.731.10-9	$1.534 \cdot 10^{-12}$	$3.442 \cdot 10^{-16}$	94
MgO	$\frac{3098 \cdot T}{T_{sol,o}}$	$1.236 \cdot 10^{-2}$	$3.792 \cdot 10^{-1}$	$5.394 \cdot 10^{-4}$	4.150.10-7	$1.758 \cdot 10^{-10}$	$3.806 \cdot 10^{-14}$	$3.291 \cdot 10^{-18}$	94
SiO ₂	$\frac{1996 \cdot T}{T_{sol,o}}$	22.56	$1.042 \cdot 10^{-1}$	$2.278 \cdot 10^{-4}$	$2.354 \cdot 10^{-7}$	9.425.10-11			94
Fe_3O_4	$\frac{1870 \cdot T}{T_{sol,o}}$	4.14							94

¹ Polynomial curve fit to the exponential expression recommended by Brandt and Neuer^[93]

and $T_{sol,m}$ and $T_{liq,m}$ denote the metal phase solidus/liquidus temperatures, respectively.

For the melt oxide phase below the oxide solidus, the effective thermal conductivity is also evaluated through a volume weighting of the individual constituent conductivities,

$$k_o = \sum_{oxides} V_i \, k_i, \tag{B-28}$$

where

$$V_i = \frac{h_i}{\sum_{oxides} h_i},\tag{B-29}$$

and k_i is given through Eq. B-22. Above the oxide liquidus, the effective thermal conductivity is currently assumed to equal the thermal conductivity at the oxide solidus, i.e.,

$$k_{liq,o} = k_o (T_{sol,o}), \tag{B-30}$$

where $k_o(T_{sol,o})$ is evaluated through Eq. B-28.

Given the thermal conductivities of the metal and oxide phases, the effective mixture conductivity is evaluated as the weighted geometric mean of the metal/oxide phase conductivities using the correlation of Lichteneker,^[95]

$$k_{eff} = k_c^{V_c} k_d^{1-V_c} , (B-31)$$

where

 V_c = volume fraction of the continuous phase,

$$V_c = \begin{cases} V_m, V_m \ge 0.5, \\ V_o, V_m < 0.5, \end{cases}$$
(B-32)

 V_m = metal volume fraction in melt,

$$V_m = \frac{\sum_{metals} h_i}{\sum_i h_i} , \qquad (B-33)$$

 V_o = oxide volume fraction in melt,

$$V_o = \frac{\sum_{oxides} h_i}{\sum_i h_i} , \qquad (B-34)$$

$$k_c = \begin{cases} k_m, V_m \ge 0.5, \\ k_o, V_m < 0.5, \end{cases}$$
(B-35)

$$k_d = \begin{cases} k_o, V_m \ge 0.5, \\ k_m, V_m < 0.5, \end{cases}$$
(B-36)

Given the melt temperature and collapsed melt constituent heights, subroutine VISCF evaluates the bulk melt dynamic viscosity. In this subroutine, the melt is assumed to consist of distinct oxide and metal phases, each of which is characterized by a solidus and liquidus temperature. The solidus and liquidus temperatures are required to be distinct, and the solid fraction in each phase is assumed to vary linearly between the solidus and liquidus values. The oxide and metal liquid phase viscosities are evaluated using the Da Andrade formula^[89] at a melting temperature corresponding to the solidus for each phase. For the metal liquid phase, the viscosity is evaluated through the equation,

$$\mu_m(T) = 6.12 \cdot 10^{-5} \frac{\left(T_{sol,m}A_m\right)^{1/2}}{V_m^{2/3}} exp\left(\frac{Q_m}{RT} - \frac{Q_m}{RT_{sol,m}}\right),\tag{B-37}$$

where

 A_m = gram-atomic weight of metal phase

$$=\frac{10^{3}\cdot\sum_{metals}X_{i}M_{i}}{\sum_{metals}X_{i}},$$
(B-38)

 V_m = molar volume of metal phase in cm^3

$$=\frac{10^{6} \cdot \sum_{metals} X_{i} M_{i} / \rho_{i}}{\sum_{metals} X_{i}} , \qquad (B-39)$$

R = gas constant = 8.3143 J/(mol·K),

$$Q_m = 1.8033 \ T_{sol,m}^{1.348}. \tag{B-40}$$

Similarly, the oxide liquid phase viscosity is evaluated through the expression,

$$\mu_o(T) = 6.12 \cdot 10^{-5} \frac{\left(T_{sol,o}A_o\right)^{1/2}}{V_o^{2/3}} exp\left(\frac{Q_o}{RT_{ev}} - \frac{Q_o}{RT_{sol,o}}\right),\tag{B-41}$$

where

$$A_o = \frac{10^3 \cdot \sum_{oxides} X_i M_i}{\sum_{oxides} X_i} , \qquad (B-42)$$

$$V_o = \frac{10^6 \cdot \sum_{oxides} X_i M_i / \rho_i}{\sum_{oxides} X_i} , \qquad (B-43)$$

$$Q_o = 1.8033 \ T_{sol,o}^{1.348}. \tag{B-44}$$

$$T_{ev} = \begin{cases} T; T \ge T_{sol,o} \\ T_{sol,o}; T < T_{sol,o} \end{cases}$$
(B-45)

When the oxide phase contains an appreciable amount of silica (SiO_2) , the viscosity is increased substantially by the formation of bonded chains of SiO_4 tetrahedra.^[96] In this case, the viscosity of the liquid oxide phase is evaluated using the Shaw¹² model,^[96]

$$\mu_o(T) = \exp[s(10^4/T_{ev} - 1.5) - 6.40], \qquad (B-46)$$

where

$$s = \frac{(\sum_i X_i Y_i S_i) X_{SiO_2}}{\sum_i X_i Y_i (\sum_i X_i + X_{SiO_2})}, \qquad (B-47)$$

and the factors Y_i and S_i are provided in Table B-5. These factors are initialized in subroutine CPROPI. In subroutine VISCF, the actual oxide liquid phase viscosity, $\mu_o(T)$, is set equal to the larger of the two viscosities predicted by the De Andrade^[89] and Shaw viscosity^[96] models (i.e., Eqs. B-41 and B-46, respectively).

Table B-5 FACTORS EMPLOYED IN THE SHAW VISCOSITY METHODOLOGY^[96] FOR OXIDE MIXTURES CONTAINING SILICA

Index	Constituent ¹³	Y _i	S_i
9	TiO ₂	1.0	4.5
11	CaO	1.0	4.5
12	MgO	1.0	3.4
13	Al_2O_3	2.0	6.7
14	FeO	1.0	3.4
15	Fe_2O_3	2.0	3.4
24	Cr_2O_3	2.0	3.4
26	UO_2	1.0	4.5
27	ZrO_2	1.0	4.5

Given the above expressions for the temperature-dependent metal and oxide phase viscosities, the effective liquid-solid mixture viscosity is evaluated using either the expression proposed by Ishii and Zuber^[47] or by Ramacciotti et al.^[25] Implementation of the Ishii-Zuber model requires the specification of the liquid (continuous) and solid (dispersed) phase viscosities, as well as the total volume fraction of the liquid and solid phases in the melt. As described earlier, it is currently assumed that the liquid fraction of the metal varies linearly between

¹² The Shaw viscosity model has also been implemented in CORCON MOD2.^[97]

 $^{^{13}}$ Y_i and S_i are set equal to zero for any constituents not shown in the table.

the liquidus and solidus (i.e., see Eq. B-27). For the oxide phase, one user option is to assume that the solid fraction also varies linearly, i.e.,

$$\phi_o = \frac{T - T_{sol,o}}{T_{liq,o} - T_{sol,o}}; \ T_{sol,o} \le T \le T_{liq,o}, \tag{B-48}$$

A second user option is that the solid fraction can be input as a user-specified function of temperature; see Section 4. In either case, the total solid fraction in the melt is then given through the expression

$$V_{sol} = (1 - \phi_o)V_o + (1 - \phi_m)V_m, \tag{B-49}$$

where the overall melt metal and oxide fractions, V_m and V_o , are defined in Eqs. B-33 and B-34, respectively. The metal and oxide fractions in the solid phase are then evaluated through the expressions:

$$V_{sol,m} = \frac{(1 - \emptyset_m)V_m}{V_{sol}},\tag{B-50}$$

$$V_{sol,o} = \frac{(1 - \phi_o)V_o}{V_{sol}},$$
(B-51)

Similarly, the metal and oxide fractions in the liquid phase are given by:

$$V_{liq,m} = \frac{\phi_m V_m}{1 - V_{sol}},\tag{B-52}$$

$$V_{liq,o} = \frac{\phi_o V_o}{1 - V_{sol}},\tag{B-53}$$

Given the above expressions, the continuous and dispersed phase viscosities are can then be calculated as,

$$\mu_c = V_{liq,m} \,\mu_m(T) + V_{liq,o} \,\mu_o(T), \tag{B-54}$$

$$\mu_{d} = V_{sol,m} \,\mu_{m}(T_{sol,m}) + V_{sol,o} \,\mu_{o}(T_{sol,o}), \tag{B-55}$$

where $\mu_m(T)$ and $\mu_m(T_{sol,m})$ are evaluated from Eq. B-37, $\mu_o(T_{sol,o})$ is evaluated from Eq. B-41, and $\mu_o(T)$ is evaluated from the larger of Eqs. B-41 and B-46. Given the viscosities of the continuous and dispersed phases, one user option for evaluating the effective liquid/solid mixture viscosity is to use the Ishii-Zuber^[47] correlation:

$$\mu = \mu_c \left(1 - \frac{V_{sol}}{V_{sol,max}} \right)^{-2.5 \, V_{sol,max} \left(\frac{\mu_d + 0.4 \, \mu_c}{\mu_d + \mu_c} \right)},\tag{B-56}$$

where $V_{sol,max}$ is the maximum solid phase packing fraction which is a userdefined constant (See Table 4-1).

As noted, the second user option for evaluating the effective mixture viscosity is to use the correlation by Ramacciotti et al.;^[25] i.e.,

$$\mu = \mu_c e^{2.5C_R V_{sol}},\tag{B-57}$$

where C_R is a user-supplied empirical constant that depends upon experiment conditions and varies between 4 and $8^{[25]}$

Given the collapsed melt constituent heights, subroutine EMISF evaluates the effective radiative emissivity based on a volumetric weighting of the emissivities for the metal and oxide phases. Currently, the emissivities of the metal and oxide phases are treated as constants using the following representative values for iron^[91] and UO_2 ,^[87] respectively.

$$\varepsilon_m = 0.30,$$
 (B-58)

$$\varepsilon_o = 0.83. \tag{B-59}$$

The effective metal/oxide mixture emissivity is thus evaluated through the equation,

$$\varepsilon = V_m \,\varepsilon_m + V_o \,\varepsilon_o, \tag{B-60}$$

where V_m and V_o have been defined in Eqs. B-33 and B-34, respectively.

Given the collapsed melt constituent heights, subroutine TEN evaluates the effective melt surface tension based on a volumetric weighting of the surface tensions for the metal and oxide phases. Currently, the surface tensions of the metal and oxide phases are treated as constants using representative values suggested by Kao and Kazimi, ^[49]

$$\sigma_m = 1.73, \tag{B-61}$$

$$\sigma_o = 0.52.$$
 (B-62)

The effective metal/oxide mixture surface tension is thus evaluated through the equation,

$$\sigma = \sigma_m V_m + \sigma_o V_o, \tag{B-63}$$

where V_m and V_o are defined in Eqs. B-33 and B-34, respectively.
Given the local collapsed melt constituent heights, subroutines MASFRA and MASFRD¹⁴ evaluate the average melt density based on a volumetric weighting of the densities for the individual melt constituents. The assumed liquid and solid phase densities for the various melt constituents currently modeled in MELTSPREAD3 are shown in Table B-6. The average density of the metal/oxide mixture is calculated through the expression

$$\rho = \frac{\sum_{i} \rho_{i} h_{i}}{\sum_{i} h_{i}}.$$
 (B-64)

Table B-6	ASSUMED LIQUID AND SOLID PHASE DENSITIES FOR THE VARIOUS MELT CONSTITUENTS MODELED BY
	MELTSPREAD3

Index	Constituent	Solid Phase Density Reference		Solid Phase Density	Reference
		(kg/m^3)		(kg/m^3)	
1	<i>Ca</i> (<i>OH</i>) ₂	2240	42		
2	CaCO ₃	2710	42		
3	$MgCa(CO_3)_2$	2872	42		
4	H ₂ O, liq			997	71
5	H ₂ 0, vap				
6	K ₂ O,sol	2320	42	2320	footnote ¹⁵
7	К ₂ 0, vар				
8	Na ₂ O	2270	42	2270	footnote ⁴
9	TiO ₂	4260	42	4021	100
10	SiO ₂	2200	42	2130	100
11	Сао	3250	42	2879	100
12	MgO	3580	42	3144	100
13	Al_2O_3	3965	42	3741	100
14	FeO	5700	42	5329	100
15	Fe_2O_3	5240	42	4950	100
16	Fe_3O_4	5180	42	4725	100
17	Fe	7867	69	7010	99
18	Cr	7190	69	6280	69
19	Ni	8908	69	7770	99
20	Zr	6500	69	6060	99
21	U	19000	42	17905	100
22	B_4C	2520	42	2396	101
23	В	2370	42	2080	98
24	Cr_2O_3	5210	42	4942	100
25	NiO	6670	42	6043	100
26	UO_2	10970	58	8739	87
27	ZrO ₂	5991	59	5800	100
28	$B_2 O_3$	1812	42	1812	footnote ⁴

¹⁴ Subroutines MASFRA and MASFRD perform essentially the same function, with the exception that MASFRA evaluates the density based on a column from a 2-D array, while subroutine MASFRD evaluates the density based on a column from 3-D array.

¹⁵ Data not available; liquid phase density assumed equal to solid phase density.

CONCRETE PROPERTY SUBROUTINES

The property subroutines in MELTSPREAD3 that evaluate the enthalpytemperature relationship for concrete implicitly account for the decomposition enthalpies associated with the generation of noncondensable gases. The concrete decomposition reactions currently modeled in MELTSPREAD3 are summarized in Tables 2-5 and B-2. The chemical composition of concrete is normally given in terms of stable binary metal oxides which reflect the actual elemental composition of the concrete. (See Tables 2-6 through 2-8). However, as shown in Table B-2, the actual mineral composition of the concrete is required to mechanistically calculate the release of H_2O and CO_2 gases. The user-specified concrete composition in terms of the stable binary oxides is converted to the corresponding mineral composition in the initialization subroutine CPROPI. The conversion methodology^[102] is described below.

Water is assumed to be present in concrete in two forms: (i) free water, and (ii) bound water, principally in the form of calcium hydroxide, $Ca(OH)_2$. Bound water is assumed to be present at a level of 2 wt%, which is based on an equation developed by Harmathy.^[103] The balance of the H_2O is assumed to be in the form of condensed phase free water. Carbon dioxide is assumed to be present as dolomite, $MgCa(CO_3)_2$, and calcium carbonate, $CaCO_3$. Dolomite is taken to be the principal carbonate form; the mole % of this constituent in the concrete is set equal to the minimum of the MgO and CaO mole %'s after accounting for the CaO that has been allotted to $Ca(OH)_2$. If any CO_2 remains after the formation of dolomite, it is assumed to be present in the form of calcium carbonate. The mineral compositions of the default concretes (see Table 2-6 through 2-8) evaluated using the above approach are shown in Tables B-7 and B-8.

Given the initial concrete temperature, subroutine ETC evaluates the initial concrete specific enthalpy and the derivative of the temperature with respect to specific enthalpy. Conversely, given the specific enthalpy and the initial mineral composition, subroutine TEC evaluates the concrete temperature and the derivative of temperature with respect to specific enthalpy. Subroutine TEC also monitors and stores the maximum specific enthalpy attained in the concrete such that the correct degassing rate is predicted on reheating of concrete which has cooled down following onset of decomposition.

Each of the principal decomposition reactions shown in Table 2-5 is assumed to be characterized by distinct, user specified, "solidus" and "liquidus" temperatures (i.e., the temperatures at the inception and completion of the decomposition reaction, respectively). In addition to these principal decomposition processes, the decomposition temperatures for K_2O and Fe_2O_3 (see Table B-2) are assumed to correspond to the $CaCO_3$ decomposition and concrete ablation solidus/liquidus temperatures, respectively. The effective molar enthalpy for a given decomposition process is assumed to vary linearly between the reactant and product enthalpies evaluated at the decomposition inception and completion temperatures, respectively. For example, the effective reactant/product molar enthalpy within the $CaCO_3$ decomposition temperature range expressed as:

$$e_{CaCO_3} = Y_{CaCO_3} e_{sol,CaCO_3}(T) + Z_{CaCO_3} e_{sol,CaO}(T),$$
(B-65)

		Mole % Constituent in Concrete:					
Index	Constituent	Limestone/Common	Siliceous	Limestone/Limestone			
		Sand					
1	$Ca(OH)_2$	8.85	6.29	9.46			
2	CaCO ₃	0.72	0.00	33.41			
3	$MgCa(CO_3)_2$	19.38	0.64	15.42			
4	H ₂ O,liq	9.29	7.72	11.59			
5	H ₂ 0, vap	9.29	7.72	11.59			
6	K ₂ O, sol	0.51	0.84	0.36			
7	К ₂ 0, vap	0.00	0.00	0.00			
8	Na ₂ O	1.41	0.64	0.00			
9	TiO ₂	0.14	0.57	0.10			
10	SiO ₂	38.21	65.74	9.93			
11	Сао	8.57	6.91	6.11			
12	MgO	0.00	0.34	0.00			
13	Al_2O_3	2.81	2.22	1.59			
14	FeO	0.00	0.00	0.00			
15	Fe_2O_3	0.80	0.35	0.43			
16	Fe_3O_4	0.00	0.00	0.00			
17	Fe	0.00	0.00	0.00			
18	Cr	0.00	0.00	0.00			

Table B-7 MINERAL COMPOSITION OF DEFAULT CONCRETES

Table B-8 THE BREAKDOWN OF CaO, MgO, H_2O , and CO_2 INTO DOLOMITE, CALCIUM CARBONATE, CALCIUM HYDROXIDE, AND FREE WATER FOR DEFAULT CONCRETES

Constituent	Weight % Constituent in Concrete:					
	Limestone/Common Sand	Siliceous	Limestone/Limestone			
H ₂ 0	4.29	5.04	5.03			
Ca(OH) ₂	8.40	8.44	8.43			
CaCO ₃	0.93	0.00	19.78			
$MgCa(CO_3)_2$	45.79	2.15	34.24			

where

$$Y_{CaCO_{3}} = \begin{cases} 1; \ e_{max} \leq e(T_{in,CaCO_{3}}), \\ \frac{e(T_{CP,CaCO_{3}}) - e_{max}}{e(T_{CP,CaCO_{3}}) - e(T_{in,CaCO_{3}})}; \ e(T_{in,CaCO_{3}}) < e_{max} < e(T_{CP,CaCO_{3}}), \\ 0; \ e_{max} \geq e(T_{CP,CaCO_{3}}), \end{cases}$$
(B-66)

$$Z_{CaCO_3} = 1 - Y_{CaCO_3} \tag{B-67}$$

$$T_{in,CaCO_3} = \text{temperature at the inception of } CaCO_3 \text{ decomposition,}$$

$$T_{CP,CaCO_3} = \text{temperature at completion of } CaCO_3 \text{ decomposition,}$$

$$e(T_{in,CaCO_3}) = \text{concrete specific enthalpy at the inception of } CaCO_3 \text{ decomposition,}$$

$$e(T_{CP,CaCO_3}) = \text{concrete specific enthalpy at completion of } CaCO_3 \text{ decomposition,}$$

$$e_{max} = \text{maximum enthalpy attained by the concrete over the course of the calculation.}$$

and the $CaCO_3$ and CaO solid phase molar specific enthalpies, $e_{sol,CaCO_3}$ and $e_{sol,CaO}$, are evaluated from Eq. B-1. The evaluation of the concrete specific enthalpy at inception and completion of the calcium carbonate decomposition process (i.e., $e(T_{in,CaCO_3})$ and $e(T_{CP,CaCO_3})$, respectively) is described below. Note that similar expressions apply to the decomposition of $Ca(OH)_2, H_2O$ and K_2O . For dolomite, the reactant/product molar enthalpy within the decomposition temperature range is written as:

$$e_{CaMg(CO_3)_2} = Y_{CaMg(CO_3)_2} e_{sol,CaMg(CO_3)_2} + Z_{CaMg(CO_3)_2} (e_{sol,CaO} + e_{sol,MgO})$$
(B-68)

where $Y_{CaMg(CO_3)_2}$ and $Z_{CaMg(CO_3)_2}$ are defined in the same manner as Y_{CaCO_3} and Z_{CaCO_3} (see Eqs. B-66 and B-67). With the above expressions, the coefficients of the general concrete enthalpy-temperature relationship, Eq. B-7, are written as:

$$A = \frac{1}{\overline{M}} \sum_{i} \overline{X}_{i} \ a_{i}, \tag{B-69}$$

$$B = \frac{1}{\overline{M}} \sum_{i} \overline{X}_{i} \ b_{i}, \tag{B-70}$$

$$C = \frac{1}{\overline{M}} \sum_{i} \overline{X}_{i} c_{i}, \tag{B-71}$$

$$\overline{M} = \sum_{i} \overline{X}_{i} \ M_{i}, \tag{B-72}$$

$$\bar{X}_{i} = \begin{cases} X_{i} Y_{i}; & i = CaCO_{3}, Ca(OH)_{2}, CaMg(CO_{3})_{2}, K_{2}O, sol, H_{2}O, liq, \\ X_{i} + X_{CaCO_{3}} Z_{CaCO_{3}} + X_{CaMg(CO_{3})_{2}} Z_{CaMg(CO_{3})_{2}} + X_{Ca(OH)_{2}} Z_{Ca(OH)_{2}}; i = CaO, \\ X_{i} + X_{CaMg(CO_{3})_{2}} Z_{CaMg(CO_{3})_{2}}; & i = MgO, \\ X_{i} + X_{K_{2}O,sol} Z_{CaCO_{3}}; & i = K_{2}O, vap, \\ X_{i} + X_{H_{2}O,liq} Z_{H_{2}O,liq}; & i = H_{2}O, vap, \end{cases}$$
(B-73)

and

 X_i = initial mineral composition of the concrete.

Given the above set of equations, the concrete specific enthalpy-temperature relationship is completely determined once the specific enthalpies at inception and completion of the various concrete decomposition processes are specified in Eq. B-66. The concrete decomposition enthalpies are initialized in subroutine CPROPI. For example, the concrete specific enthalpy at inception of free water release, $e(T_{in,H_20})$, is found by setting $T=T_{in,H_20}$ in Eq. B-7; the coefficients A, B, and C are evaluated from Eqs. B-69 through B-72 by setting $Y_i = 1$ for all decomposition reactions. Similarly, the specific enthalpy at completion of free water release is found by setting $T = T_{CP,H_20}$ in Eq. B-7; the enthalpy coefficients are evaluated from Eqs. B-69 through B-73 by setting $Y_{H_20} = 0$ with $Y_{CaCO_3} = Y_{Ca(OH)_2} = Y_{CaMg(CO_3)_2} = Y_{K_20} = 1$. Similar reasoning is used to evaluate the specific enthalpies at dryout of $Ca(OH)_2$, $CaMg(CO_3)_2$, and $CaCO_3$, in addition to the concrete solidus/liquidus specific enthalpies.

Given the initial concrete temperature, subroutine ETC evaluates the initial concrete specific enthalpy and the derivative of temperature with respect to specific enthalpy through Eqs. B-7 and B-16, respectively, assuming that the initial temperature lies below the value at which free water is released (i.e., Y_i is set equal to one for all concrete decomposition reactions in Eqs. B-69 through Conversely, given the current concrete specific enthalpy and the B-73). maximum specific enthalpy which has been attained over the course of the calculation, e_{max} , subroutine TEC evaluates the concrete temperature through Eqs. B-20, B-21, and Eqs. B-65 through B-73. If the current concrete specific enthalpy lies below e_{max} , then decomposition reactions are not occurring and the derivative of temperature with respect to enthalpy is evaluated directly from If the current specific enthalpy meets or exceeds e_{max} , then Eq. B-16. decomposition reactions are occurring and the derivative of temperature with respect to specific enthalpy is evaluated from the differentiated form of Eq. B-7, viz.,

$$\frac{dT}{de} = \left(1 - \dot{A}T^2 - \dot{B}T - \dot{C}\right)(2AT + B)^{-1},\tag{B-74}$$

where () denotes a derivative with respect to specific enthalpy and:

$$\dot{A} = \frac{1}{\bar{M}} \sum_{i} \dot{\bar{x}} a_{i}, \tag{B-75}$$

$$\dot{B} = \frac{1}{\bar{M}} \sum_{i} \dot{\bar{x}} b_{i}, \qquad (B-76)$$

$$\dot{C} = \frac{1}{\bar{M}} \sum_{i} \dot{\bar{x}} c_i, \tag{B-77}$$

$$\dot{\bar{x}} = \begin{cases} X_i \dot{Y}_i; & i = CaCO_3, Ca(OH)_2, CaMg(CO_3)_2, K_2O, sol, H_2O, liq, \\ -X_{CaCO_3} \dot{Y}_{CaCO_3} - X_{CaMg(CO_3)_2} \dot{Y}_{CaMg(CO_3)_2} - X_{Ca(OH)_2} \dot{Y}_{Ca(OH)_2}; & i = CaO, \\ -X_{CaMg(CO_3)_2} \dot{Y}_{CaMg(CO_3)_2}; & i = MgO, \\ -X_{K_2O,sol} \dot{Y}_{CaCO_3}; & i = K_2O, vap, \\ -X_{H_2O,liq} \dot{Y}_{H_2O,liq}; & i = H_2O, vap, \end{cases}$$
(B-78)

and, for example,

$$\dot{Y}_{CaCO_3} = \frac{-1}{e(T_{CP,CaCO_3}) - e(T_{in,CaCO_3})}.$$
(B-79)

In addition to evaluating the local concrete temperature, subroutine TEC also calculates the relative concrete density given the maximum specific enthalpy attained by the concrete over the course of the calculation. The ratio of the current concrete density to the initial value is evaluated as,

$$R = \frac{\rho(e_{max})}{\rho_o} = \frac{\sum_i \bar{X}_i M_i}{\sum_i X_i M_i},\tag{B-80}$$

where

 ρ_o = initial concrete density.

Given the initial mineral composition of the concrete, subroutines DENSC evaluates the initial concrete density based on a molar average, i.e.,

$$\rho_o = \frac{\sum_i X_i M_i}{\sum_i \frac{X_i M_i}{\rho_i}}.$$
(B-81)

Given the concrete temperature and composition, subroutine CONDC evaluates the concrete thermal conductivity. For the default limestone/common sand and siliceous concretes (See Tables 2-6, 2-7, and B-7), as well as user-specified concrete compositions (see Section 4), the thermal conductivity is evaluated through the following polynomial curve fit to the basalt concrete data of Baker et. al., ^[104]

$$k = -21.79 + 2.102 \cdot 10^{-1} T - 7.243 \cdot 10^{-4} T^2 + 1.245 \cdot 10^{-6} T^3$$

-1.139 \cdot 10^{-9} T^4 + 5.299 \cdot 10^{-13} T^5 - 9.871 \cdot 10^{-17} T^6 (B-82)

For default limestone/limestone concrete (See Tables 2-8 and B-7), the thermal conductivity is evaluated through the following polynomial curve fit to the limestone concrete data of Baker et. al., ^[104]

$$k = -76.32 + 7.925 \cdot 10^{-1} T - 3.115 \cdot 10^{-3} T^{2} + 6.199 \cdot 10^{-6} T^{3} + 6.668 \cdot 10^{-9} T^{4} + 3.701 \cdot 10^{-12} T^{5} - 8.325 \cdot 10^{-16} T^{6}.$$
 (B-83)

Given the concrete temperature and composition, subroutine EMISC is set up to evaluate the concrete radiative emissivity. The emissivity is currently assumed constant at a value of 0.83.

STEEL STRUCTURE PROPERTY SUBROUTINES

Given the wide range of steels which may be encountered in a given plant configuration, the steel properties are described mainly in terms of properties for pure iron. The properties for iron were taken from Reference [91] with the following exceptions: (i) the liquid iron density was taken from Reference [99], and (ii) the thermal conductivity below the iron Curie temperature (1043 K) was taken equal to that recommended in Reference [105] for a representative 1.0% Mn, 0.5% Mo, 0.5% Ni medium carbon, low alloy steel. The resulting thermal conductivity is about 50% that of pure iron at room temperature and rises to ~90% of the iron value near the Curie temperature. The molten iron thermal conductivity at the liquidus was assumed to equal the value at the solidus divided by a factor of 1.6. As described earlier, this ratio^[89] is appropriate for a metal such as iron which immediately below the solidus has a crystal structure in which each atom has eight nearest neighbors.

Given the local steel temperature, subroutine ETSS evaluates the specific enthalpy and the derivative of temperature with respect to specific enthalpy. Conversely, given the steel specific enthalpy, subroutine TESS evaluates the temperature and the derivative of temperature with respect to enthalpy. In these subroutines, a linear relationship between specific enthalpy and temperature is assumed,

$$e = BT + C, \tag{B-84}$$

where

$$B = \begin{cases} \frac{e_{sol,s}}{T_{sol,s} - T_{ref}}; & T \leq T_{sol,s}, \\ \frac{e_{liq,s} - e_{sol,s}}{T_{liq,s} - T_{sol,s}}; & T_{sol,s} < T < T_{liq,s}, \\ C_{liq,s}; & T \geq T_{liq,s}. \end{cases}$$
(B-85)

$$C = \begin{cases} -\frac{T_{ref} e_{sol,s}}{T_{sol,s} - T_{ref}}; & T \leq T_{sol,s} \\ e_{sol,s} - \frac{(e_{liq,s} - e_{sol,s})T_{sol,s}}{T_{liq,s} - T_{sol,s}}; & T_{sol,s} < T < T_{liq,s}, \\ e_{liq,s} - C_{liq,s} & T_{liq,s}; & T \geq T_{liq,s}. \end{cases}$$
(B-86)

The nomenclature and assumed input data to Eqs. B-85 and B-86 are provided in Table B-9. Given the steel temperature, subroutine ETSS evaluates the specific enthalpy directly through Eqs. B-84, B-85, and B-86. The derivative of temperature with respect to enthalpy is then evaluated through Eq. B-16 with $A \equiv 0, i.e.,$

$$\frac{dT}{de} = \frac{1}{B}.$$
 (B-87)

Table B-9 ASSUMED PROPERTIES FOR STRUCTURAL STEEL

Property	Designation	Value
Solidus Temperature, K	T _{sol,s}	1810
Liquidus Temperature, K	$T_{liq,s}$	1811
Specific Enthalpy Reference Temperature, K	T _{ref}	298
Specific Enthalpy at Solidus, MJ/kg	e _{sol,s}	1.045
Specific Enthalpy at Liquidus, MJ/kg	e _{liq,s}	1.293
Specific Heat at Liquidus, J/(Kg·K)	$C_{liq,s}$	835

Given the specific enthalpy, subroutine TESS evaluates the temperature through Eq. B-20 in conjunction with the following expressions, which are revised versions of Eqs. B-85 and B-86,

$$B = \begin{cases} \frac{e_{sol,s}}{T_{sol,s} - T_{ref}}; & e \le e_{sol,s}, \\ \frac{e_{liq,s} - e_{sol,s}}{T_{liq,s} - T_{sol,s}}; & e_{sol,s} < T < T_{liq,s}, \\ C_{liq,s}; & e \ge e_{liq,s}. \end{cases}$$
(B-88)
$$C = \begin{cases} -\frac{T_{ref} e_{sol,s}}{T_{sol,s} - T_{ref}}; & e \le e_{sol,s}, \\ -\frac{(e_{liq,s} - e_{sol,s})T_{sol,s}}{T_{liq,s} - T_{sol,s}}; & e_{sol,s} < e < e_{liq,s}, \\ e_{liq,s} - C_{liq,s} T_{liq,s}; & e \ge e_{liq,s}. \end{cases}$$
(B-89)

Given the coefficient B through Eq. B-88, subroutine TESS then evaluates the derivative of temperature with respect to specific enthalpy through Eq. B-87.

Given the temperature, subroutines CONDSS evaluates the local steel thermal conductivity through the following series of expressions. For T < 477.59 K,

$$k = 41.19.$$
 (B-90)

For 477.59 K <u><</u> T < 1043 K,

 $k = 8.623 \cdot 10^{2} - 7.083 T + 2.504 \cdot 10^{-2} T^{2} - 4.630 \cdot 10^{-5} T^{3} + 4.718 \cdot 10^{-8} T^{4}$ $-2.515 \cdot 10^{-11} T^{5} + 5.478 \cdot 10^{-15} T^{6}.$ (B-91)

For 1043 K <u><</u> T < 1185 K,

For 1185 K < T < 1811 K,

$$k = 30.4 - 1.002 \cdot 10^{-2} \text{ (T-1185)}. \tag{B-93}$$

For T > 1811 K,

$$k = 24.13.$$
 (B-94)

Given the temperature, subroutines DENSS evaluates the local steel density through the following series of expressions. For T<1811 K (i.e., below the steel liquidus),

$$\rho = \frac{7867}{(1+1.0\cdot10^{-2}\,F_L)^3}\tag{B-95}$$

where, for T < 1185 K,

$$F_L = 9.0 \cdot 10^{-3} + 1.21 \cdot 10^{-3} (T - 300) + 6.504 \cdot 10^{-7} (T - 300)^2 - 3.140 \cdot 10^{-10} (T - 300)^3, \text{ (B-96)}$$

and for 1185 K <u><</u> T < 1811 K,

$$F_L = -1.7681 + 2.330 \cdot 10^{-3} T . \tag{B-97}$$

For $T \ge 1811$ K (i.e., above the steel liquidus),

$$\rho = 7010 - 8.342 \cdot 10^{-1} \left(T - 1811 \right). \tag{B-98}$$

WATER PROPERTY SUBROUTINES

Subroutine CONWAT evaluates the water coolant properties as a function of temperature and system pressure. The properties are evaluated using polynomial curve fits to the tabulated data found in several on-line sources.^[106-109] Given the system absolute pressure, the saturation temperature is evaluated from^[109]

$$T_{sat}[K] = \frac{5132.0}{13.766 - \log(P[bar])}$$
(B-99)

Given the saturation temperature (defined below as T for brevity), the thermal conductivity, density, specific heat, dynamic viscosity, specific enthalpy, and surface tension are respectively evaluated from the following curve fits to data provided in References [106-108]:

$$k = -0.5841 + 6.9066 \cdot 10^{-3}T - 1.0916 \cdot 10^{-5}T^2 + 4.000 \cdot 10^{-9}T^3$$
 (B-100)

$$\rho = 689.7904 + 2.6667 T - 6.5756 \cdot 10^{-3} T^2 + 3.6400 \cdot 10^{-6} T^3$$
(B-101)

$$C_P = 4481.727 - 1.4345 T + 6.6160 \cdot 10^{-4} T^2 + 2.9333 \cdot 10^{-6} T^3$$
 (B-102)

$$\mu = 10^{-6} (30032.04 - 216.82 T + 0.52811 T^2 - 4.3093 \cdot 10^{-4} T^3)$$
 (B-103)

$$e = 10^{3} (-1274.5669 + 5.4424T - 3.9744 \cdot 10^{-3} T^{2} + 4.1733 \cdot 10^{-6} T^{3})$$
 (B-104)

$$\sigma = 10^{-3}(82.0450 + 0.1261T - 6.5932 \cdot 10^{-4} T^2 + 4.1333 \cdot 10^{-7} T^3)$$
(B-105)

where as a reminder all units are SI. The water latent heat of vaporization is then calculated by taking the difference between the vapor (see Eq. B-119 below) and liquid (see Eq. B-104 above) phase specific enthalpies.

GAS PROPERTY SUBROUTINES

Given the gas temperature and system pressure, the water vapor and CO_2 gas properties are evaluated in subroutines CONH2O and CONCO2, respectively. Simple linear curve fits to the property data in Reference [110] are currently employed. For CO_2 gas, the expressions for the thermal conductivity, specific heat, and viscosity are of the form,

$$k = 1.657 \cdot 10^{-2} + 8.832 \cdot 10^{-5} (T - 300), \tag{B-106}$$

$$C_P = 1326.5,$$
 (B-107)

$$\mu = 1.496 \cdot 10^{-5} + 3.957 \cdot 10^{-8} (T - 300), \tag{B-108}$$

where T is in °K. For carbon monoxide in the range $300 \le T \le 600$ K,

$$k = 2.525 \cdot 10^{-2} + 6.4033 \cdot 10^{-5}(T - 300), \tag{B-109}$$

$$C_P = 1048.4,$$
 (B-110)

$$\mu = 1.7483 \cdot 10^{-5} + 3.919 \cdot 10^{-8} (T - 300), \tag{B-111}$$

For hydrogen in the range $300 \le T \le 1333$ K,

$$k = 0.182 + 3.853 \cdot 10^{-4} (T - 300), \tag{B-112}$$

$$C_P = 14,537.0$$
 (B-113)

$$\mu = 1.095 \cdot 10^{-4} + 1.1796 \cdot 10^{-6} (T - 300), \tag{B-114}$$

Finally the water vapor thermal conductivity, density, specific heat, specific enthalpy, and viscosity are evaluated along the saturation line for $300 \le T \le 443$ K from quadratic curve fits to data provided in References [111-112]:

$$k = 10^{-3}(-35.6212 + 0.403494T - 1.094794 \cdot 10^{-3}T^2 + 1.199994 \cdot 10^{-6}T^3)$$
(B-116)

$$\rho = -56.33799 + 0.53218 T - 1.68066 \cdot 10^{-3} T^2 + 1.77744 \cdot 10^{-6} T^3$$
 (B-117)

$$C_P = -817.0310 + 27.598 T - 9.6764 \cdot 10^{-2} T^2 + 1.1600 \cdot 10^{-4} T^3$$
 (B-118)

$$e = 10^{3} (2313.321 - 1.3080 T + 1.0590 \cdot 10^{-2} T^{2} - 1.200 \cdot 10^{-5} T^{3})$$
(B-119)

$$\mu = 10^{-6} (-0.36792 + 1.62815 \cdot 10^{-2} T + 7.70341 \cdot 10^{-5} T^2 - 8.39984 \cdot 10^{-8} T^3) \text{ (B-110)}$$

where in the above T denotes the saturation temperature that is evaluated from Eq. A-84.

The binary diffusion coefficients for H_2O/H_2 and CO_2/CO are evaluated in subroutine TTODAB using Hershfelder's correlation,^[44] which is defined in Eq. 2-17. The Lennard-Jones force constants for the various gases are, ^[43]

$$\sigma_{CO_2} = 3.941 \, \text{\AA}, \mathcal{E}_{CO_2} = 195.2 \, \text{K}, \tag{B-111}$$

$$\sigma_{CO} = 3.690 \, \dot{A}, \mathcal{E}_{CO} = 91.7 \, K, \tag{B-112}$$

$$\sigma_{H_20} = 2.641 \, \dot{A}, \mathcal{E}_{H_20} = 809.1 \, K, \tag{B-113}$$

$$\sigma_{H_2} = 2.827 \, \dot{A}, \, \mathcal{E}_{H_2} = 59.7 \, K. \tag{B-114}$$

The force constants for the binary gas mixtures are evaluated through the expressions,

$$\bar{\sigma} = \frac{1}{2}(\sigma_A + \sigma_B), \tag{B-115}$$

$$\mathcal{E} = (\mathcal{E}_A \, \mathcal{E}_B)^{1/2}.\tag{B-116}$$

The collision integrals are evaluated through polynomial curve fits to the tabulated data in Reference [43],

$$\Omega_{H_2}^{H_2 0} = 1.579 - .352 X + .0567 X^2 - .00317 X^3, \tag{B-117}$$

$$\Omega_{CO}^{CO_2} = 1.070 - .06267 X + .0039 X^2 - 8.70 \cdot 10^{-5} X^3$$
 (B-118)

where

$$X \equiv T/\mathcal{E},\tag{B-119}$$

and T is the temperature of the gas mixture in °K.

Appendix C

COMPILATION OF MELTSPREAD VALIDATION CALCULATIONS

This appendix presents the results of the various validation calculations that have been carried out with the beta version of MELTSPREAD3¹⁶. The matrix of calculations is shown in Table C-1, while the available information from each solution/experiment is shown in Table C-2. The validation database can be broken down into the following categories: i) analytical solutions, ii) simulant fluid isothermal spreading tests, iii) high temperature flow and freezing tests with simulant oxide melts, iv) high temperature flow and freezing tests using metallic melts, and v) reactor material melt spreading tests. The results are presented under these same generalized headings.

ANALYTICAL SOLUTIONS

As a starting point for the verification of the hydrodynamics modeling, the code was compared with the analytical solution for the one-dimensional dam break problem.^[27] Details for the input file assembled for this case are shown in Table C-3. Since this problem contains no heat transfer effects, the code was executed using the 'adiabatic' spreading option. Further, the analytical solution is based on inviscid flow theory, and so the 'inviscid flow' modeling option was also selected in which case the friction shear stress term in the momentum equation is set to zero.

The particular case that is modeled assumes a 20 m long, 15 cm wide channel that is initially filled with a 10 cm water depth over $\frac{1}{2}$ the channel length. At time t = 0, the 'dam' barrier is removed and the water is allowed to relocate under the influence of gravity. Computationally, this situation is modeled by pouring the water at a high flowrate into the nodes that cover the first half of the spreading channel to rapidly accumulating the 10 cm water depth.

According to simple gravity current theory,^[27] after short term transient effects have died away, the advancing front will achieve a depth equal to ¹/₂ the initial fluid depth, and (in an Eulerian coordinate system) the advancing and receding fronts will achieve a constant velocity that is given through the equation,

$$U = \frac{\sqrt{gd}}{2} \quad , \tag{C-1}$$

 $^{^{16}}$ The beta version corresponds to version 133 (i.e., test 133.f) in the MELTSPREAD developmental version archive library.

Program	Test or Case	Fluid	Substrate	Flow Geometry	Cavity Condition
N/A	1-D dam break solution	Water	Inert	1-D channel	N/A
	Run no. 1	Water	"	1/10 linear scale model of Mark-I containment	"
	Run no. 2	"	"	"	"
	WAT_Q1.5_G0	Water	"	Feedbox with 24 cm weir $\rightarrow 17^{\circ}$ sector	"
	WAT_Q0.5_G0	"	"	"	"
	HEC_3_G0_0.1ª	HECa	"	п	"
	HEC_3_G0_2ª	"	"	"	"
	3MDC-Ox-1	Oxide simulant ^b	Concrete	Feedbox \rightarrow 1-D channel	Dry
	3MDS-Ox-1	"	Steel	"	"
	3MDS-Ox-2	"	"	"	"
	2MWS-Ox-1	"	"	"	12 cm H ₂ O
	2MWS-Ox-2	"	"	п	"
	2MWS-Ox-3	"	"	"	"
		Iron	Ceramic	Feedbox \rightarrow 1-D channel	Dry
		Oxide simulant ^c	"	"	"
		Iron	Concrete	"	
		Oxide simulant ^c	"	"	"
		Iron	Ceramic	"	"
		Oxide simulant ^c	"	"	
	V1	Oxide simulant ^d	Ceramic	"	"
	1	"	Concrete	Feedbox \rightarrow 1-D channel \rightarrow 2-D floor	"
	2	"	"	"	"
	Test 15	Stainless steel	"	Cylindrical cavity with door $\rightarrow 180^{\circ}$ sector	"
	Test 21	"	"	"	7 cm H ₂ O
		Core oxides + iron	Concrete	Feedbox with 5 cm weir \rightarrow 1-D channel	Dry
		"	Ceramic	п	"
		"	Steel	"	"
		Core oxides	Concrete	"	"
		"	Ceramic	"	"
		"	Steel	"	"
	EU-4	Core oxides + iron	"	Feedbox with 5 cm weir \rightarrow 1-D channel \rightarrow 45° sector	"
	L-26S	"	"	Cylindrical cavity with 4 cm weir $\rightarrow 17^{\circ}$ sector	"
	L-32S	"	"	"	1 cm H ₂ O
		"	Concrete	Feedbox box with 0.5 cm weir \rightarrow 9.5° sector	Dry
		"	Ceramic	"	"

Table C-1 MELTSPREAD3 VALIDATION TEST MATRIX (35 cases in total)

^aHydroxyl ethyl cellulose; ^b30/70 wt% CaO/B₂O₃; ^c83/8.5/6/1.5/1 wt% Al₂O₃/ SiO₂/FeO/MgO/MnO; ^d41/24/19/16 wt% Al₂O₃/FeO/CaO/SiO₂

		Available Information						
Program	Case	Leading Edge vs. Time	Spreading Distance	Posttest Debris Profile	Sub. Ablation Profile	Sub. Thermal Response	Local Melt Temperatures	Local Melt Height
N/A	Dam break sol.	Х	N/A	N/A	N/A	N/A	N/A	X
	Run no. 1	Х	N/A	N/A	N/A	N/A	N/A	Х
	Run no. 2	Х	N/A	N/A	N/A	N/A	N/A	Х
	WAT_Q1.5_G0	Х	N/A	N/A	N/A	N/A	N/A	
	WAT_Q0.5_G0	Х	N/A	N/A	N/A	N/A	N/A	
	HEC_3_G0_0.1ª	Х	N/A	N/A	N/A	N/A	N/A	
	HEC_3_G0_2a	Х	N/A	N/A	N/A	N/A	N/A	
	3MDC-Ox-1	Х	Х	Х		Х		
	3MDS-Ox-1	Х	Х	Х				
	3MDS-Ox-2	Х	Х	Х				
	2MWS-Ox-1		Х					
	2MWS-Ox-2		Х					
	2MWS-Ox-3		Х					
		Х	Х	Х			Х	
		Х	Х	Х			Х	
		Х	Х	Х			Х	
		Х	Х	Х			Х	
		Х	Х	Х	Х		Х	
		Х	Х	Х			Х	
	V1	Х	Х	Х				
	1	Х	Х			Х		
	2	Х				Х	Х	
	Test 15		Х	Х				
	Test 21		Х	Х				
		Х	Х					
		Х	Х					
		Х	Х			Х		
		Х	Х					
		Х	Х					
		Х	Х					
	EU-7	Х	Х					
	L-26S	Х	Х	Х				
	L-32S	Х	Х	Х				
		Х	Х	Х		Х		
		Х	X	X		X		

Table C-2 OPEN LITERATURE VALIDATION TEST MATRIX DATA AVAILABILITY

where d is the initial fluid depth in the channel (10 cm). Thus, for the particular example under consideration, the advancing front should eventually achieve a constant velocity of 0.5 m/sec.

The calculated height distributions at various times are shown in Figure C-1, while leading edge location is shown in Figure C-2. As is evident from Figure C-1, the model slightly under-predicts (by ~ 10 %) the theoretical advancing front depth of 5 cm throughout the calculated time domain. In addition, examination of Figure C-2 indicates that the model reasonably predicts the location of the leading edge based on a spreading velocity of 0.5 m/sec. Thus, the results of this comparison indicate that the fluid mechanics algorithm in MELTSPREAD reasonably reproduces a simple analytical solution for the dam break problem.

Test parameter	Value
Test name	1-D Dam Break Problem
Fluid composition (wt %)	100 H ₂ O
Fluid delivery technique	Water assumed to be poured rapidly into the first 10 m of
5 1	the spreading channel to establish a uniform water depth
	of 10 cm over the first 10 meters
Total pour mass	150 kg
Spreading geometry	20 m long channel with a uniform width of 15 cm
Code input parameter(s)	Value(s)
Fluid composition (wt %)	100 H ₂ O
Fluid pour rate and duration	Uniform injection water at a flowrate of 300 kg/sec over a
	time interval of 0.5 seconds; injection flow spread
	uniformly over $\frac{1}{2}$ of the spreading channel to establish the
	initial 10 cm fluid depth.
Fluid material property evaluation ^a	User-specified property data used: ρ = 1000 kg/m ³ and σ =
	0.073 N-m
Heat transfer modeling	Flow is "adiabatic"
Fluid mechanics modeling	Flow is "inviscid"
Spreading cavity nodalization	20 m cavity length subdivided into 200 cells each with a
	width of 15 cm and a length of 10 cm. All nodes cell-
	centered.
Timestep	0.05 seconds

Table C-3 INPUT FILE DATA SHEET FOR 1-D DAM BREAK PROBLEM

^aAs is applicable, in this table and the tables that follow, c = specific heat, $\Delta h_f = \text{latent heat of fusion}$, $\rho = \text{density}$, k = thermal conductivity, $\mu_o = \text{viscosity at the liquidus}$, $\sigma = \text{surface tension}$, M = molecular weight, $\epsilon = \text{emissivity}$. Subscripts s and 1 denote solid and liquid phases, respectively.







Figure C-28 Comparison of leading edge locations for 1-D Dam Break Problem

SIMULANT FLUID ISOTHERMAL SPREADING TESTS

The code was also benchmarked against isothermal spreading tests to verify proper behavior before moving on to tests that involved heat transfer and freezing effects. Tests considered in this area include the water spreading tests of Theofanous et al.,^[6] in addition to the Corine program^[29] water and glycerol spreading tests.

Theofanous Water Spreading Tests

Theofanous et al.^[6] conducted water spreading tests in a 1/10 linear scale model of the Mark I BWR containment. Local depth versus time profiles were reported at four different positions within the apparatus: i) Position A, just inside the pedestal doorway to the drywell, ii) Position C, adjacent to the annulus directly across from the doorway, iii) Position D, in the annulus 90° from the doorway, and Position E, in the annulus 180° from the doorway. Two tests were conducted; Run 1 was considered to be a 'high flowrate' case simulating the flow at reactor scale of a 10 m³ pour volume at a flowrate of 6.5 m³/minute. Based on a scaling analysis in which the flow characteristics were preserved on the basis of conserving the Froude number, the corresponding flowrate at test scale was deduced to be 0.325 liters/second. The test characteristics, as well as code input information that was compiled to simulate Run No. 1, are described in Table C-4. A comparison of the predicted water leading edge penetration through the apparatus as a function of time is provided in Figure C-3, while local responses at Positions A, C, D, and E are compared with the data in Figures C-4 to C-7, respectively. Finally, local depth profiles throughout the apparatus at several different times are shown in Figure C-8. As is evident from these figures, calculations were carried out for two cases; i.e., both non-wetted and wetted (surface tension ~ 0) surfaces. Examination of the figures indicates that the wetted surface solution provides a better overall fit to the test data. The code seems to provide a reasonable estimate of arrival times (viz. leading edge penetration rate) and subsequent depth profiles at the positions where data were reported in the apparatus.

Run No. 2 also simulated a 10 m³ pour volume but at $\frac{1}{2}$ the flowrate (i.e., 3.25 m³/minute). Test characteristics and the corresponding code input are summarized in Table C-5, while analogous plots of leading edge penetration, local depth responses, and depth profiles at several times are shown in Figures C-9 through C-14. Again, the wetted surface calculation seems to provide a better agreement, and overall predictions of arrival times and depth profiles seem to reasonably replicate the behavior observed in the experiments.

Test parameter	Value
Test name	Theofanous Test No. 1
Fluid composition (wt %)	100 H ₂ O
Melt delivery technique	Water poured into a 28.3 cm radius cylindrical cavity that simulated the pedestal of a Mark I containment.
Total pour mass	10.2 kg
Spreading geometry	1/10 linear scale model of a Mark I containment: A 28.3 cm inner radius cylindrical cavity with a 9.5 cm wide doorway leading to an annular spreading region with a radius of 56.5 cm. The wall thickness of the pedestal was 3.2 cm.
	-
Code input parameter(s)	Value(s)
Fluid composition (wt %)	100 H ₂ O
Fluid pour rate and duration	Flowrate constant at 0.325 kg/sec for 31.5 seconds.
Melt material property evaluation	User-specified property data: ρ = 997 kg/m³, μ_o = 0.826 mPa-s, and σ = 0.073 N-m
Heat transfer modeling	Flow is "adiabatic"
Spreading cavity nodalization	Automated Mark I shell meshing option used: melt pour into the sump with assumed radius of 19.9 cm and flush with the concrete surface; balance of pedestal interior meshed with 2 nodes that were 4.2 cm long. The 9.5 cm wide doorway was meshed with 2 cells that were 1.6 cm long. The water was assumed to spread outside the doorway with a spreading angle of 90°. The distance from the doorway to the shell was meshed with 7 cells that were 3.57 cm long. The balance of the annulus was meshed using 25 cells. All nodes cell-centered.
Timestep	0.05 seconds

Table C-4 INPUT FILE DATA SHEET FOR THEOFANOUS WATER SPREADING TEST NO. 1



Figure C-29 Leading edge penetration comparison for Theofanous et al. Run No. 1



Figure C-30 Comparison of local depth response at Position A for Theofanous Run No. 1



Figure C-31 Comparison of local depth response at Position C for Theofanous Run No. 1







Figure C-33 Comparison of local depth response at Position E for Theofanous Run No. 1





Table C-5	INPUT FILE DATA	SHEET FOR	THEOFANOUS	WATER 9	SPREADING	TEST NO. 2
			THEORANOOS		JINLADING	1231 140.2

Test parameter	Value
Test name	Theofanous Test No. 2
Fluid composition (wt %)	100 H ₂ O
Melt delivery technique	Water poured into a 28.3 cm radius cylindrical cavity that simulated the pedestal of a Mark I containment.
Total pour mass	10.2 kg
Spreading geometry	1/10 linear scale model of a Mark I containment: A 28.3 cm inner radius cylindrical cavity with a 9.5 cm wide doorway leading to an annular spreading region with a radius of 56.5 cm. The wall thickness of the pedestal was 3.2 cm.
Code input parameter(s)	Value(s)
Fluid composition (wt %)	100 H ₂ O
Fluid pour rate and duration	Flowrate constant at 0.1625 kg/sec for 63.0 seconds.
Melt material property evaluation	User-specified property data: $\rho = 997 \text{ kg/m}^3$, $\mu_o = 0.826 \text{ mPa-s}$, and $\sigma = 0.073 \text{ N-m}$
Heat transfer modeling	Flow is "adiabatic"
Spreading cavity nodalization	Automated Mark I shell meshing option used: melt pour into the sump with assumed radius of 19.9 cm and flush with the concrete surface; balance of pedestal interior meshed with 2 nodes that were 4.2 cm long. The 9.5 cm wide doorway was meshed with 2 cells that were 1.6 cm long. The water was assumed to spread outside the doorway with a spreading angle of 90°. The distance from the doorway to the shell was meshed with 7 cells that were 3.57 cm long. The balance of the annulus was meshed using 25 cells. All nodes cell-centered.
Timestep	0.05 seconds







Figure C-36 Comparison of local depth response at Position A for Theofanous Run No. 2



Figure C-37 Comparison of local depth response at Position C for Theofanous Run No. 2



Figure C-38 Comparison of local depth response at Position D for Theofanous Run No. 2



Figure C-39 Comparison of local depth response at Position E for Theofanous Run No. 2



Figure C-40 Predicted local depth profiles at various times for Theofanous Run No. 2

<u>Corine Water and HEC Spreading Tests</u>

The second validation exercise involving isothermal spreading consisted of comparing code predictions with water and glycerol spreading data obtained as part of the Corine^[29] program. These were large-scale simulant experiments involving the spreading of ~ 40 liters of fluid within an instrumented 19° sector. The principal parameters that were varied in the test matrix included pour rate and fluid viscosity. As shown in Table C-1, four tests were selected from this experiment series for analysis: two water tests at different flowrates (i.e., 0.5 and 1.5 liters/second), and two glycerol tests at the same flowrate but with different fluid viscosities (i.e., 0.1 and 2.0 Pa-sec). Test characteristics and the corresponding code input for the low water flowrate test WAT_Q0.5_GO are described in Table C-6. A comparison of the predicted water leading edge penetration rate with the test data is provided in Figure C-15, while local depth profiles at several times are shown in Figure C-16. In Figure C-15, results are again provided for both wetted and non-wetted surface conditions. For this case, the non-wetted surface solution seems to provide slightly better agreement, although the difference is not dramatic. In general, the code reasonably predicts the leading edge penetration rate for this experiment.

Test parameter	Value
Test name	WAT_Q0.5_GO
Fluid composition (wt %)	100 H ₂ O
Fluid delivery technique	Water pumped from below into a fluid delivery reservoir that was
	circular with a cross-sectional area of 0.1064 m ² . The reservoir
	was separated from the spreading channel by a weir that was
	24.0 cm high and had a wall thickness of 1.4 cm.
Total pour mass	65 (25 kg to fill the reservoir, 40 kg spread)
Spreading geometry	6.5 m long, 19° angular sector
	-
Code input parameter(s)	Value(s)
Fluid composition (wt %)	100 H ₂ O
Fluid pour rate and duration	Injection flowrate into the reservoir constant at 0.5 kg/sec over a
	time interval of 130 seconds.
Fluid material property	User-specified property data: ρ = 1000 kg/m ³ , μ_0 = 0.826 mPa-s,
evaluation	and $\sigma = 0.073$ N-m
Heat transfer modeling	Flow is "adiabatic"
Spreading cavity nodalization	Reservoir modeled as a single cell with area 0.1064 m^2 ,
	spreading arc length of 19.05 cm, node length of 41.1 cm, and
	elevation flush with the spreading surface. The weir was
	modeled with a single cell that was 24.0 cm above the spreading
	surface and had a thickness (length) of 1.4 cm. The spreading
	channel modeled as a 19° angular sector; the 6.5 m radial length
	was subdivided into 200 nodes of equal radial length of 3.25 cm.
Timestep	0.05 seconds

	E DATA CUEET EOD	CODINE TECT WAAT	ODE CO	water in a 100 costor)
I ADIE C-O INPUT FIL	E DAIA SHEET FUR	CORINE LEST WAT	Q0.5 GU	(water in a 19= Sector)



Figure C-41 Leading edge penetration comparison for Corine Test WAT_Q0.5_GO



Figure C-42 Predicted local depth profiles at various times for Corine Test WAT_Q0.5_GO

Test characteristics and the corresponding code input for the high water flowrate test WAT_Q1.5_GO are summarized in Table C-7, while the analogous plots of leading edge penetration and depth profiles at several times are shown in Figures C-17 and C-18. For this test, the non-wetted surface solution provides a slightly better fit to the leading edge penetration data, and the solution reasonably replicates the overall trends observed in the experiment.

Test parameter	Value
Test name	WAT_Q1.5_GO
Fluid composition (wt %)	100 H ₂ O
Fluid delivery technique	Water pumped from below into a fluid delivery reservoir that was
	circular with a cross-sectional area of 0.1064 m ² . The reservoir was
	separated from the spreading channel by a weir that was 24.0 cm high
	and had a wall thickness of 1.4 cm.
Total pour mass	65 (25 kg to fill the reservoir, 40 kg spread)
Spreading geometry	6.5 m long, 19° angular sector
Code input parameter(s)	Value(s)
Fluid composition (wt %)	100 H ₂ O
Fluid pour rate and duration	Injection flowrate into the reservoir constant at 1.5 kg/sec over a time
	interval of 43.3 seconds.
Fluid material property	User-specified property data: ρ = 1000 kg/m ³ , μ_o = 0.826 mPa-s, and σ
evaluation	= 0.073 N-m
Heat transfer modeling	Flow is "adiabatic"
Spreading cavity nodalization	Reservoir modeled as a single cell with area 0.1064 m ² , spreading arc
	length of 19.05 cm, node length of 41.1 cm, and elevation flush with
	the spreading surface. The weir was modeled with a single cell that
	was 24.0 cm above the spreading surface and had a thickness (length)
	of 1.4 cm. The spreading channel was modeled as a 19° angular
	sector; the 6.5 m radial length was subdivided into 200 nodes of equal
	radial length of 3.25 cm.
Timestep	0.05 seconds

Table C-7 INPUT FILE DATA SHEET FOR CORINE TEST WAT_Q1.5_GO (water in a 19^o sector)



Figure C-43 Leading edge penetration comparison for Corine Test WAT_Q1.5_GO



Figure C-44 Predicted local depth profiles at various times for Corine Test WAT_Q1.5_GO

Aside from the water spreading experiments, test characteristics and corresponding code input for the Corine low viscosity (0.1 Pa-sec) glycerol spreading test HEC_3_GO_0.1 are summarized in Table C-8, while plots of leading edge penetration and depth profiles at several different times are shown in Figures C-19 and C-20. For this test, the non-wetted surface solution provides a slightly better fit to the leading edge penetration data, and the overall shape of the position vs. time curve is reasonably reproduced. However, the code systematically under-predicts the leading edge penetration distance by ~ 30 cm for times past ~ 20 seconds into the test. The reason for the discrepancy is not clear, but one possibility is offered; i.e., edge effects may play an important role in these higher viscosity tests, and so penetration at the centerline (where progression was measured) was systematically greater than at the edges, and so the average penetration distance was less than reported at any given time. Recall that MELTSREAD is a one-dimensional code, and so edge effects cannot be accurately modeled.

Test parameter	Value	
Test name	HEC_3_GO_0.1	
Fluid composition (wt %)	100 Hydroxyl ethyl cellulose (HEC)	
Melt delivery technique	Fluid pumped from below into a delivery reservoir that was circular	
	with a cross-sectional area of 0.1064 m^2 . The reservoir was	
	separated from the spreading channel by a weir that was 24.0 cm	
	high and had a wall thickness of 1.4 cm.	
Total pour mass	65 (25 kg to fill the reservoir, 40 kg spread)	
Spreading geometry	6.5 m long, 19° angular sector	
Code input parameter(s)	Value(s)	
Fluid composition (wt %)	100 Hydroxyl ethyl cellulose (HEC)	
Fluid pour rate and duration	Injection flowrate into the reservoir constant at 3.0 kg/sec over a	
	time interval of 21.67 seconds.	
Melt material property	User-specified property data: ρ = 1000 kg/m ³ , μ_0 = 0.1 Pa-s, and σ =	
evaluation	0.04 N-m	
Heat transfer modeling	Flow is "adiabatic"	
Spreading cavity nodalization	Reservoir modeled as a single cell with area 0.1064 m ² , spreading	
	arc length of 19.05 cm, node length of 41.1 cm, and elevation flush	
	with the spreading surface. The weir was modeled with a single cell	
	that was 24.0 cm above the spreading surface and had a thickness	
	(length) of 1.4 cm. The spreading channel was modeled as a 19°	
	angular sector; the 6.5 m radial length was subdivided into 200	
	nodes of equal radial length of 3.25 cm.	
Timestep	0.05 seconds	

Table C-8 INPUT FILE DATA SHEET FOR CORINE TEST HEC_3_GO_0.1 (glycol in a 19^o sector)



Figure C-45 Leading edge penetration comparison for Corine Test HEC_3_GO_0.1



Figure C-46 Predicted local depth profiles at various times for Corine Test HEC_3_GO_0.1

Test information and modeling details for the Corine high viscosity (2.0 Pa-sec) spreading test HEC_3_GO_0.1 are summarized in Table C-9. Conversely, plots of leading edge penetration and depth profiles at several different times are shown in Figures C-21 and C-22. As for the previous case, the non-wetted surface solution provides a slightly better fit to the leading edge penetration data, and the overall shape of the position vs. time curve is reasonably reproduced. However, as for the previous case, the code systematically underpredicts the leading edge penetration distance by ~ 30 cm for all times past ~ 20 seconds into the experiment sequence. A possible explanation for the discrepancy was provided above.

Test parameter	Value
Test name	HEC_3_GO_2.0
Fluid composition (wt %)	100 Hydroxyl ethyl cellulose (HEC)
Fluid delivery technique	Fluid pumped from below into a delivery reservoir that was circular
	with a cross-sectional area of 0.1064 m^2 . The reservoir was
	separated from the spreading channel by a weir that was 24.0 cm
	high and had a wall thickness of 1.4 cm.
Total pour mass	65 (25 kg to fill the reservoir, 40 kg spread)
Spreading geometry	6.5 m long, 19° angular sector
Code input parameter(s)	Value(s)
Fluid composition (wt %)	100 Hydroxyl ethyl cellulose (HEC)
Fluid pour rate and duration	Injection flowrate into the reservoir constant at 3.0 kg/sec over a
	time interval of 21.67 seconds.
Fluid material property	User-specified property data: ρ = 1000 kg/m ³ , μ_o = 2.0 Pa-s, and σ =
evaluation	0.04 N-m
Heat transfer modeling	Flow is "adiabatic"
Spreading cavity nodalization	Reservoir modeled as a single cell with area 0.1064 m ² , spreading
	arc length of 19.05 cm, node length of 41.1 cm, and elevation flush
	with the spreading surface. The weir was modeled with a single cell
	that was 24.0 cm above the spreading surface and had a thickness
	(length) of 1.4 cm. The spreading channel was modeled as a 19°
	angular sector; the 6.5 m radial length was subdivided into 200
	nodes of equal radial length of 3.25 cm.
Timestep	0.05 seconds

Table C-9 INPUT FILE DATA SHEET FOR CORINE TEST HEC_3_GO_2.0 (glycol in a 19^o sector)



Figure C-47 Leading edge penetration comparison for Corine Test HEC_3_GO_2.0



Figure C-48 Predicted local depth profiles at various times for Corine Test HEC_3_GO_2.0

HIGH TEMPERATURE TESTS WITH SIMULANT OXIDE MELTS

The code has also been applied to experiments involving heat transfer and freezing effects. The first class of tests considered were those that utilized simulant oxide materials. Tests that fall into this category include those by Engel et al.^[31] and Eppinger et al.^[32] in the KATS test facility, and those by Foit^[33] and Alsmeyer et al.^[34] in the ECOKATS facility. In addition, high temperature calcia – boria eutectic spreading experiments were carried out under both wet and dry cavity conditions by Dinh et al.^[30] at the Royal Institute of Technology (RIT) in Sweden. Comparisons with these various tests are provided in this section.

In order to analyze the flow and freezing tests presented in the balance of this appendix, the metal and oxide phase solid fraction variations as a function of temperature between the liquidus and solidus must be supplied as part of the code input (see Section 4). The assumed functions used in this work are shown in Figure C-23; these data are taken from Reference [15].



Figure C-49 Oxide and metal phase solid fraction functions assumed for the various melt compositions in this study^[15]

KATS Oxide Simulant Spreading Tests

These tests involved spreading of high temperature oxide melts that principally contained concrete decomposition byproducts, but with a small amount of FeO (i.e., 83.0/8.5/6.0/1.5/1.0 wt % Al₂O₃/SiO₂/FeO/MgO/MnO). These melts were generated using a modified iron-alumina thermite reaction. The reaction

byproduct consisted of a superheated iron metal phase that was segregated from the oxide, thereby allowing both the metal and oxide phases to be spread in separate one-dimensional channels. The counterpart metal tests are analyzed later in this section.

For the oxide test series, the KATS-12, -13, and -14 experiments were selected for analysis (see Table C-1). KATS-12 and -13 parameterized on substrate composition, with KATS-12 utilizing ceramic (Corderite), and KATS-13 utilizing concrete. KATS-14 was also conducted with a ceramic substrate, but the melt pour rate was reduced relative to KATS-12.

The accumulator design in these tests was somewhat novel, with a base that was slightly elevated relative to the spreading surface. The general characteristics are shown in Figure C-24, while the corresponding dimensions for each test are summarized in Table C-10. As is evident, a small incline connected the accumulator to the spreading channel.

Test characteristics and the code input that was developed for the KATS-12 test are summarized in Table C-11. As is evident from the table, an effort was made with the meshing scheme to physically mock up the details of the melt accumulator, gate, and incline leading to the spreading channel. The experimenters^[32] provided detailed specifications of melt pour rate vs. time as well as the material properties of the melt and ceramic substrate. This information was used as part of the input for the calculation.



Figure C-50 Melt accumulator characteristics for the KATS tests

	Spreading Device Dimension (mm):						
Test	$\mathbf{L}_{\mathbf{B}}$	WB	$\mathbf{L}_{\mathbf{G}}$	WG	$\mathbf{H}_{\mathbf{G}}$	$\mathbf{L}_{\mathbf{f}}$	$\mathbf{H}_{\mathbf{f}}$
KATS-12 Metal	302	170	43	80	50	100	70
KATS-12 Oxide	382	367	43	140	50	110	70
KATS-13 Metal	302	170	43	80	50	100	90
KATS-13 Oxide	382	367	43	140	50	110	90
KATS-14 Metal	200	180	43	140	30	30	50
KATS-14 Oxide	300	300	43	240	40	80	100

Table C-10 MELT ACCUMULATOR DIMENSIONS FOR KATS TESTS (see Figure C-24 for nomenclature)

The calculated leading edge penetration vs. time for KATS-12 is compared to the test data in Figure C-25, while local melt temperature and post-spreading material profile predictions are compared with the data in Figures C-26 and C-27, respectively. The pour rate in this test was relatively high and so the spreading rate was initially dominated by inertial effects. As is evident from Figure C-26, despite discrepancies in melt arrival times, peak melt temperatures are predicted to within ~ 30 K near the melt injection point, but the discrepancy grows to ~ 70 K near the channel midpoint. As shown in Figure C-27, the debris profile is reasonably predicted. The large structure to the left in this figure is the melt accumulator. Given this design and high melt injection rate, the possibility exists that the melt jetted out of feedbox, causing overshoot of some (unknown) distance of the spreading surface and an initial spreading velocity that would exceed what the code would calculate based on gravity-driven spreading alone. This may explain at least part of the discrepancy in initial spreading rate seen early in the sequence, as the code assumes continuous flow through the mesh with no possibility of bypass.

Test parameter	Value
Test name	KATS-12 oxide, ceramic channel
Melt composition (wt %)	83.0 Al ₂ O ₃ , 8.5 SiO ₂ , 6.0 FeO, 1.5 MgO, 1.0 MnO
Melt delivery technique	Melt poured into an accumulator box that was 36.7
	cm wide, 38.2 cm long, and 7.0 cm above the
	spreading surface. Pour initiated by opening a gate to
	the spreading channel.
Melt temperature	2300 K
Total pour mass	186 kg
Substrate material	Cordierite
Spreading geometry	1-D channel, 12 m long by 25 cm wide
Code input parameter(s)	Value(s)
Melt composition (wt %)	83.0 Al ₂ O ₃ , 8.5 SiO ₂ , 6.0 FeO, 1.5 MgO, 1.0 MnO
Melt pour temperature	2300 K
Melt oxide phase solidus – liquidus	1850 К – 2200 К
Melt metal phase solidus – liquidus	1810 К – 1820 К
Melt pour rate and duration	Linear decrease in pour rate from 37.1 kg/sec to zero
	over 10 second interval
Melt material property evaluation	User-specified property data used: $c_s = 1280 \text{ J/kg-K}$,
	$c_1 = 1423 \text{ J/kg-K}, \Delta h_f = 802 \text{ kJ/kg}, \rho_s = \rho_1 = 2800$
	kg/m^3 , $k_s = k_1 = 5.4 W/m-K$, $\mu_0 = 0.05 Pa-s$, $\sigma = 0.5 N-t$
	m, M = 91.7 g/mole, and ε = 0.8
Substrate composition	Corderite (modeled using user-specified material input
	properties)
Substrate initial temperature	298 K
Substrate material properties evaluation	$c_s = c_l = 840 \text{ J/kg-K}, \Delta h_l = 1.0 \text{ MJ/kg}, \rho_s = \rho_l = 2200$
	kg/m^3 , $k_s = k_l = 3.8 \text{ W/m-K}$, and $\epsilon = 0.3$
Substrate solidus - liquidus temperatures	1893 K – 1923 K
Substrate nodalization	are used; all nodes are cell-centered.
Spreading cavity nodalization	Accumulator: modeled as a single cell that is 36.7 cm
	wide, 38.2 cm long, and 7.0 cm above the channel
	surface. Gate: modeled as a single cell that is 14 cm
	wide, 4.3 cm long, and 7.0 cm above the channel.
	Incline down to channel: modeled as a single cell that
	is 11 cm long, 25 cm wide, and 3.5 cm above the
	channel. Channel: modeled using 120 cells; each is
	25 cm wide and 10 cm long. All nodes cell-centered.
Cavity condition	Dry
Upper atmosphere temperature	300 K
Upper atmosphere emissivity	0.7
Ambient pressure	0.1 MPa
Melt/substrate heat transfer coefficient model	Dittus - Boelter
Melt/substrate interfacial heat transfer	Not modeled
resistance	
Constant in Ramacciotti correlation	2.34 (Average for oxide type [15])
Solid-fraction variation	See Figure C-23
Timestep	0.02 seconds

Table C-11 INPUT FILE DATA SHEET FOR THE KATS-12 OXIDE MELT TEST WITH CERAMIC CHANNEL






Figure C-52 Comparison of local melt temperature predictions with KATS-12 oxide data



Figure C-53 Comparison of posttest debris profile prediction with KATS-12 oxide data

Test characteristics and modeling input for the KATS-13 test are summarized in Table C-12. As for the KATS-12 simulation, the experimental specifications^[32] for melt pour rate vs. time and the melt thermo-physical properties were used, but the code default composition for siliceous concrete was assumed since the data report did not provide this information. The calculated leading edge penetration vs. time is compared to the test data in Figure C-28, while local melt temperature and post-spreading material profile predictions are compared with the data in Figures C-29 and C-30, respectively. As discussed in Reference [15], this test was an outlier in terms of predicting the maximum melt penetration distance using the Ramacciotti melt viscosity correlation. The results shown here were obtained using the best fit C_R value in the Ramacciotti correlation (i.e. Eq. 2-24) of 10.28 for this particular test.

As for KATS-12, this was a high flowrate test and so the spreading rate was initially dominated by inertial effects. As noted previously, given the accumulator design and high melt flowate, the possibility exists that the melt overshot some distance of the spreading surface near the accumulator, leading to an apparent spreading velocity that was initially larger than the code prediction.

Test parameter	Value
Test name	KATS-13 oxide, concrete channel
Melt composition (wt %)	83.0 Al ₂ O ₃ , 8.5 SiO ₂ , 6.0 FeO, 1.5 MgO, 1.0 MnO
Melt delivery technique	Melt poured into an accumulator box that was
	36.7 cm wide, 38.2 cm long, and 9.0 cm above
	the spreading surface. Pour initiated by opening
	a gate to the spreading channel.
Melt temperature	2320 K
Total pour mass	186 kg
Substrate material	Siliceous concrete
Spreading geometry	1-D channel, 12 m long by 25 cm wide
Code input parameter(s)	Value(s)
Melt composition (wt %)	83.0 Al ₂ O ₃ , 8.5 SiO ₂ , 6.0 FeO, 1.5 MgO, 1.0 MnO
Melt pour temperature	2320 K
Melt oxide phase solidus – liquidus	1850 К – 2200 К
Melt metal phase solidus – liquidus	1810 К – 1820 К
Melt pour rate and duration	Linear decrease in pour rate from 37.1 kg/sec to
	zero over 10 second interval
Melt material property evaluation	User-specified property data used: $c_s = 1280$
	J/kg-K, c_l = 1423 J/kg-K, Δh_f = 802 kJ/kg, ρ_s = ρ_l
	= 2800 kg/m ³ , $k_s = k_l = 5.4$ W/m-K, $\mu_o = 0.05$ Pa-
	s, $\sigma = 0.5$ N-m, M = 91.7 g/mole, and $\varepsilon = 0.8$
Substrate composition	Default siliceous concrete
Substrate initial temperature	298 K
Substrate material properties evaluation	Code subroutines
Substrate solidus - liquidus temperatures	1403 – 1523 K (Code default values)
Substrate nodalization	At each substrate nodal location, twelve 6.0 mm
	cells are used; all nodes cell-centered.
Spreading cavity nodalization	Accumulator: modeled as a single cell that is 36.7
	cm wide, 38.2 cm long, and 9.0 cm above the
	channel surface. Gate: modeled as a single cell
	that is 14 cm wide, 4.3 cm long, and 9.0 cm
	above the channel. Incline down to channel:
	modeled as a single cell that is 11 cm long, 25 cm
	wide, and 4.5 cm above the channel. Channel:
	modeled using 120 cells; each is 25 cm wide and
	10 cm long. All nodes cell-centered.
Lange streaghters temperature	
Upper atmosphere emigricuity	500 K
Ambient pressure	0.7
Molt / substrate heat transfer coefficient model	U.I. MFa
Meit/substrate fleat transfer coefficient model	slog film heat transfer coefficients
Melt/substrate interfacial heat transfer	Not modeled
meny substrate internacial field transfer	
Constant in Romacointti correlation	10.28 (Best fit for this test [15])
Solid-fraction variation	See Figure C_{23}
Timesten	$0.02 \operatorname{seconds}$
imesich	0.04 30001103

Table C-12 INPUT FILE DATA SHEET FOR THE KATS-13 OXIDE MELT TEST WITH CONCRETE CHANNEL



Figure C-54 Leading edge penetration comparison for the KATS-13 oxide spreading test



Figure C-55 Comparison of local melt temperature predictions with KATS-13 oxide data



Figure C-56 Comparison of posttest debris profile prediction with KATS-13 oxide data

As is evident from Figure C-29, despite discrepancies in melt arrival times, peak melt temperatures are predicted to within ~ 40 K over the first 3.5 m of the spreading channel, but at the 6.5 m location, the code overpredicts the temperature by ~ 100 K. As shown in Figure C-30, local depths in the solidified debris are under-predicted, but the code calculates solidification assuming a fully dense melt condition, whereas the debris most likely solidified with porosity present from gas sparging due to concrete decomposition.

Test characteristics and the corresponding code input developed for KATS-14 are summarized in Table C-13. As for KATS-12, the experimenter's specifications^[32] for melt pour rate, as well as the melt and substrate thermophysical properties, were used. The calculated leading edge penetration versus time is compared to the test data in Figure C-31, while local melt temperature and post-spreading material profile predictions are compared with the data in Figures C-32 and C-33, respectively. The pour rate in this test was lower compared to the counterpart test KATS-12, and so the penetration for this case is reduced relative to KATS-12 (see Figure C-25). The code appears to capture this effect reasonably well. In general, the initial rate of spreading from the accumulator box is better captured for this case in comparison to KATS-12.

Test parameter	Value
Test name	KATS-14 oxide, ceramic channel
Melt composition (wt %)	83.0 Al ₂ O ₃ , 8.5 SiO ₂ , 6.0 FeO, 1.5 MgO, 1.0 MnO
Melt delivery technique	Melt poured into an accumulator box that was
	30.0 cm wide, 30.0 cm long, and 10.0 cm above
	the spreading surface. Pour initiated by opening
	a gate to the spreading channel.
Melt temperature	2245 K
Total pour mass	176 kg
Substrate material	Cordierite
Spreading geometry	1-D channel, 12 m long by 25 cm wide
Code input parameter(s)	Value(s)
Melt composition (wt %)	83.0 Al ₂ O ₃ , 8.5 SiO ₂ , 6.0 FeO, 1.5 MgO, 1.0 MnO
Melt pour temperature	2245 K
Melt oxide phase solidus – liquidus	1850 К – 2200 К
Melt metal phase solidus – liquidus	1810 K – 1820 K
Melt pour rate and duration	Linear decrease in pour rate from 5.95 kg/sec to
	3.57 kg/sec over a 37 second interval
Melt material property evaluation	User-specified property data used: $c_s = 1280$
	$J/kg-K$, $c_l = 1423 J/kg-K$, $\Delta h_f = 802 kJ/kg$, $\rho_s = \rho_l$
	= 2800 kg/m ³ , k_s = k_l = 5.4 W/m-K, μ_o = 0.05 Pa-
	s, $\sigma = 0.5$ N-m, M = 91.7 g/mole, and $\varepsilon = 0.8$
Substrate composition	Corderite (modeled using user-specified material
	input properties)
Substrate initial temperature	298 K
Substrate material properties evaluation	$c_s = c_l = 840 \text{ J/kg-K}, \Delta h_f = 1.0 \text{ MJ/kg}, \rho_s = \rho_l =$
	2200 kg/m ³ , $k_s = k_l = 3.8$ W/m-K, and $\epsilon = 0.3$
Substrate solidus - liquidus temperatures	1893 К – 1923 К
Substrate nodalization	At each substrate nodal location, twelve 6.0 mm
	cells are used; all nodes are cell-centered.
Spreading cavity nodalization	Accumulator: modeled as a single cell that is 30.0
	cm wide, 30.0 cm long, and 10.0 cm above the
	channel surface. Gate: modeled as a single cell
	that is 24 cm wide, 4.3 cm long, and 10.0 cm
	above the channel. Incline down to channel:
	wide and 5.0 cm above the channel. Channel:
	modeled using 120 cells: each is 25 cm wide and
	10 cm long All nodes cell-centered
Cavity condition	Dry
Upper atmosphere temperature	300 K
Upper atmosphere emissivity	0.7
Ambient pressure	0.1 MPa
Melt/substrate heat transfer coefficient model	Dittus – Boelter
Melt/substrate interfacial heat transfer	Not modeled
resistance	
Constant in Ramacciotti correlation	2.34 (Average for oxide type [15])
Solid-fraction variation	See Figure C-23
Timestep	0.02 seconds

Table C-13 INPUT FILE DATA SHEET FOR THE KATS-14 OXIDE MELT TEST WITH CERAMIC CHANNEL







Figure C-58 Comparison of local melt temperature predictions with KATS-14 oxide data



Figure C-59 Comparison of posttest debris profile prediction with KATS-14 oxide data

Examination of the melt temperature data in Figure C-32 indicates that despite discrepancies in melt arrival times, peak melt temperatures are predicted to within ~ 50 K at the 1meter location, and to within ~ 10 K at the 3 m location. The code under-predicts the melt temperature by ~ 120 K at the 5 m location, but note that the recorded peak here exceeds that at 3 m by ~ 30 K, which does not seem physically plausible. As shown in Figure C-33, the debris thickness after spreading is slightly under-predicted, but this is again due to the fact that the code assumes a fully dense condition upon solidification, whereas experience has shown that melts solidify with some porosity present.

ECOKATS Oxide Simulant Spreading Tests

These tests followed the KATS spreading tests described in the previous section, but the experiments were increased in scale and flow complexity to provide a more diverse database, and to examine some additional phenomenology (i.e. coolability) that was not considered in KATS. The experimenters again used a modified thermite reaction to generate the melts, but the resultant oxide was slightly different compared to KATS (i.e., 41.0/24.0/19.0/16.0 % Al₂O₃/FeO/CaO/SiO₂ wt for ECOKATS vs. 83.0/8.5/6.0/1.5/1.0 wt % Al₂O₃/SiO₂/FeO/MgO/MnO for KATS). As shown in Table C-1, ECOKATS-V1 was a 1-D spreading test with a ceramic substrate, whereas ECOKATS-1 and -2 were 2-D tests using concrete substrates.

ECOKATS-2 had the added dimension of a multi-component melt pour in which the iron phase was spread first, followed by the oxide.

Test characteristics and code input for the ECOKATS-V1 test are summarized in Table C-14, while leading edge penetration and the post-spreading material profile predictions are compared with the data in Figures C-34 and C-35, respectively. The experimentally specified melt pour rate, as well as the material properties of the melt and ceramic substrate, was input as part of the calculation.

Examination of these figures indicates that the overall rate of melt propagation during the spreading transient is captured reasonably well by the code. In addition, the shape of material depth profile after spreading is reasonably predicted, but overall thickness of the layer is again somewhat under-predicted due to the fact the code does not include porosity during solidification.

Test characteristics and code input for ECOKATS-1 are summarized in Table C-15. As for the ECOKATS-V1 simulation, the experimental specifications^[33] for melt pour rate vs. time and the melt thermo-physical properties were used, but the code default composition for siliceous concrete was assumed since the data report did not provide the detailed concrete composition. This test featured a melt accumulator box and a 2.6 m long 1-D spreading channel that entered into a 4 m long by 3 m wide rectilinear box on the centerline of one of the 3 m wide sides. The test data indicates that the melt roughly spread as a 180° sector, stopping just short of the outer wall of the box. On this basis, the system was modeled assuming flow into a 180° sector outside the 1-D channel.

The calculated leading edge penetration versus time in the 1-D channel section is compared to the test data in Figure C-36, while the floor area coverage versus time in the balance of the system is compared in Figure C-37. In addition, predictions of the basemat thermal response 20 cm outside the channel exit are compared to the data in Figure C-38. Finally, the debris profile following spreading is shown in Figure C-39. Results for leading edge penetration indicate that the overall spreading velocity is reasonably predicted. Examination of Figure C-38 indicates that, despite the offset in melt arrival time, the code does a reasonable job predicting the overall shape of the thermal response in the basemat, but temperatures are over-predicted by 50 to 80 K depending upon depth into the concrete. As shown in Figure C-39, the code predicts a few millimeters of concrete ablation in the last meter of the 1-D spreading channel. It is not known if this is physically reasonable since no mention is made of it in the documentation.

Test parameter	Value
Test name	ECOKATS-V1
Melt composition (wt %)	41.0 Al ₂ O ₃ , 24.0 FeO, 19.0 CaO, and 16.0 SiO ₂
Melt delivery technique	Melt poured into an accumulator box that was
	modeled as a 29.3 cm wide, 22.5 cm long, and flush
	with the spreading surface. Pour initiated by melt
	injection into the accumulator box.
Melt temperature	1893 K
Total pour mass	193 kg
Substrate material	Cordierite
Spreading geometry	1-D channel, 8 m long by 29.3 cm wide
Code input parameter(s)	Value(s)
Melt composition (wt %)	41.0 Al ₂ O ₃ , 24.0 FeO, 19.0 CaO, and 16.0 SiO ₂
Melt pour temperature	1893 K
Melt oxide phase solidus – liquidus	1373 К – 1822 К
Melt metal phase solidus – liquidus	1810 K – 1820 K
Melt pour rate and duration	For 0 – 13.7 sec, 4.238 kg/sec pour rate; for 13.7 –
	40.5 sec, 3.463 kg/sec; for 40.5 – 47.6 sec, 3.291
	kg/sec; for $47.6 - 54.7$, 2.61 kg/sec; for t > 54.7
	sec, pour rate is zero.
Melt material property evaluation	User-specified property data used: $c_s = 1055 \text{ J/kg}$
	K, c _l = 1220 J/kg-K, Δh _f = 1162 kJ/kg, $\rho_s = \rho_l = 3263$
	kg/m^3 , $k_s = k_1 = 5.4$ W/m-K, $\mu_0 = 0.2$ Pa-s, $\sigma = 0.5$ N-
Orthographic communities	m, M = 74.6 g/mole, and $\varepsilon = 0.95$
Substrate composition	Cordenite (modeled using user-specified material
Substrate initial temperature	
Substrate material properties evaluation	270 K
Substrate material properties evaluation	$k_{\rm s} = c_{\rm l} = 0.4007$ kg·K, $\Delta m_{\rm l} = 1.0$ MJ/kg, $p_{\rm s} = p_{\rm l} = 2200$
Substrate solidus - liquidus temperatures	1893 K – 1923 K
Substrate podalization	At each substrate nodal location, three 2.0 mm
	cells one 4.0 mm cell and eight 6.0 mm cells are
	used: all nodes are cell-centered.
Spreading cavity nodalization	Accumulator: modeled as a single cell that is a 29.3
	cm wide, 22.5 cm long, and flush with the spreading
	channel. Channel: modeled using 80 cells; each is
	29.3 cm wide and 10 cm long. All nodes cell-
	centered.
Cavity condition	Dry
Upper atmosphere temperature	300 K
Upper atmosphere emissivity	0.7
Ambient pressure	0.1 MPa
Melt/substrate heat transfer coefficient model	Dittus - Boelter
Melt/substrate interfacial heat transfer	Not modeled
resistance	
Constant in Ramacciotti correlation	2.34 (Average for oxide type [15])
Solid-fraction variation	See Figure C-23
Timestep	0.02 seconds

Table C-14 INPUT FILE DATA SHEET FOR THE ECOKATS-V1 TEST



Figure C-60 Leading edge penetration comparison for the ECOKATS-V1 spreading test



Figure C-61 Comparison of posttest debris profile prediction with ECOKATS-V1 data

Test parameter	Value
Test name	ECOKATS-1
Melt composition (wt %)	41.0 Al ₂ O ₃ , 24.0 FeO, 19.0 CaO, and 16.0 SiO ₂
Melt delivery technique	Melt poured into an accumulator box that was
	modeled as a 28.8 cm wide, 32.5 cm long, and flush
	with the spreading surface. Pour initiated by melt
	injection into the accumulator box.
Melt temperature	1873 K
Total pour mass	547 kg
Substrate material	Siliceous concrete
Spreading geometry	1-D channel, 2.6 m long, followed by a 4 m long by
	3 m wide rectilinear spreading surface
Code input parameter(s)	Value(s)
Melt composition (wt %)	$41 \text{ 0 Al}_2\text{O}_3$ 24 0 FeO 19 0 CaO and 16 0 SiO ₂
Melt pour temperature	1873 K
Melt oxide phase solidus – liquidus	1373 K – 1822 K
Melt metal phase solidus – liquidus	1810 K – 1820 K
Melt pour rate and duration	For 0 – 16.0 sec, 7.84 kg/sec pour rate; for 16.0 –
1	69.9 sec, 6.66 kg/sec; for 69.9 – 79.5 sec, 4.78
	kg/sec; for 79.5 – 84.8 sec, 3.08 kg/sec; for t > 84.8
	sec, pour rate is zero.
Melt material property evaluation	User-specified property data used: cs = 1055 J/kg-
	K, c _l = 1220 J/kg-K, Δ h _f = 1162 kJ/kg, ρ _s = ρ _l = 3263
	kg/m^3 , $k_s = k_l = 5.4 W/m$ -K, $\mu_0 = 0.2 Pa$ -s, $\sigma = 0.5 N$ -
	m, M = 74.6 g/mole, and ε = 0.95
Substrate composition	Default siliceous concrete
Substrate initial temperature	298 К
Substrate material properties evaluation	Code subroutines
Substrate solidus - liquidus temperatures	1403 – 1523 K (Code default values)
Substrate nodalization	At each substrate nodal location, three 2.0 mm
	cells, one 4.0 mm cell, and eight 6.0 mm cells are
	used; all nodes are cell-centered.
Spreading cavity nodalization	Accumulator: modeled as a single cell that is a 28.8
	channel. Channel modeled using 50 cells, each is
	28.8 cm wide and 5 cm long 2 D spreading surface:
	modeled as a 180° sector using 30 nodes; nodes
	uniformly divided into 5 19 cm radial increments
	All nodes cell-centered.
Cavity condition	Dry
Upper atmosphere temperature	300 K
Upper atmosphere emissivity	1.0
Ambient pressure	0.1 MPa
Melt/substrate heat transfer coefficient model	Locally, largest of Dittus – Boelter and Bradley slag
	film heat transfer coefficients
Melt/substrate interfacial heat transfer	Not modeled
resistance	
Constant in Ramacciotti correlation	2.34 (Average for oxide type [15])
Solid-fraction variation	See Figure C-23
Timestep	0.02 seconds

Table C-15 INPUT FILE DATA SHEET FOR THE ECOKATS-1 TEST



Figure C-62 Leading edge comparison (1-D channel section) for the ECOKATS-1 spreading test







Figure C-64 Comparison of substrate thermal response predictions with ECOKATS-1 data 20 cm outside of 1-D channel exit



Figure C-65 Debris profile prediction for ECOKATS-1

Test characteristics and code input for ECOKATS-2 are summarized in Table C-16. Similar to ECOKATS-1, this test featured a 2.7 m long, 1-D channel that issued into a 2 m long by 2 m wide spreading area. The substrate material was also siliceous concrete. However, for this test the channel entered adjacent to one of the spreading area walls and so, with the symmetry boundary condition, the experiment simulated a larger 2 m long by 4 m wide spreading surface. A second difference between the two tests was that the metal (iron) reaction byproduct from the thermite reaction was spread first, followed by the oxide, which offered the opportunity to examine a more complicated melt pour sequence. A third difference was that the melt was also flooded following spreading in this test to investigate the coolability of the simulant spread melt. On this basis, a substantial pour mass (i.e., 3200 kg) was used so that a nontrivial post-spreading melt depth of ~ 15 cm was obtained in the apparatus. Since the melt covered the entire surface, this test could not be used to assess ultimate melt penetration distance with the code. The data also indicated that the melt spread roughly in a 45° sector after exiting the 1-D channel, and on that basis, the spreading geometry was modeled assuming a 45° sector flow outside the channel opening up until the melt reached the opposite side of the spreading box. Past this point, the material was assumed to relocate into two large nodes simulating the balance of the surface. Data for leading edge penetration was only provided up to the point when the melt contacted the opposite wall of the spreading box, and so a more detailed meshing beyond this point was not warranted.

The final note regarding modeling for this test is that since a distinct metal spreading transient occurred first, the user-option of applying a melt-substrate interfacial heat transfer resistance was invoked. As discussed in Section 2, a heat transfer resistance had to be added in order to adequately fit the model to the metal melt spreading tests. As shown in Table C-16, the heat transfer resistance was set to the average value that best-fit the melt spreading test data; i.e., $h_r = 4800 \text{ W/m}^2\text{-K}$. As further noted in Reference [15], inclusion of this resistance had little effect on the predicted spreading behavior for oxide melts since the low convective heat transfer coefficients from the bulk melt to the interface that are typically calculated for these materials controls heat losses to the underlying substrate. Thus, with the model applied in this manner, the code should provide reasonable estimates of the spreading behavior for both metal and oxide phase pour streams.

Test parameter Value Test name ECOKATS-2 Two-phases, initial is 100 Fe metal, and the second is oxide: 41.0 Al₂O₃, 24.0 Melt composition (wt %) FeO, 19.0 CaO, and 16.0 SiO₂ Melt delivery technique Melt poured into an accumulator box that was modeled as 25 cm long by 25 cm wide, and flush with the spreading surface. Pour initiated by melt injection into the accumulator box. 2103 K Melt temperature Total pour mass 3200 kg (2305 kg oxide, 895 kg metal) Substrate material Siliceous concrete Spreading geometry 1-D channel, 2.7 m long, followed by a 2 m long by 2 m wide rectilinear spreading surface. Code input parameter(s) Value(s) Metal phase: 100 Fe, oxide phase: 41.0 Al₂O₃, 24.0 FeO, 19.0 CaO, Melt composition (wt %) and 16.0 SiO_2 2103 K Melt pour temperature 1273 K – 1823 K Melt oxide phase solidus - liquidus Melt metal phase solidus - liquidus 1810 K – 1820 K Melt pour rate and duration For 0 – 7.1 sec, 126.06 kg/sec Fe metal; for 7.1 – 33.2 sec, 88.3 kg/sec oxide; for t > 88.3 sec, pour rate is zero. Melt material property evaluation For iron phase, code subroutines are used; for oxide phase, userspecified property data used: $c_s = 1055 \text{ J/kg-K}$, $c_l = 1220 \text{ J/kg-K}$, $\Delta h_{f} = 1162 \text{ kJ/kg}, \rho_{s} = \rho_{l} = 3263 \text{ kg/m}^{3}, k_{s} = k_{l} = 5.4 \text{ W/m-K}, \mu_{o} = 0.2$ Pa-s, $\sigma = 0.5$ N-m, M = 74.6 g/mole, and $\epsilon = 0.95$ Default siliceous concrete Substrate composition 298 K Substrate initial temperature Code subroutines Substrate material properties evaluation Substrate solidus - liquidus 1403 – 1523 K (Code default values) temperatures Substrate nodalization At each substrate nodal location, seven 2.0 mm cells and five 4.0 mm cells are used; all nodes are cell-centered. Spreading cavity nodalization Accumulator: modeled as single cell 25 cm long by 25 cm wide, and flush with spreading surface. Channel: modeled using 54 cells; each is 30 cm wide and 5 cm long. 2-D spreading surface: from channel outlet to opposing wall, modeled as a 45° sector using 40 nodes uniformly divided into 4.69 cm radial increments. Outside of sector, the balance of the 2-D spreading surface modeled using 2 large notes to catch melt deflected from wall. All nodes cell-centered. Cavity condition Dry Upper atmosphere temperature 300 K 1.0 Upper atmosphere emissivity Ambient pressure 0.1 MPa Melt/substrate heat transfer Locally, largest of Dittus - Boelter and Bradley slag film heat coefficient model transfer coefficients 4800 W/m²-K Melt/substrate interfacial heat transfer resistance Constant in Ramacciotti correlation 2.34 (Average for oxide type [15]) Solid-fraction variation See Figure C-23

Table C-16 INPUT FILE DATA SHEET FOR THE ECOKATS-2 TEST

0.01 seconds

Timestep

The calculated leading edge penetration versus time is compared with the test data in Figure C-40. Conversely, predictions of the basemat thermal response at four different locations within the 2-D spreading area are compared with data in Figures C-41 through C-44. Finally, predicted melt depth and temperature profiles at four different times are provided in Figure C-45. Examination of Figure C-40 indicates that the code somewhat under-predicts the leading edge penetration rate for this test, particularly in the latter half of the 1-D channel that ends at 3 m (length includes that of the accumulator also). Examination of Figures C-41 through C-44 indicates mixed results. The overall shape of the thermal response curves seems to be captured in most In addition, the code predicts onset and progression of basemat cases. ablation as observed in the test. However, temperatures seem to be somewhat over-predicted, particularly near the channel exit. Finally, Figure C-45 reveals a computational strength of the code, as well as a weakness. The strength is that complicated flow configurations can be addressed in which distinct metal and oxide pours occur. However, as illustrated by the plot at 25 seconds, the weakness is that the code does not properly handle the fluid mechanics later in the spreading transient when the stratified melt layers, behaving as two interacting gravity currents, would gradually relocate into a well-defined oxideover metal pool configuration. This is due to the fact that the two phases are assumed to be intermixed during spreading and so they relocate with the same velocity through the mesh. A more thorough analysis would treat the two distinct gravity currents with heat and mass transfer between them. However, this would be a major modeling change to the code which lies beyond the current scope of work.







Figure C-67 Comparison of substrate thermal response predictions with ECOKATS-2 data 20 cm from channel exit



Figure C-68 Comparison of substrate thermal response predictions with ECOKATS-2 data 1.8 m directly across from channel exit



Figure C-69 Comparison of substrate thermal response predictions with ECOKATS-2 data at centerline of rectilinear spreading box



Figure C-70 Comparison of substrate thermal response predictions with ECOKATS-2 data diametrically across from channel exit

<u>RIT Calcia-Boria Simulant Spreading Tests</u>

These tests^[30] involved spreading of high temperature CaO-B₂O₃ melts that were produced in a resistance heated furnace and poured into instrumented test sections. A summary of the test matrix is provided in Table C-17. A total of six experiments were conducted; all tests were in a 1-D channel flow geometry. The first three tests were conducted under dry conditions and parameterized on substrate composition and initial melt temperature. One of the unique aspects of this program was that three of the tests were conducted under water. As is evident, the tests with water principally parameterized on the mass of melt spread in the experiment.

Test	Substrate Material	Melt Temp. (K)	Pour Mass (kg)	Pour Rate (kg/sec)	Cavity Condition	Water Temp. (K)	Water Depth (cm)
3MDC-Ox-1	Concrete	1473	30.0	0.75	Dry	N/A	N/A
3MDS-Ox-1	Steel	"	"	"	"	N/A	N/A
3MDS-Ox-2	"	1373	"	"	"	N/A	N/A
2MWS-Ox-1	"	"	5.0	"	Wet	353	12
2MWS-Ox-2	"	"	12.5	"	"	358	12
2MWS-Ox-3	"	"	25.0	"	"	363	12

Table C-17 SUMMARY OF TEST PARAMETERS FOR RIT SPREADING TESTS



Figure C-71 Melt depth and temperature profiles at 2, 5, 10, and 25 seconds for the ECKOTAS-2 test

Test characteristics and the corresponding code input for the dry spreading test on concrete, 3MDC-OX-1, are summarized in Table C-18. As is evident, the melt thermal-physical property data recommended by the experimentalist's was used as part of the input, while the code default siliceous concrete composition was selected since the concrete property data was not provided.

The calculated leading edge penetration vs. time is compared to the test data in Figure C-46, while local melt substrate temperature and post-spreading material profile predictions are compared in Figures C-47 to C-49. The code under-predicts the spreading velocity early in the transient, but in general captures the overall characteristics. As is evident from Figure C-47 and C-48, the code seems to overpredict the heat transfer to the substrate, particularly at the 110 cm location. The information in Figure C-49 indicates that the code provides a reasonable estimate of the debris distribution following the spreading transient.

Test characteristics and the corresponding code input for the second dry spreading test, 3MDS-OX-1, are summarized in Table C-19. This was a counterpart test to 3MDC-OX-1 with the substrate material being the parametric variation (i.e. steel vs. concrete). The melt thermal-physical property data recommended by the experimenters was used as input, while the code default steel property data were utilized for the substrate.

The calculated leading edge penetration vs. time is compared to the test data in Figure C-50, while the post-spreading material profile prediction is compared in Figure C-51. As for the previous test with the concrete substrate, the spreading velocity early in the sequence is under-predicted, but the overall characteristics are captured. Data in Figure C-51 indicates that the code reasonably predicts the debris distribution following the spreading transient.

Test characteristics and corresponding code input for the 3MDS-OX-2 test are summarized in Table C-20. This was a counterpart test to 3MDS-OX-1 with initial melt temperature being the parametric variation (i.e. 1473 K vs. 1373 K).

Comparisons of leading edge penetration and material distribution following spreading with the test data are provided in Figures C-52 and C-53, respectively. In terms of melt penetration, the code seems to do a better job in predicting the leading edge penetration rate for this test compared to the other two dry experiments that had higher initial melt temperatures (see Table C-17). The information in Figure C-53 indicates that the code does a fair job in estimating the debris distribution following spreading.

Table C-18 INPUT FILE DATA SHEET FOR RIT TEST 3MDC-OX-1 WITH A DRY CONCRETE CHANNEL

Test parameter	Value
Test name	3MDC-Ox-1
Melt composition (wt %)	30 CaO, 70 B ₂ O ₃
Melt delivery technique	Melt poured from a furnace through a 2.8 cm
	diameter nozzle at an average rate of 0.75 kg/sec into
	one end of a rectilinear spreading channel.
Melt temperature	1473 К
Total pour mass	30.0 kg
Substrate material	Siliceous concrete
Spreading geometry	1-D channel, 347.5 cm long by 20 cm wide
Code input parameter(s)	Value(s)
Melt composition	30 CaO, 70 B ₂ O ₃
Melt pour temperature	1473 К
Melt oxide phase solidus – liquidus	1225 К – 1323 К
Melt metal phase solidus – liquidus	1810 – 1820 K
Melt pour rate and duration	0.75 kg/sec over 40.0 sec
Melt material property evaluation	User-specified property data used: $c_s = 1530 \text{ J/kg-K}$,
	$c_1 = 2200 \text{ J/kg-K}, \Delta h_f = 460 \text{ kJ/kg}, \rho_s = 3300 \text{ kg/m}^3, \rho_1$
	= 2500 kg/m ³ , k _s = 2.0 W/m-K, k _l = 3.0 W/m-K, μ_0 =
	0.2 Pa-s, σ = 0.75 N-m, M = 65.1 g/mole, and ϵ = 0.3
Substrate composition	Default siliceous concrete
Substrate initial temperature	298 K
Substrate material properties evaluation	Code subroutines
Substrate solidus - liquidus temperatures	1403 – 1523 K (Code default values)
Substrate nodalization	At each substrate nodal location, first cell is 2.0 mm,
	second is 3.0 mm, and these are followed by ten 5.0
	mm cells. All nodes cell-centered.
Spreading cavity nodalization	Accumulator: modeled as a single cell that is 40 cm
	wide, 25 cm long, and 5 cm deep. Channel: modeled
	using 120 cells; each is 40 cm wide and 5.33 cm long.
	All nodes cell-centered.
Cavity condition	Dry
Upper atmosphere temperature	300 K
Upper atmosphere emissivity	0.6
Ambient pressure	0.1 MPa
Melt/substrate heat transfer coefficient model	Locally, largest of Dittus – Boelter and Bradley slag
Malt/auhatrata interfacial heat transfer	
resistance	
Constant in Ramacciotti correlation	4.75 (Average for oxide type [15])
Solid-fraction variation	See Figure C-23
Timestep	0.02 seconds







Figure C-73 Comparison of substrate thermal response predictions with RIT 3MDC-Ox-1 data 31 cm from channel inlet



Figure C-74 Comparison of substrate thermal response predictions with RIT 3MDC-Ox-1 data 110 cm from channel inlet



Figure C-75 Comparison of posttest debris profile prediction with RIT 3MDC-Ox-1 data

Test parameter	Value
Test name	3MDS-Ox-1
Melt composition (wt %)	30 CaO, 70 B ₂ O ₃
Melt delivery technique	Melt poured from a furnace through a 2.8 cm
1	diameter nozzle at an average rate of 0.75 kg/sec into
	one end of a rectilinear spreading channel.
Melt temperature	1473 K
Total pour mass	30.0 kg
Substrate material	Steel
Spreading geometry	1-D channel, 347.5 cm long by 20 cm wide
Code input parameter(s)	Value(s)
Melt composition	30 CaO, 70 B ₂ O ₃
Melt pour temperature	1473 K
Melt oxide phase solidus – liquidus	1225 К – 1323 К
Melt metal phase solidus – liquidus	1810 K – 1820 K
Melt pour rate and duration	0.75 kg/sec over 40.0 sec
Melt material property evaluation	User-specified property data used: $c_s = 1530 \text{ J/kg-K}$,
	$c_1 = 2200 \text{ J/kg-K}, \Delta h_f = 460 \text{ kJ/kg}, \rho_s = 3300 \text{ kg/m}^3, \rho_1$
	= 2500 kg/m ³ , k _s = 2.0 W/m-K, k _l = 3.0 W/m-K, μ_0 =
	0.2 Pa-s, σ = 0.75 N-m, M = 65.1 g/mole, and ε = 0.3
Substrate composition	Steel (code default composition)
Substrate initial temperature	298 K
Substrate material properties evaluation	Code subroutines
Substrate solidus - liquidus temperatures	1810 K – 1811 K (code default values)
Substrate nodalization	At each substrate nodal location, first cell is 2.0 mm,
	second is 3.0 mm, and these are followed by ten 5.0
	mm cells. All nodes cell-centered.
Spreading cavity nodalization	Melt injection zone: modeled as a single cell that is 2.8
	cm long, 20 cm wide, and flush with the spreading
	surface. Channel: modeled using 80 cells; each is
	4.31 cm long and 20 cm wide. All nodes cell-centered.
Cavity condition	
Upper atmosphere temperature	300 K
Opper atmosphere emissivity	0.0 0.1 MDs
Ambient pressure	0.1 MPa
Melt/substrate heat transfer coefficient model	Dillus – Boeiler
weil/substrate internacial neat transfer	U
Constant in Ramacojotti correlation	4.75 (Average for oxide type [15])
Solid-fraction variation	See Figure C-23
Timesten	0.02 seconds

Table C-19 INPUT FILE DATA SHEET FOR RIT TEST 3MDS-OX-1 WITH A DRY STEEL CHANNEL



Figure C-76 Leading edge comparison for RIT 3MDS-Ox-1 spreading test



Figure C-77 Comparison of posttest debris profile prediction with RIT 3MDS-Ox-1 data

Table C-20 INPU	T FILE DATA SHEET	FOR RIT TEST 3MDS-OX-2	WITH A DRY STEEL CHANNEL
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Test parameter	Value
Test name	3MDS-Ox-2
Melt composition (wt %)	30 CaO, 70 B ₂ O ₃
Melt delivery technique	Melt poured from a furnace through a 2.8 cm diameter nozzle at an average rate of 0.75 kg/sec into
	one end of a rectilinear spreading channel.
Melt temperature	1373 К
Total pour mass	30.0 kg
Substrate material	Steel
Spreading geometry	1-D channel, 347.5 cm long by 20 cm wide
Code input parameter(s)	Value(s)
Melt composition	30 CaO, 70 B ₂ O ₃
Melt pour temperature	1373 К
Melt oxide phase solidus – liquidus	1225 К – 1323 К
Melt metal phase solidus – liquidus	1810 K – 1820 K
Melt pour rate and duration	0.75 kg/sec over 40.0 sec
Melt material property evaluation	User-specified property data used: c _s = 1530 J/kg-K,
	$c_1 = 2200 \text{ J/kg-K}, \Delta h_f = 460 \text{ kJ/kg}, \rho_s = 3300 \text{ kg/m}^3, \rho_1$
	= 2500 kg/m ³ , k _s = 2.0 W/m-K, k _l = 3.0 W/m-K, μ_0 =
	0.2 Pa-s, σ = 0.75 N-m, M = 65.1 g/mole, and ϵ = 0.3
Substrate composition	Steel (code default composition)
Substrate initial temperature	298 K
Substrate material properties evaluation	Code subroutines
Substrate solidus - liquidus temperatures	1810 K – 1811 K (code default values)
Substrate nodalization	At each substrate nodal location, first cell is 2.0 mm,
	second is 3.0 mm, and these are followed by ten 5.0
	mm cells. All nodes cell-centered.
Spreading cavity nodalization	Melt injection zone: modeled as a single cell that is 2.8
	cm long, 20 cm wide, and flush with the spreading
	surface. Channel: modeled using 80 cells; each is
	4.31 cm long and 20 cm wide. All nodes cell-centered.
Cavity condition	Dry
Upper atmosphere temperature	300 K
Upper atmosphere emissivity	0.6
Ambient pressure	0.1 MPa
Melt/substrate heat transfer coefficient model	Dittus – Boelter
Melt/substrate interfacial heat transfer	0
resistance	
Constant in Ramacciotti correlation	4.75 (Average for oxide type [15])
Solid-fraction variation	See Figure C-23
Timestep	0.02 seconds



Figure C-78 Leading edge comparison for RIT 3MDS-Ox-2 spreading test



Figure C-79 Comparison of posttest debris profile prediction with RIT 3MDS-Ox-2 data

The next three spreading tests in the RIT series all were conducted with a 12 cm water depth with a small amount of subcooling. These tests were more difficult to execute, and as a result, the only data that was reported was the maximum melt penetration distance. Thus, it was not possible to compare spreading velocities or posttest debris profiles with the test results. On this basis, the plots of spreading rate and debris distribution are provided for these three tests to be consistent with the material presented for the others.

The primary parametric variation in the wet spreading tests was the mass of the melt, which increased from 5 to 12.5 and then 25 kg for the three tests. The melt pour rate was the same as that used for the dry tests, the spreading surface was steel, and initial melt temperature was fixed at 1373 K.

The tables of test characteristics and modeling assumptions, leading edge penetration, and posttest material distribution for tests 2MWS-OX-1, -2, and -3 are provided in sequential order at the end of this subsection. Examination of this collection of information indicates that the code predictions and test data exhibit a systematic increase in ultimate melt penetration distance with pour mass when all other parameters are fixed. Unlike other experiments in this and other test series that were conducted under cavity dry conditions, the code predicts substantial debris solidification at the leading edge near the end of the spreading transient which is attributable to the increased heat transfer rate to overlying water. As shown, the code locally nodalizes the solidified debris into the basemat mesh so that the solidified material becomes a physical impediment that the melt must spread over to further propagate down the channel.

Test reserves	Value
Test parameter	
Molt composition (wt %)	20.000 70 P-0-
Melt delivery technique	Molt noured from a furnade through a 0.8 cm
Meit denvery technique	diameter pozzle et en evereze rete ef 0.75 kg/ace inte
	one end of a rectilinear aprending channel
Melt temperature	1372 K
Total pour mass	5 0 kg
Substrate material	Steel
Spreading geometry	1-D channel 200 cm long by 20 cm wide
Spreading geometry	1-D channel, 200 chi long by 20 chi wide
Code input parameter(s)	Value(s)
Melt composition	30 CaO, 70 B ₂ O ₃
Melt pour temperature	1373 K
Melt oxide phase solidus – liquidus	1225 К – 1323 К
Melt metal phase solidus – liquidus	1810 – 1820 K
Melt pour rate and duration	0.75 kg/sec over 6.66 sec
Melt material property evaluation	User-specified property data used: c _s = 1530 J/kg-K,
	$c_1 = 2200 \text{ J/kg-K}, \Delta h_f = 460 \text{ kJ/kg}, \rho_s = 3300 \text{ kg/m}^3, \rho_1$
	= 2500 kg/m ³ , k _s = 2.0 W/m-K, k _l = 3.0 W/m-K, μ_0 =
	0.2 Pa-s, σ = 0.75 N-m, M = 65.1 g/mole, and ϵ = 0.3
Substrate composition	Steel (code default composition)
Substrate initial temperature	298 K
Substrate material properties evaluation	Code subroutines
Substrate solidus - liquidus temperatures	1403 – 1523 K (Code default values)
Substrate nodalization	At each substrate nodal location, first cell is 2.0 mm,
	second is 3.0 mm, and these are followed by ten 5.0
	mm cells. All nodes cell-centered.
Spreading cavity nodalization	Melt injection zone: modeled as a single cell that is 2.8
	cm long, 20 cm wide, and flush with the spreading
	surface. Channel: modeled using 80 cells; each is
	4.31 cm long and 20 cm wide. All nodes cell-centered.
Cavity condition	Wet
Water temperature (subcooling)	353 (20) K
Ambient pressure	0.1 MPa
Water depth	12 cm
Melt/substrate heat transfer coefficient model	Dittus – Boelter
Melt/substrate interfacial heat transfer	0
resistance	
Constant in Ramacciotti correlation	4.75 [Average for oxide type [15]]
Solid-iraction variation	See Figure C-23
Timestep	0.02 seconds

Table C-21 INPUT FILE DATA SHEET FOR RIT TEST 2MWS-OX-1 WITH A WET STEEL CHANNEL



Figure C-80 Leading edge comparison for RIT 2MWS-Ox-1 spreading test



Figure C-81 Comparison of posttest debris profile prediction with RIT 2MWS-Ox-1 data

Toot noromotor	Value
Test parameter	
Molt composition (wt %)	20 CoO 70 PoOo
Melt delivery technique	Molt noured from a furnace through a 2.8 am
Meit denvery teeninque	diameter pozzle at an average rate of 0.75 kg/sec into
	one end of a rectilinear spreading channel
Melt temperature	1373 K
Total pour mass	12.5 kg
Substrate material	Steel
Spreading geometry	1-D channel 200 cm long by 20 cm wide
	The channel, 200 cm long by 20 cm white
Code input parameter(s)	Value(s)
Melt composition	30 CaO, 70 B ₂ O ₃
Melt pour temperature	1373 К
Melt oxide phase solidus – liquidus	1225 K – 1323 K
Melt metal phase solidus – liquidus	1810 K – 1820 K
Melt pour rate and duration	0.75 kg/sec over 16.66 sec
Melt material property evaluation	User-specified property data used: c _s = 1530 J/kg-K,
	$c_1 = 2200 \text{ J/kg-K}, \Delta h_f = 460 \text{ kJ/kg}, \rho_s = 3300 \text{ kg/m}^3, \rho_1$
	= 2500 kg/m ³ , k _s = 2.0 W/m-K, k _l = 3.0 W/m-K, μ_0 =
	0.2 Pa-s, σ = 0.75 N-m, M = 65.1 g/mole, and ϵ = 0.3
Substrate composition	Steel (code default composition)
Substrate initial temperature	298 K
Substrate material properties evaluation	Code subroutines
Substrate solidus - liquidus temperatures	1810 K – 1811 K (code default values)
Substrate nodalization	At each substrate nodal location, first cell is 2.0 mm,
	second is 3.0 mm, and these are followed by ten 5.0
	mm cells. All nodes cell-centered.
Spreading cavity nodalization	Melt injection zone: modeled as a single cell that is 2.8
	cm long, 20 cm wide, and flush with the spreading
	surface. Channel: modeled using 80 cells; each is
	2.46 cm long and 20 cm wide. All nodes cell-centered.
Cavity condition	Wet
Water temperature (subcooling)	358 (15) K
Ambient pressure	0.1 MPa
Water depth	12 cm
Melt/substrate heat transfer coefficient model	Dittus – Boelter
Melt/substrate interfacial heat transfer	0
resistance	
Constant in Ramacciotti correlation	4.75 (Average for oxide type [15])
Solid-fraction variation	See Figure C-23
Timestep	0.02 seconds

Table C-22 INPUT FILE DATA SHEET FOR RIT TEST 2MWS-OX-2 WITH A WET STEEL CHANNEL



Figure C-82 Leading edge comparison for RIT 2MWS-Ox-2 spreading test



Figure C-83 Comparison of posttest debris profile prediction with RIT 2MWS-Ox-2 data

Test parameter	Value
Test name	2MWS-Ox-3
Melt composition (wt %)	30 CaO, 70 B ₂ O ₃
Melt delivery technique	Melt poured from a furnace through a 2.8 cm
	diameter nozzle at an average rate of 0.75 kg/sec into
	one end of a rectilinear spreading channel.
Melt temperature	1373 К
Total pour mass	25.0 kg
Substrate material	Steel
Spreading geometry	1-D channel, 200 cm long by 20 cm wide
Code input parameter(s)	Value(s)
Melt composition	30 CaO, 70 B ₂ O ₃
Melt pour temperature	1373 К
Melt oxide phase solidus – liquidus	1225 К – 1323 К
Melt metal phase solidus – liquidus	1810 K – 1820 K
Melt pour rate and duration	0.75 kg/sec over 33.33 sec
Melt material property evaluation	User-specified property data used: cs = 1530 J/kg-K,
	$c_1 = 2200 \text{ J/kg-K}, \Delta h_f = 460 \text{ kJ/kg}, \rho_s = 3300 \text{ kg/m}^3, \rho_1$
	= 2500 kg/m ³ , k _s = 2.0 W/m-K, k _l = 3.0 W/m-K, μ_0 =
	0.2 Pa-s, σ = 0.75 N-m, M = 65.1 g/mole, and ϵ = 0.3
Substrate composition	Steel (code default composition)
Substrate initial temperature	298 K
Substrate material properties evaluation	Code subroutines
Substrate solidus - liquidus temperatures	1810 K – 1811 K (code default values)
Substrate nodalization	At each substrate nodal location, first cell is 2.0 mm,
	second is 3.0 mm, and these are followed by ten 5.0
	mm cells. All nodes cell-centered.
Spreading cavity nodalization	Melt injection zone: modeled as a single cell that is 2.8
	cm long, 20 cm wide, and flush with the spreading
	surface. Channel: modeled using 80 cells; each is
	2.46 cm long and 20 cm wide. All nodes cell-centered.
Cavity condition	Wet
Water temperature (subcooling)	363 (10) K
Ambient pressure	0.1 MPa
Water depth	12 cm
Melt/substrate heat transfer coefficient model	Dittus – Boelter
Melt/substrate interfacial heat transfer	0
resistance	
Constant in Ramacciotti correlation	4.75 (Average for oxide type [15])
Solid-fraction variation	See Figure C-23
Timestep	0.02 seconds

Table C-23 INPUT FILE DATA SHEET FOR RIT TEST 2MWS-OX-3 WITH A WET STEEL CHANNEL



Figure C-84 Leading edge comparison for RIT 2MWS-Ox-3 spreading test



Figure C-85 Comparison of posttest debris profile prediction with RIT 2MWS-Ox-3 data
SPREADING TESTS WITH MOLTEN STEEL

Following the benchmarking exercise against oxide simulant melt spreading tests, the code was further exercised against tests conducted with molten iron and stainless steel. Tests that fall into this category include those carried out by Eppinger et al.^[32] in the KATS test facility, and the SPREAD tests conducted in Japan by Suzuki et al.^[28] The code assessment against these tests is provided in this section.

KATS Iron Spreading Tests

As previously discussed, these tests involved spreading of high temperature oxide and iron melts that were generated by a modified iron-alumina thermite reaction. The previous subsection addressed spreading tests conducted with the oxide phase of that reaction, while the current discussion focuses on the spreading tests with the metal phase.

The KATS-12, -13, and -14 metal tests were selected for analysis (see Table C-1). KATS-12 and -13 parameterized on substrate material, with KATS-12 utilizing ceramic (Corderite), and KATS-13 utilizing concrete. KATS-14 was also conducted with a ceramic substrate, but the melt pour rate was reduced relative to KATS-12.

The accumulator design in these tests was novel, with a base that was elevated slightly above that of the spreading surface. The general characteristics were shown previously in Figure C-24, while the corresponding dimensions for the metal tests are summarized in Table C-10. As is evident, a small incline connected the accumulator box to the spreading channel. An effort was made to mock up the details of the melt accumulator, gate, and incline leading to the spreading channel with the meshing scheme.

Test characteristics and the corresponding model input that was developed for the KATS-12 metal test are summarized in Table C-24. The ceramic substrate thermal-physical properties were input as user-defined quantities based on project documentation.^[32] The iron melt properties were calculated using code subroutines. As discussed in Reference [15], the approach for the metal tests was to set the constant in the Ramacciotti viscosity correlation to the best-fit value for the oxide tests (i.e., $C_R = 7.26$), and then to develop statistical data on the melt-substrate interfacial heat transfer resistance, h_r , that best fit the collection of steel spreading penetration test data. The results shown in this section use the best fit value of $h_r = 4800 \text{ W/m}^2\text{-K}$.^[15]

Test parameter	Value
Test name	KATS-12, metal, ceramic channel
Melt composition (wt %)	100 Fe
Melt delivery technique	Melt poured into an accumulator box that was 17.0
	cm wide, 30.2 cm long, and 7.0 cm above the
	spreading surface. Pour initiated by opening a gate
	to the spreading channel.
Melt temperature	2170 К
Total pour mass	135 kg
Substrate material	Cordierite
Spreading geometry	1-D channel, 15 m long by 15 cm wide
Code input parameter(s)	Value(s)
Melt composition (wt %)	100 Fe
Melt pour temperature	2170 К
Melt oxide phase solidus – liquidus	1893 K – 1923 K
Melt metal phase solidus – liquidus	1806 К – 1816 К
Melt pour rate and duration	Linear decrease in pour rate from 40.3 kg/sec to
	zero over 6.7 second interval
Melt material property evaluation	Code subroutines
Substrate composition	Corderite (modeled using user-specified material
-	input properties)
Substrate initial temperature	298 K
Substrate material properties evaluation	$c_s = c_l = 840 \text{ J/kg-K}, \Delta h_f = 1.0 \text{ MJ/kg}, \rho_s = \rho_l = 2200$
	kg/m^3 , $k_s = k_l = 3.8 W/m-K$, and $\epsilon = 0.3$
Substrate solidus - liquidus temperatures	1893 K – 1923 K
Substrate nodalization	At each substrate nodal location, twelve 6.0 mm
	cells are used; all nodes are cell-centered.
Spreading cavity nodalization	Accumulator: modeled as a single cell that is 17.0
	cm wide, 30.2 cm long, and 7.0 cm above the
	channel surface. Gate: modeled as a single cell that
	is 8 cm wide, 4.3 cm long, and 7.0 cm above the
	channel. Incline down to channel: modeled as a
	single cell that is 10 cm long, 15 cm wide, and 3.5
	cm above the channel. Channel: 12 m modeled
	using 120 cells; each is 15 cm wide and 10 cm long.
	All nodes cell-centered.
Cavity condition	Dry
Upper atmosphere temperature	300 K
Upper atmosphere emissivity	0.7
Ambient pressure	0.1 MPa
Melt/substrate heat transfer coefficient model	Dittus - Boelter
Melt/substrate interfacial heat transfer	4800 W/m ² -K
resistance	
Constant used in Ramacciotti correlation	7.26
Solid-fraction variation	See Figure C-23
Timestep	0.02 seconds

Table C-60 INPUT FILE DATA SHEET FOR THE KATS-12 METAL MELT TEST WITH CERAMIC CHANNEL

The calculated leading edge penetration vs. time is compared to the KATS-12 metal test data in Figure C-60, while local melt temperature and post-spreading material profile predictions are compared with data in Figures C-61 and C-62, respectively. As for the counterpart KATS-12 oxide test, the pour rate was relatively high and so the spreading rate was initially dominated by inertial effects. As a result, viscous forces that retard spreading do not show up until late in the transient; see Figure C-60.

As is evident from Figure C-61, peak melt temperature is predicted quite well 1 m from the melt accumulator, but is under-predicted by ~ 80 K 3.5 m from the The debris profile comparison in Figure C-62 shows some accumulator. discrepancies between the calculation and the experiment. The large accumulation that develops at the leading edge in the calculation is a byproduct of the melt flowrate function for the test, viz., initially large, and then a linear decline. The large structure to the left in Figure C-62 is the melt accumulator. As discussed earlier, this design may have caused overshoot of some (unknown) distance of the spreading surface and a corresponding initial spreading velocity that would exceed what the code would calculate based on gravity-driven spreading alone. This may explain at least part of the discrepancy in initial spreading rate seen early in Figure C-60 since the code assumes continuous frictional flow through the mesh with no bypass.



Figure C-86 Leading edge penetration comparison for the KATS-12 metal spreading test



Figure C-87 Comparison of local melt temperature predictions with KATS-12 metal data



Figure C-88 Comparison of posttest debris profile prediction with KATS-12 metal data

Test characteristics and the corresponding modeling input data for the KATS-13 metal test are summarized in Table C-25. Code subroutines were used to evaluate melt properties, and the code default composition for siliceous concrete was assumed since the data report did not provide this information. Local melt temperature and post-spreading material profile predictions are compared with the data in Figures C-64 and C-65, respectively. As for KATS-12, this was a high flowrate test, and so the possibility exists that the melt overshot some distance of the spreading surface near the accumulator, leading to an apparent spreading velocity that was initially larger than the prediction.

As is evident from Figure C-64, peak melt temperature 1 m from the gate was under-predicted by ~ 70 K, and the discrepancy grows to almost 100 K at the 3.5 m distance. There are also some discrepancies in the overall shape of the posttest debris distribution (Figure C-65). The code predicts up to 1 cm of basemat erosion, but data on basemat erosion was not collected as part of the posttest exams for this experiment.

Test characteristics and the corresponding code input for the KATS-14 metal test are summarized in Table C-26. As for KATS-12, the recommended substrate thermal-physical property data was used, but the melt properties were calculated using code subroutines. The calculated leading edge

penetration versus time is compared to the test data in Figure C-66, while local melt temperature and post-spreading material profile predictions are compared with the data in Figures C-67 and C-68, respectively. The pour rate in this test was lower compared to the counterpart test KATS-12, and so the time interval over which the spreading characteristics were governed by inertial effects was reduced. In general, the code does a much better job capturing the initial rate of melt spreading from the accumulator box in comparison to KATS-12.

Examination of the melt temperature data in Figure C-67 indicates that despite discrepancies in melt arrival times, peak melt temperatures are predicted to within ~ 40 K at the 1 meter location, ~ 100 K at the 4 m location, and ~ 50 K at the 7 m location. As shown in Figure C-68, there are again some discrepancies in the overall shape of the debris, but the code does a good job of replicating the shape of the basemat erosion profile; for this experiment, that information was provided.

Test parameter	Value
Test name	KATS-13, metal, concrete channel
Melt composition (wt %)	100 Fe
Melt delivery technique	Melt poured into an accumulator box that was 17.0
	cm wide, 30.2 cm long, and 9.0 cm above the
	spreading surface. Pour initiated by opening a gate
	to the spreading channel.
Melt temperature	2220 K
Total pour mass	135 kg
Substrate material	Siliceous concrete
Spreading geometry	1-D channel, 15 m long by 15 cm wide
Code input parameter(s)	Value(s)
Melt composition (wt %)	100 Fe
Melt pour temperature	2220 К
Melt oxide phase solidus – liquidus	1403 K – 1523 K
Melt metal phase solidus – liquidus	1806 K – 1816 K
Melt pour rate and duration	Linear decrease in pour rate from 40.3 kg/sec to
	zero over 6.7 second interval
Melt material property evaluation	Code subroutines
Substrate composition	Default siliceous concrete
Substrate initial temperature	298 K
Substrate material properties evaluation	Code subroutines
Substrate solidus - liquidus temperatures	1403 – 1523 K (Code default values)
Substrate nodalization	At each substrate nodal location, twelve 6.0 mm
	cells are used; all nodes cell-centered.
Spreading cavity nodalization	Accumulator: modeled as a single cell that is 17.0
	cm wide, 30.2 cm long, and 9.0 cm above the
	channel surface. Gate: modeled as a single cell that
	is 8 cm wide, 4.3 cm long, and 9.0 cm above the
	channel. Incline down to channel: modeled as a
	single cell that is 10 cm long, 15 cm wide, and 4.5
	cm above the channel. Channel: 12 m modeled
	using 120 cells; each is 15 cm wide and 10 cm long.
	All nodes cell-centered.
Cavity condition	Dry
Upper atmosphere temperature	300 K
Upper atmosphere emissivity	0.7
Ambient pressure	0.1 MPa
Melt/substrate heat transfer coefficient model	Locally, largest of Dittus – Boelter and Bradley slag
	film heat transfer coefficients
Meit/substrate interfacial heat transfer	4800 W/m²-K
resistance	7.06
Constant used in Ramacciotti correlation	(.20 Dec Figure 0.02
Solid-iraction variation	See Figure C-23
Timestep	0.01 seconds

Table C-25 INPUT FILE DATA SHEET FOR THE KATS-13 METAL MELT TEST WITH CONCRETE CHANNEL



Figure C-89 Leading edge penetration comparison for the KATS-13 metal spreading test



Figure C-90 Comparison of local melt temperature predictions with KATS-13 metal data



Figure C-91 Comparison of posttest debris profile prediction with KATS-13 metal data

Test parameter	Value
Test name	KATS-14, metal, ceramic channel
Melt composition (wt %)	100 Fe
Melt delivery technique	Melt poured into an accumulator box that was 18.0
	cm wide, 20.0 cm long, and 5.0 cm above the
	spreading surface. Pour initiated by opening a gate
	to the spreading channel.
Melt temperature	2440 K
Total pour mass	154 kg
Substrate material	Cordierite
Spreading geometry	1-D channel, 12 m long by 15 cm wide
Code input parameter(s)	Value(s)
Melt composition (wt %)	100 Fe
Melt pour temperature	2440 K
Melt oxide phase solidus – liquidus	1893 K – 1923 K
Melt metal phase solidus – liquidus	1806 K – 1816 K
Melt pour rate and duration	Linear increase in pour rate from 6.16 to 9.24
	kg/sec over a 20 second interval
Melt material property evaluation	Code subroutines
Substrate composition	Corderite (modeled using user-specified material
	input properties)
Substrate initial temperature	298 К
Substrate material properties evaluation	$c_s = c_l = 840 \text{ J/kg-K}, \Delta h_f = 1.0 \text{ MJ/kg}, \rho_s = \rho_l = 2200$
	kg/m^3 , $k_s = k_l = 3.8 W/m$ -K, and $\epsilon = 0.3$
Substrate solidus - liquidus temperatures	1893 K – 1923 K
Substrate nodalization	At each substrate nodal location, twelve 6.0 mm
	cells are used; all nodes are cell-centered.
Spreading cavity nodalization	Accumulator: modeled as a single cell that is 18.0
	cm wide, 20.0 cm long, and 5.0 cm above the
	channel surface. Gate: modeled as a single cell that
	is 14.0 cm wide, 4.3 cm long, and 5.0 cm above the
	channel. Incline down to channel: modeled as a
	single cell that is 3.0 cm long, 15 cm wide, and 2.5
	cm above the channel. Channel: 12 m modeled
	using 120 cells; each is 15 cm wide and 10 cm long.
	All nodes cell-centered.
Cavity condition	Dry
Upper atmosphere temperature	300 K
Upper atmosphere emissivity	0.7
Ambient pressure	0.1 MPa
Melt/substrate heat transfer coefficient model	Dittus - Boelter
Melt/substrate interfacial heat transfer	4800 W/m ² -K
resistance	
Constant used in Ramacciotti correlation	7.26
Solid-fraction variation	See Figure C-23
Timestep	0.02 seconds

Table C-26 INPUT FILE DATA SHEET FOR THE KATS-14 METAL MELT TEST WITH CERAMIC CHANNEL







Figure C-93 Comparison of local melt temperature predictions with KATS-14 metal data



Figure C-94 Comparison of posttest debris profile prediction with KATS-14 metal data

SPREAD Stainless Steel Spreading Tests

These tests involved spreading of stainless steel melts in test sections that mimicked the key features of the GE BWR Mark I containment. In particular, melt was poured into a cylindrical cavity that represented the reactor pedestal. The melt then spread into a large open region simulating the cavity annulus through a doorway. Although many spreading tests were conducted in this program, minimal data was reported in the open literature. Sufficient information was gathered to examine two tests: i) Test 15, which was a dry experiment, and ii) Test 21, which was similar to Test 15 but with water.

Test characteristics and code input for Test 15 are summarized in Table C-27, while comparisons with maximum melt penetration distance and the posttest debris profile are provided in Figures C-69 and C-70, respectively. The analogous set of information for Test 21 that was conducted with water present is provided in Table C-28 and Figures C-71 and C-72, respectively. Both tests used stainless steel melts with siliceous concrete. MELTSPREAD was originally developed for Mark I applications; thus, the code has an automated meshing scheme for this containment geometry. This option was used to generate the cavity nodalization for these tests. The melt spreading angle outside the pedestal doorway was set to the experimentally observed value of 130°. Code subroutines were used to calculate the melt and substrate properties.

Table C-27 INPUT FILE DATA SHEET FOR SPREAD TEST 15 WITH METAL MELT IN A MOCKUP OF THE MARK I CONTAINMENT WITH DRY CONCRETE FLOOR

Test name SPREAD Test 15 Meit composition (wt %) 70 Fe, 20 Cr, 10 N (stainless steel) Melt delivery technique Meit poured into a 17.5 cm radius cylindrical cavity that simulated the pedestal of a Mark I containment. Melt megrerature 1804 K Total pour mass 63.6 kg Substrate material Siliceous concrete Spreading geometry Mockup of a Mark I containment: A 17.5 cm inner radius cylindrical cavity with a 5 cm wide doorway leading to an annular spreading region with a radius of 1.275 m. The wall thickness of the pedestal was 5 cm. Code input parameter(s) Value(s) Melt our temperature 1804 K Melt our temperature 1804 K Melt our temperature 1804 K Melt neut al phase solidus – liquidus 1403 K – 1523 K Melt metral phase solidus – liquidus 1601 K – 1727 K Melt material property evaluation Code subroutines Substrate naterial properties evaluation Code subroutines Substrate initial temperature 298 K Substrate nodalization At each substrate nodal location, six 5.0 mm cells followed by six 10 mm cells; all nodes cell-centered. Spreading cavity nodalization At each substrate nodal location, six 6.0 mm cel	Test parameter	Value
Mett composition (wt %) 70 Fe, 20 Cr, 10 Ni (stainless steel) Melt delivery technique Melt poured into a 17.5 cm radius cylindrical cavity that simulated the pedestal of a Mark I containment. Melt temperature 1804 K Total pour mass 63.6 kg Substrate material Siliceous concrete Spreading geometry Mockup of a Mark I containment: A 17.5 cm inner radius cylindrical cavity with a 5 cm wide doorway leading to an annular spreading region with a radius of 1.275 m. The wall thickness of the pedestal was 5 cm. Code input parameter(s) Value(s) Melt composition (wt %) 70 Fe, 20 Cr, 10 Ni Melt outer phase solidus - liquidus 1403 K - 1523 K Melt metal phase solidus - liquidus 1671 K - 1727 K Melt metal phase solidus - liquidus 1671 K - 1727 K Melt metal phase solidus - liquidus 1671 K - 1727 K Melt material property evaluation Code subroutines Substrate composition Default siliceous concrete Substrate nodalization Default siliceous concrete Substrate nodalization At each substrate nodal location, six 5.0 mm cells followed by six 10 mm cells; all nodes cell-centered. Spreading cavity nodalization At each substrate nodal location, six 3.0 mm cells anodes t	Test name	SPREAD Test 15
Melt delivery technique Melt poured into a 17.5 cm radius cylindrical cavity that simulated the pedestal of a Mark I containment. Melt temperature 1804 K Total pour mass 63.6 kg Substrate material Siliceous concrete Spreading geometry Mockup of a Mark I containment: A 17.5 cm inner radius cylindrical cavity with a 5 cm wide doorway leading to an annular spreading region with a radius of 1.275 m. The wall thickness of the pedestal was 5 cm. Code input parameter(s) Yo Fe, 20 Cr, 10 Ni Melt composition (wt %) 70 Fe, 20 Cr, 10 Ni Melt toxide phase solidus - liquidus 1403 K - 1523 K Melt toxide phase solidus - liquidus 1671 K - 1727 K Melt metarial property evaluation Code subroutines Substrate composition Default siliceous concrete Substrate material property evaluation Code subroutines Substrate material properties evaluation Code subroutines Substrate material properties evaluation Code subroutines Substrate modalization At cach substrate nodal location, six 5.0 mm cells followed by six 10 mm cells; all nodes cell-centered. Syreading cavity nodalization At cach substrate nodal location, six 5.0 mm cells followed to synead outside the doorway with a spreading angle of 130°. The distance from the	Melt composition (wt %)	70 Fe, 20 Cr, 10 Ni (stainless steel)
Intaliated the pedestal of a Mark I containment. Melt temperature 1804 K Total pour mass 63.6 kg Substrate material Siliceous concrete Spreading geometry Mockup of a Mark I containment: A 17.5 cm inner radius cylindrical cavity with a 5 cm wide doorway leading to an annular spreading region with a radius of 1.275 m. The wall thickness of the pedestal was 5 cm. Code input parameter(s) Value(s) Melt composition (wt %) 70 Fe, 20 Cr, 10 Ni Melt oxied phase solidus - liquidus 1403 K - 1523 K Melt metal phase solidus - liquidus 1671 K - 1727 K Melt pour rate and duration Steady pour rate of 9.5 kg/sec over a 6.7 second interval Melt material property evaluation Code subroutines Substrate composition Default siliceous concrete Substrate nodalization At each substrate nodal location, six 5.0 mm cells followed by six 10 mm cells; all nodes cell-centered. Substrate nodalization At each substrate nodal location, six 5.0 mm cells assumed pour into the sum which was atken to have a radius of 10 cm and was flux with the concrete surface; balance of pedestal interior meshed with 3 nodes that were 2.5 cm wide. As concluded by the experimenters, the melt was assumed to spreading angle of 130°. The distance from the doorway was meshed with 61 cells that were 2.17 cm wide. All nodes cell-centered. <t< td=""><td>Melt delivery technique</td><td>Melt poured into a 17.5 cm radius cylindrical cavity</td></t<>	Melt delivery technique	Melt poured into a 17.5 cm radius cylindrical cavity
Melt temperature 1804 K Total pour mass 63.6 kg Substrate material Siliceous concrete Spreading geometry Mockup of a Mark I containment: A 17.5 cm inner radius cylindrical cavity with a 5 cm wide doorway leading to an annular spreading region with a radius of 1.275 m. The wall thickness of the pedestal was 5 cm. Code input parameter(s) Value(s) Melt composition (wt %) 70 Fe, 20 Cr, 10 Ni Melt pour temperature 1804 K Melt oxide phase solidus – liquidus 1671 K – 1727 K Melt material property evaluation Steady pour rate of 9.5 kg/sec over a 6.7 second interval Melt material property evaluation Code subroutines Substrate initial temperature 298 K Substrate nodalization At each substrate nodal location, six 5.0 mm cells followed by six 10 mm cells; all nodes cell-centered. Synaptic cavity nodalization At each substrate nodal location, six 5.0 mm cells followed by six 10 mm cells; all nodes cell-centered. Spreading cavity nodalization Dr and was fush with the concrete surface; balance of pedestal interior meshed with 3 nodes that were 2.5 cm wide. The 5 cm wide doorway was meshed with 2 cells that were 2.5 cm wide that concrete surface; balance of pedestal interior meshed with 3 nodes that were 2.5 cm wide. He os rem wide doorway was meshed with 4 cells that were 2.5 cm wide. He os rem wide doorway was meshed with 2 cells that were 2.5 cm wide. He		that simulated the pedestal of a Mark I containment.
Total pour mass 63.6 kg Substrate material Silicous concrete Spreading geometry Mockup of a Mark I containment: A 17.5 cm inner radius cylindrical cavity with a 5 cm wide doorway leading to an annular spreading region with a radius of 1.275 m. The wall thickness of the pedestal was 5 cm. Code input parameter(s) Value(s) Melt composition (wi %) 70 Fe, 20 Cr, 10 Ni Melt nor temperature 1804 K Melt our temperature 1804 K Melt pour rate and duration Steady pour rate of 9.5 kg/sec over a 6.7 second interval Melt metal phase solidus - liquidus 1671 K - 1727 K Substrate composition Default silicous concrete Substrate composition Default silicous concrete Substrate notalization Code subroutines Substrate nodalization At each substrate nodal location, six 5.0 mm cells followed by six 10 mm cells; all nodes cell-centered. Spreading cavity nodalization At each substrate nodal location, six 5.0 mm cells followed by six 10 cm and was fluch with a spreading angle of 130°. The distance from the doorway to the shell was meshed with 3 nodes that were 2.5 cm wide. As concluded by the experimenters, the melt was assumed to spread outside the doorway with a spreading angle of 130°. The distance from the doorway to the shell was meshed with 61 cells that were 2.17 cm wide. All nodes cell-centered.	Melt temperature	1804 K
Substrate material Siliceous concrete Spreading geometry Mockup of a Mark I containment: A 17.5 cm inner radius cylindrical cavity with a 5 cm wide doorway leading to an annular spreading region with a radius of 1.275 m. The wall thickness of the pedestal was 5 cm. Code input parameter(s) Value(s) Melt composition (wt %) 70 Fe, 20 Cr, 10 Ni Melt mount temperature 1804 K Melt nout temperature 1804 K Melt nout and duration Steady pour rate of 9.5 kg/sec over a 6.7 second interval Melt material property evaluation Code subroutines Substrate indicate maperature 298 K Substrate material properties evaluation Code subroutines Substrate modalization At each substrate nodal location, six 5.0 mm cells followed by six 10 mm cells; all nodes cell-centered. Spreading cavity nodalization At each substrate nodal location, six 5.0 mm cells followed by six 10 mm cells; all nodes cell-centered. Spreading cavity nodalization At each substrate nodal location, six 5.0 mm cells followed by six 10 mm cells; all nodes cell-centered. Cavity condition Dry Query to the shell was meshed with 3 nodes that were 2.5 cm wide. All nodes cell-centered. Cavity condition Dry Query atmosphere emissivity 0.6 <tr< td=""><td>Total pour mass</td><td>63.6 kg</td></tr<>	Total pour mass	63.6 kg
Spreading geometry Mockup of a Mark I containment: A 17.5 cm inner radius cylindrical cavity with a 5 cm wide doorway leading to an annular spreading region with a radius of 1.275 m. The wall thickness of the pedestal was 5 cm. Code input parameter(s) Value(s) Melt composition (wt %) 70 Fe, 20 Cr, 10 Ni Melt parameter(s) Value(s) Melt with a S cm 1804 K Melt with a se solidus - liquidus 1403 K - 1523 K Melt metal phase solidus - liquidus 1671 K - 1727 K Melt metal phase solidus - liquidus 1671 K - 1727 K Melt metal phase solidus - liquidus 1662 Code subroutines Substrate composition Default siliceous concrete Substrate composition Default siliceous concrete Substrate material properties evaluation Code subroutines Substrate nodalization At each substrate nodal location, sits 5.0 mm cells followed by sit 10 mm cells; all nodes cell-centered. Substrate nodalization At each substrate nodal location, sits 5.0 m wide. Nave assumed to spread outside the doorway was meshed with 3 nodes that were 2.5 cm wide. As concluded by the experimenters, the melt was assumed to spread outside the doorway was assumed to spread outside the doorway with a spreading angle of 130°. The distance from the doorway to the shell was meshed with 61 cells that were 2.17 cm wide. All nodes cell-centered. Cavity condition Dry	Substrate material	Siliceous concrete
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Opper atmosphere emissivity 0.6 Ambient pressure 0.1 MPa Melt/substrate heat transfer coefficient model Locally, largest of Dittus – Boelter and Bradley slag film heat transfer coefficients Melt/substrate interfacial heat transfer resistance 4800 W/m²-K Constant used in Ramacciotti correlation 7.26 Solid-fraction variation See Figure C-23	Upper atmosphere temperature	300 K
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Meit/substrate neat transfer coefficient model Locally, largest of Dittus – Boelter and Bradley slag film heat transfer coefficients film heat transfer coefficients Melt/substrate interfacial heat transfer 4800 W/m²-K resistance 7.26 Solid-fraction variation See Figure C-23 Timester 0.02 accords	Alliblent pressure	U.I. MIPA
Millin neat transfer coefficients Melt/substrate interfacial heat transfer resistance Constant used in Ramacciotti correlation Solid-fraction variation See Figure C-23	Meny substrate neat transfer coefficient model	Locally, largest of Dittus – Boelter and Bradley slag
Metry substrate interfactal fleat transfer 4000 W/III ² -K resistance 7.26 Solid-fraction variation See Figure C-23 Timester 0.02 seconds	Molt (aubatrata interfacial bast transfor	A800 W/m ² K
Constant used in Ramacciotti correlation 7.26 Solid-fraction variation See Figure C-23 Timester 0.02 seconds	meny substrate internacial neat transfer	4000 W/III"-K
Solid-fraction See Figure C-23	Constant used in Romaniatti correlation	7.26
Solid-fraction SCC Figure C-25	Solid-fraction variation	See Figure C-23
		0.02 seconds







Figure C-96 Comparison of posttest debris profile prediction with SPREAD Test 15 data

Table C-28 INPUT FILE DATA SHEET FOR SPREAD TEST 21 WITH METAL MELT IN A MOCKUP OF THE MARK I CONTAINMENT WITH WET CONCRETE FLOOR

Test parameter	Value
Test name	SPREAD Test 21
Melt composition (wt %)	70 Fe, 20 Cr, 10 Ni (stainless steel)
Melt delivery technique	Melt poured into a 17.5 cm radius cylindrical cavity
	that simulated the pedestal of a Mark I containment.
Melt temperature	1778 К
Total pour mass	69.2 kg
Substrate material	Siliceous concrete
Spreading geometry	Mockup of a Mark I containment: A 17.5 cm inner
	radius cylindrical cavity with a 5 cm wide doorway
	leading to an annular spreading region with a radius
	of 1.275 m. The wall thickness of the pedestal was 5
	cm.
Code input parameter(s)	Value(s)
Melt composition (wt %)	70 Fe, 20 Cr, 10 Ni
Melt pour temperature	1778 К
Melt oxide phase solidus – liquidus	1403 К – 1523 К
Melt metal phase solidus – liquidus	1671 К – 1727 К
Melt pour rate and duration	Steady pour rate of 9.5 kg/sec over a 7.27 second
	interval
Melt material property evaluation	Code subroutines
Substrate composition	Default siliceous concrete
Substrate initial temperature	298 K
Substrate material properties evaluation	Code subroutines
Substrate solidus - liquidus temperatures	1403 – 1523 K (Code default values)
Substrate nodalization	At each substrate nodal location, six 5.0 mm cells
	followed by six 10 mm cells; all nodes cell-centered.
Spreading cavity nodalization	Automated Mark I shell meshing option used: melt
	assumed pour into the sump which was taken to have
	a radius of 10 cm and was flush with the concrete
	surface; balance of pedestal interior meshed with 3
	was mashed with 2 cells that were 2.5 cm wide doorway
	concluded by the experimenters, the melt was
	assumed to spread outside the doorway with a
	spreading angle of 130°. The distance from the
	doorway to the shell was meshed with 61 cells that
	were 2.17 cm wide. All nodes cell-centered.
Cavity condition	Wet
Water temperature (subcooling)	298 (75) K
Ambient pressure	0.1 MPa
Water depth	4.0 cm
Melt/substrate heat transfer coefficient model	Locally, largest of Dittus – Boelter and Bradley slag
	film heat transfer coefficients
Melt/substrate interfacial heat transfer	4800 W/m ² -K
resistance	
Constant used in Ramacciotti correlation	7.26
Solid-fraction variation	See Figure C-23
Timestep	0.01 seconds



Figure C-97 Leading edge penetration comparison for the SPREAD Test 21 metal spreading test



Figure C-98 Comparison of posttest debris profile prediction with SPREAD Test 21 data

As is evident from the figures, the code calculates that melt spreading would be limited by solidification at the leading edge for both tests. In addition, a few millimeters of substrate erosion are calculated for both tests, but this was not reported in the documentation.^[28] The overall shape of the debris profiles following spreading are also similar to the data, but depth is consistently under-predicted. This is again due to the fact that the code does not account for porosity upon solidification, and since concrete decomposition gases would have been produced as a result of heat transfer to the substrate, porosity would have been present as the melt cooled and solidified.

REACTOR MATERIAL MELT SPREADING TESTS

Following the benchmarking exercise against oxide simulant and metal melt spreading tests, the code was further exercised against tests conducted with reactor materials. As reported by Cognet et al.^[35] and Journeau et al.,^[36-37] several corium melt spreading tests were carried out at CEA with varying melt compositions and substrate materials in the VULCANO facility. Two corium tests were also conducted by Magallon and Tromm^[38] as part of the FARO program, one of them under wet cavity conditions. Finally, several large scale spreading tests at up to 2 metric tons melt mass were conducted at Siempelkamp Nuklear in Germany on various types of surface materials (Sappok and Steinwarz^[39] and Steinwarz et al.^[40]) Code assessments against these tests are provided in this section.

Vulcano Spreading Tests

These tests^[36-37] involved spreading of high temperature core oxide melts that were generated using a specially designed plasma arc furnace. Once the melts had reached the desired initial condition, the furnace was tilted and the melt was poured and spread within instrumented test sections. A total of 12 tests were conducted as part of this experiment program. The VULCANO VE-U7 test was selected from the matrix for analysis here because the experiment apparatus, operating conditions, and results have been very well documented in the open literature. For this test, a 40 kg melt mass was generated and poured into an accumulator that fed two parallel spreading channels; one concrete, the other refractory ceramic. The overall spreading geometry was a 19° sector with a wall in the center dividing the two parallel channels. Thus, each channel was modeled as an isolated 9.5° sector.

Test characteristics and the corresponding code input that was used to model the concrete channel spreading test are summarized in Table C-29. As is evident, the code subroutines were used to calculate both the melt and substrate thermal-physical property data. Furthermore, as part of the specifications for the experiment, the concrete composition was provided and so this was also used as code input to improve the fidelity of the simulation. One of the modeling challenges for these tests was how to best define the melt pour rate into the two parallel channels given the fact that the code can only calculate one channel at a time. What is known regarding the test operations is the total pour mass into the accumulator, the pour duration, and the corium mass recovered from each channel. With this information, the pour rate into each channel was calculated by dividing the recovered mass in each channel by the overall pour duration.

The calculated leading edge penetration vs. time is compared to the concrete channel test data in Figure C-73, while substrate thermal response and post-spreading material profile predictions are compared with the data in Figures C-74 and C-75, respectively. Regarding the melt penetration data, the code slightly under-predicts the velocity early in the transient, but the overall trend is reasonably reproduced. As is evident from Figure C-74, the code seems to under-predict heat transfer to the substrate for this test, with local temperatures falling ~ 200 K below those measured near the surface. Finally, the overall shape of the debris profile following spreading is similar to the data, but depth is consistently under-predicted. This again is due to the fact that the code does not account for porosity upon solidification, which would be present due to concrete decomposition gases.

Test characteristics and the corresponding code input that was used to model the concrete channel spreading test are summarized in Table C-30. The calculated leading edge penetration vs. time is compared to the ceramic channel test data in Figure C-76, while substrate thermal response and postspreading material profile predictions are compared with data in Figures C-77 and C-78, respectively. For this test, the code seems to do a reasonable job of predicting the leading edge propagation, including both the initial transient and longer term viscous deceleration phase (Figure C-76). However, consistent with the concrete test results, the basemat heatup is under-predicted later in the transient (i.e., after ~ 20 seconds). Finally, the shape of the posttest debris distribution is reasonably replicated (Figure C-78), but depths are again slightly under-predicted since the code does not account for the presence of porosity during solidification.

Test nemeter	Walue
Test yarameter	
Nelte some esition (est 0())	$\begin{array}{c} \text{VOLCANO VE-07, concrete channel} \\ \text{(1 UO 20.7 co. 2 E-0.2 C-0.0 C-0.0 A} \\ \end{array}$
Melt composition (wt %)	Al_2O_3 , 1 Fe
Melt delivery technique	Melt poured into a common accumulator that fed both the
	concrete and ceramic channels of the apparatus. The
	accumulator had an average width of 20 cm, length of 15
	cm, and was 0.5 cm deep relative to spreading surface.
	The total 40 kg melt mass was poured at an average rate
	of 3.0 kg/sec from a furnace into the accumulator.
Melt temperature	2450 K
Total pour mass	18.5 kg ^a for the concrete channel side
Substrate material	Siliceous concrete
Spreading geometry	9.5° sector with an opening width of 9.5 cm from the
	accumulator; overall channel length was 1.084 m.
Code input parameter(s)	Value(s)
Melt composition (wt %)	61 UO ₂ , 30 ZrO ₂ , 3 FeO,1, Fe, 5 slag (slag is 3 SiO ₂ , 1.6
	CaO, 0.4 Al ₂ O ₃)
Melt pour temperature	2450 K
Melt oxide phase solidus – liquidus	1270 К – 2640 К
Melt metal phase solidus – liquidus	1810 K – 1820 K
Melt pour rate and duration	Steady pour of 21.7 kg melt mass into the accumulator
	over a 13.3 second interval; average pour rate of 1.62
	kg/sec.
Melt material property evaluation	Code subroutines
Substrate composition	$4.2 \text{ CO}_2, 3.7 \text{ H}_2\text{O}, 1.4 \text{ K}_2\text{O}, 0.7 \text{ N}_2\text{O}, 0.8 \text{ TiO}_2, 69.8 \text{ SiO}_2,$
	13.7 CaO, 0.7 MgO, 4.0 Al ₂ O ₃ , 1.0 Fe ₂ O ₃
Substrate initial temperature	300 K
Substrate material properties evaluation	Code subroutines
Substrate solidus - liquidus temperatures	1390 К – 1960 К
Substrate nodalization	At each substrate nodal location, six 5.0 mm cells,
	followed by six 10 mm cells. All nodes cell-centered.
Spreading cavity nodalization	Accumulator: modeled as a single cell that is 10 cm wide,
	15 cm long, and 0.5 cm deep. Spreading surface: modeled
	as 9.5° sector with 50 cells with a radial length of 2.17 cm.
Operite and litica	All nodes cell-centered.
Upper atmosphere temperature	300 K
Auchieute ausonaute	
Ambient pressure	U.I MPa
melt/substrate neat transfer coefficient	Locally, larger of the Dittus – Boelter and Bradley slag film
Molt (ashetuate interfected heat transfer	
meny substrate interfactal neat transfer	U
Constant in Pamagaistti correlation	7.26 (Average for evide type [15])
Solid fraction variation	20 Figure C 22
	0.02 seconds
ιμμεδιεμ	0.04 SCLUIIUS

Table C-29 INPUT FILE DATA SHEET FOR THE VULCANO VE-U7 TEST WITH CONCRETE CHANNEL

^aEstimate. Reported information: total pour mass was 40 kg, with 14 kg recovered from the ceramic channel and 12 kg from the concrete channel. The missing 12 kg was assumed to be retained in the accumulator, and was split between the concrete and ceramic channel sides according to the mass % recovered from each channel.



Figure C-99 Leading edge penetration comparison for the VULCANO VE-U7 core oxide spreading test over a concrete surface



Figure C-100 Comparison of substrate thermal response predictions with VULCANO VE-U7 concrete channel data 12 cm from channel inlet



Figure C-101 Comparison of posttest debris profile prediction with VULCANO VE-U7 concrete channel data

Test parameter	Value
Test name	VULCANO VE-U7, ceramic channel
Melt composition (wt %)	61 UO ₂ , 30 ZrO ₂ , 3 FeO, 2 CaSiO ₃ , 2 SiO ₂ , 0.6 CaO, 0.4 Al ₂ O ₃ , 1 Fe
Melt delivery technique	Melt poured into a common accumulator that fed both the concrete and ceramic channels of the apparatus. The
	accumulator had an average width of 20 cm, length of 15 cm,
	and was 0.5 cm deep relative to spreading surface. The total 40
	kg melt mass was poured at an average rate of 3.0 kg/sec from a
	furnace into the accumulator.
Melt temperature	2450 K
Total pour mass	21.7 kg ^a for the ceramic channel side
Substrate material	
Spreading geometry	9.5° sector with an opening width of 9.5 cm from the
	accumulator; overall channel length was 1.084 m.
Code input parameter(s)	Value(s)
Melt composition (wt %)	$\sqrt{auc(s)}$ 61 UO ₂ 30 ZrO ₂ 3 FeO 1 Fe 5 slag (slag is 3 SiO ₂ 1 6 CaO
ment composition (we vo)	0.4 Al2O3
Melt pour temperature	2450 K
Melt oxide phase solidus – liquidus	1270 K – 2640 K
Melt metal phase solidus – liquidus	1810 K – 1820 K
Melt pour rate and duration	Steady pour of 21.7 kg melt mass into the accumulator over a
	13.3 second interval; average pour rate of 1.62 kg/sec.
Melt material property evaluation	Code subroutines
Substrate composition	zirconia (modeled using user-specified material input properties)
Substrate initial temperature	300 K
Substrate material properties	$c_s = c_1 = 575 \text{ J/kg-K}, \Delta h_f = 0.706 \text{ MJ/kg}, \rho_s = \rho_1 = 5300 \text{ kg/m}^3, k_s$
evaluation ^b	$= k_1 = 4.7 \text{ W/m-K}$, and $\varepsilon = 0.3$
Substrate solidus - liquidus temperatures	1780 K – 2900 K
Substrate nodalization	At each substrate nodal location, six 5.0 mm cells, followed by six 10 mm cells. All nodes cell-centered.
Spreading cavity nodalization	Accumulator: modeled as a single cell that is 10 cm wide, 15 cm
	long, and 0.5 cm deep. Spreading surface: modeled as 9.5°
	sector with 50 cells with a radial length of 2.17 cm. All nodes
	cell-centered.
Cavity condition	Dry
Upper atmosphere temperature	300 K
Ambient processor	1.0 0.1 MPa
Molt (substrate best transfer	0.1 MPa
coefficient model	Dittus - Boeiter
Melt/substrate interfacial heat	0
transfer resistance	Ť
Constant in Ramacciotti correlation	7.26 (Average for oxide type [15])
Solid-fraction variation	See Figure C-23
Timestep	0.02 seconds

Table C-30 INPUT FILE DATA SHEET FOR THE VULCANO VE-U7 TEST WITH CERAMIC CHANNEL

^aEstimate. Reported information: total pour mass was 40 kg, with 14 kg recovered from the ceramic channel and 12 kg from the concrete channel. The missing 12 kg was assumed to be retained in the accumulator, and was split between the concrete and ceramic channel sides according to the mass % recovered from each channel.



Figure C-102 Leading edge penetration comparison for the VULCANO VE-U7 core oxide spreading test over a ceramic surface



Figure C-103 Comparison of substrate thermal response predictions with VULCANO VE-U7 ceramic channel data 12 cm from channel inlet



Figure C-104 Comparison of posttest debris profile prediction with VULCANO VE-U7 ceramic channel data

Faro Spreading Tests

These tests^[38] involved spreading of high temperature core oxide melt that was generated in a graphite resistance heating furnace. Once the melts had reached the desired initial condition, a plug was opened and the material was poured into a cylindrical accumulator that fed a spreading channel that was a 17° sector lined with steel. The accumulator included a 4 cm high weir that prevented splashing at pour inception. As shown in Table C-1, two tests were conducted in this experiment series; the first with a dry surface (L-26S), and the second with a thin (1 cm deep) water layer (L-32S). For both tests, code subroutines were used to calculate melt and substrate thermal-physical properties. The 4 cm high weir was modeled as part of the nodalization scheme.

Test characteristics and the corresponding code input for L-26S are summarized in Table C-31, while the leading edge penetration and post-spreading material profile predictions are shown in Figures C-79 and C-80, respectively. For this test, the initial rate of spreading is somewhat over-predicted by the model. The code predicts a thick accumulation of melt following spreading, which qualitatively agrees with the experiment results, but sufficient information was not provided^[38] for a direct comparison.

Test parameter	Value
Test name	Faro L-26S, dry steel channel
Melt composition (wt %)	80 UO ₂ , 20 ZrO ₂
Melt delivery technique	Melt poured into a circular accumulator with an ID of
	10 cm and an elevation flush with the spreading
	surface. The accumulator was separated from the
	channel by a 3.2 cm thick, 4.0 cm high weir with a
	width of 15 cm leading to the channel. The total 160.4
	kg melt mass was poured at an average rate of 16.54
	kg/sec from a furnace into the accumulator.
Melt temperature	2950 K
Total pour mass	160.4 kg
Substrate material	steel
Spreading geometry	17° sector with an opening width of 15 cm from the
	accumulator; overall channel length was 2.0 m.
Code input parameter(s)	Value(s)
Melt composition (wt %)	80 UO ₂ , 20 ZrO ₂
Melt pour temperature	2950 K
Melt oxide phase solidus – liquidus	2860 – 2910 K
Melt metal phase solidus – liquidus	1810 – 1820 K
Melt pour rate and duration	Steady pour of 160.4 kg melt mass into the
	accumulator over a 9.7 second interval; average pour
	rate of 16.54 kg/sec.
Melt material property evaluation	Code subroutines
Substrate composition	steel
Substrate initial temperature	296 K
Substrate material properties evaluation	Code subroutines
Substrate solidus - liquidus temperatures	1810 K – 1811 K (code default values)
Substrate nodalization	At each substrate nodal location, six 5.0 mm cells,
	tollowed by six 10 mm cells. All nodes cell-centered.
Spreading cavity nodalization	Accumulator: modeled as a single, cylindrical, 10 cm
	ID cell with an elevation flush with the spreading
	surface. Weir: modeled as a single 4 cm nigh, 15 cm
	wide 5.2 cm long cell spreading surface. Inodeled as a 17° soster with 80 cells with a radial length of 2.5 cm
	All nodes cell centered
Cavity condition	Dry
Upper atmosphere temperature	300 K
Upper atmosphere emissivity	10
Ambient pressure	0.1 MPa
Mildent pressure	Dittus - Boelter
model	Dittus - Dociter
Melt/substrate interfacial heat transfer	0
resistance	Ň
Constant in Ramacciotti correlation	7.26 (Average for oxide type [15])
Solid-fraction variation	See Figure C-23
Timesten	0.01 seconds

Table C-31 INPUT FILE DATA SHEET FOR THE FARO L-26S TEST WITH DRY STEEL CHANNEL



Figure C-105 Leading edge penetration comparison for FARO L-26S core oxide spreading test



Figure C-106 Posttest debris profile prediction for the FARO L-26S core oxide spreading test

Experimental details and modeling input for L-32S are summarized in Table C-32, while the leading edge penetration and post-spreading material profile predictions are shown in Figures C-81 and C-82, respectively. The code also over-predicts the initial rate of spreading for this test, but less so in comparison to L-26S. As for L-26S, a thick melt layer following spreading is predicted, which qualitatively agrees with the experiment results, but sufficient information was not provided for a direct comparison.

Test parameter	Value
Test name	Faro L-32S, wet steel channel
Melt composition (wt %)	80 UO ₂ , 20 ZrO ₂
Melt delivery technique	Melt poured into a circular accumulator with an ID
	of 10 cm and an elevation flush with the spreading
	surface. The accumulator was separated from the
	channel by a 3.2 cm thick, 4.0 cm high weir with a
	width of 15 cm leading to the channel. The total
	128 kg melt mass was poured at an average rate of
	18.55 kg/sec from a furnace into the accumulator.
Melt temperature	3000 K
Total pour mass	128 kg
Substrate material	steel
Spreading geometry	17° sector with an opening width of 15 cm from the
	accumulator; overall channel length was 2.0 m.
.	
Code input parameter(s)	
Melt composition (wt %)	80 002, 20 ZIO2
Melt pour temperature	3000 K
Melt oxide phase solidus – liquidus	2800 - 2910 K
Melt metal phase solidus – inquidus	1810 - 1820 K Stoody pour of 108 kg malt mass into the
Men pour rate and duration	scentry pour of 128 kg men mass into the
	nour rate of 18 55 kg/sec
Melt material property evaluation	Code subroutines
Substrate composition	steel
Substrate initial temperature	300 K
Substrate material properties evaluation	Code subroutines
Substrate solidus - liquidus temperatures	1810 K – 1811 K (code default values)
Substrate nodalization	At each substrate nodal location, six 5.0 mm cells.
	followed by six 10 mm cells. All nodes cell-centered.
Spreading cavity nodalization	Accumulator: modeled as a single, cylindrical, 10
F	cm ID cell with an elevation flush with the spreading
	surface. Weir: modeled as a single 4 cm high, 15
	cm wide 3.2 cm long cell Spreading surface:
	modeled as a 17° sector with 80 cells with a radial
	length of 2.5 cm. All nodes cell-centered.
Cavity condition	Wet
Water temperature (subcooling)	293 (80) K
Ambient pressure	0.1 MPa
Water depth	1.0 m
Melt/substrate heat transfer coefficient model	Dittus - Boelter
Melt/substrate interfacial heat transfer	0
resistance	
Constant in Ramacciotti correlation	7.26 (Average for oxide type [15])
Solid-fraction variation	See Figure C-23
Timestep	0.01 seconds

Table C-32 INPUT FILE DATA SHEET FOR THE FARO L-32S TEST WITH WET STEEL CHANNEL



Figure C-107 Leading edge penetration comparison for FARO L-32S core oxide spreading test



Figure C-108 Posttest debris profile prediction for the FARO L-32S core oxide spreading test

COMAS Spreading Tests

These large scale tests^[39-40] involved spreading of core melts that were produced by induction heating of the metallic (iron) component of a core oxide-metal mixture. Once the melt reached target temperature, the material was poured into an accumulator, and then a gate was opened to initiate the spreading transient. There were a variety of tests conducted as part of this program. Of this matrix, three specific tests have been selected for analysis (see Table C-1):

- 1. Comas-5a, wherein a core oxide-metal mixture was poured into a common accumulator that fed three parallel channels with different substrates (i.e., ceramic, concrete, and steel),
- 2. Comas EU-2b, which was essentially the same as Comas-5a with the exception that the metal phase was separated from the oxide before the oxide phase was spread, and
- 3. Comas EU4, which was a large scale (2000 kg) demonstration test in which a metal-oxide mixture was spread on a steel surface in geometry similar to the EPR core catcher.

This matrix embodies seven individual tests that cover spreading on ceramic, concrete, and steel surfaces with different melt compositions and flow geometries. Although the nature and extent of these tests was significant, it should be pointed out that the open literature publications did not provide a few key pieces of information that were required to construct detailed models, the most notable of which was the geometry of the accumulator and gate plug assembly. The models utilized here were developed from several different sources of information to assemble as accurate a representation as possible.

The Comas-5a experiment was a combined metal-oxide spreading test, and no mention was made in the literature regarding a stratified melt injection configuration. Thus, the metal and oxide phases in the spread melt were assumed to be well-mixed. The code subroutines were used to calculate the melt properties for all tests. The ceramic substrate was assumed to be composed of Cordierite, and the same material properties used for the KATS tests^[32] were used. The total pour mass of 1000 kg was assumed to be equally spread between the three channels. Computationally, the melt was dropped into the accumulator over a time interval of 0.1 seconds to rapidly accumulate the material and thereby simulate a dam break type spreading event, as intended with the gate plug design. Finally, the geometry of the accumulator for each 'channel' was assumed to be a 40 cm wide (same as channel width), 25 cm long rectilinear box with a surface elevation that was 5 cm below that of the channel.

Test characteristics and the corresponding code input for the COMAS 5a ceramic channel test are summarized in Table C-33, while the calculated leading edge penetration and ultimate melt penetration predictions are compared to the data in Figures C-83 and C-84. Table C-34 and Figures C-85 and C-86 provide the same information for the concrete channel test. Finally, Table C-35 summarizes characteristics and input for the steel channel test, while Figures C-87 and C-89 provide plots of leading edge penetration, substrate thermal response, and ultimate melt penetration distance, respectively.

In general, the code somewhat under-predicts spreading velocity early in the transient for all three tests, but the overall agreement is favorable. As shown in Figure C-88, the heatup in the steel substrate is overpredicted by ~ 100 K during the first ~50 seconds of the transient. Afterwards, melt solidification occurs at the measurement location, and the temperature predictions approach the measurements.

The Comas EU2b test was very similar to Comas 5a, with the exception that the oxide phase was slightly modified by the addition of SiO₂, and the metal phase was decanted so that only the oxide phase was spread. Test characteristics and the corresponding code input for the ceramic channel test are summarized in Table C-36, while the calculated leading edge penetration and ultimate melt penetration predictions are compared to the test data in Figures C-90 and C-91. Table C-37 and Figures C-92 and C-93 provide the analogous comparisons for the concrete channel test, while Table C-38 and Figures C-94 and C-95 provide the comparisons for the steel channel test. As for Comas 5a, the initial spreading velocity is under-predicted for all three cases, but the overall agreement is reasonable.

Finally, Table C-39 summarizes characteristics and model input for the COMAS EU4 2-D steel channel test, while Figures C-96 and C-97 provide comparisons of the leading edge penetration and ultimate melt penetration distance, respectively. This was a combined metal-oxide spreading test, and no mention of a stratified pour condition was made.^[39-40] Thus, the metal and oxide were assumed to spread in a well-mixed configuration. Examination of Figure C-96 indicates that the code does an excellent job in predicting spreading velocity for this experiment.

Test parameter	Value
Test name	Comas 5a, ceramic channel
Melt composition (wt %)	29 UO ₂ , 12 ZrO ₂ 18 FeO, 2 Cr ₂ O ₃ , 39 Fe
Melt delivery technique	Melt poured into an accumulator box that was 40
	cm wide (per channel), 25 cm long, and 5 cm deep
	relative to spreading surface. Pour initiated by
	opening a plug device at the bottom of the
	accumulator.
Melt temperature	2173 К
Total pour mass	333.3 kg (assumes 1000 kg pour uniformly
	distributed between the 3 channels)
Substrate material	Unspecified ceramic; assumed to be Cordierite
Spreading geometry	1-D channel, 6.4 m long by 40 cm wide
Code input parameter(s)	Value(s)
Melt composition (wt %)	29 UO ₂ , 12 ZrO ₂ 18 FeO, 2 Cr ₂ O ₃ , 39 Fe
Melt pour temperature	2173 К
Melt oxide phase solidus – liquidus	1598 К – 2223 К
Melt metal phase solidus – liquidus	1810 К – 1820 К
Melt pour rate and duration	3333.3 kg/sec over a 0.1 sec (simulating
	instantaneous deposition in the accumulator,
	followed by initiation of spreading)
Melt material property evaluation	Code subroutines
Substrate composition	Corderite (modeled using user-specified material
	input properties)
Substrate initial temperature	300 K
Substrate material properties evaluation	c_s = c_l = 840 J/kg-K, Δh_f = 1.0 MJ/kg, ρ_s = ρ_l = 2200
	kg/m^3 , $k_s = k_l = 3.8 W/m$ -K, and $\epsilon = 0.3$
Substrate solidus - liquidus temperatures	1893 К – 1923 К
Substrate nodalization	At each substrate nodal location, six 5.0 mm cells,
	followed by six 10 mm cells. All nodes cell-centered.
Spreading cavity nodalization	Accumulator: modeled as a single cell that is 40 cm
	wide, 25 cm long, and 5 cm deep. Channel:
	modeled using 120 cells; each is 40 cm wide and
	5.33 cm long. All nodes cell-centered.
Cavity condition	Dry
Upper atmosphere temperature	300 K
Upper atmosphere emissivity	1.0
Ambient pressure	
Meit/substrate heat transfer coefficient model	Dittus - Boelter
Meit/substrate interfacial heat transfer	U
resistance	
Constant in Ramacciotti correlation	1.20 [Average for oxide type [15]]
Solid-Iraction Variation	See Figure C-23
Timestep	0.025 seconds



Figure C-109 Leading edge penetration comparison for COMAS-5a core oxide spreading test with ceramic channel



Figure C-110 Posttest debris profile prediction for the COMAS 5a core oxide spreading test with ceramic channel

Test narameter	Value
Test name	Comas 5a concrete channel
Melt composition (wt %)	29 UO_2 12 $7rO_2$ 18 FeO 2 Cr_2O_2 39 Fe
Melt delivery technique	Melt poured into an accumulator box that was 40 cm
weit denvery teeninque	wide (per channel) 25 cm long and 5 cm deep relative
	to spreading surface. Pour initiated by opening a plug
	device at the bottom of the accumulator.
Melt temperature	2173 K
Total pour mass	333.3 kg (assumes 1000 kg pour uniformly
	distributed between the 3 channels)
Substrate material	Siliceous concrete
Spreading geometry	1-D channel, 6.4 m long by 40 cm wide
Code input parameter(s)	Value(s)
Melt composition (wt %)	29 UO ₂ , 12 ZrO ₂ 18 FeO, 2 Cr ₂ O ₃ , 39 Fe
Melt pour temperature	2173 K
Melt oxide phase solidus – liquidus	1598 K – 2223 K
Melt metal phase solidus – liquidus	1810 K – 1820 K
Melt pour rate and duration	3333.3 kg/sec over a 0.1 sec (simulating
-	instantaneous deposition in the accumulator,
	followed by initiation of spreading)
Melt material property evaluation	Code subroutines
Substrate composition (wt %)	4.2 CO ₂ , 3.7 H ₂ O, 1.4 K ₂ O, 0.7 Na ₂ O, 0.8 TiO ₂ , 69.8
	SiO ₂ , 13.7 CaO, 0.7 MgO, 4.0 Al ₂ O ₃ , 1.0 Fe ₂ O ₃
Substrate initial temperature	300 K
Substrate material properties evaluation	Code subroutines
Substrate solidus - liquidus temperatures	1390 К – 1960 К
Substrate nodalization	At each substrate nodal location, six 5.0 mm cells,
	followed by six 10 mm cells. All nodes cell-centered.
Spreading cavity nodalization	Accumulator: modeled as a single cell that is 40 cm
	wide, 25 cm long, and 5 cm deep. Channel: modeled
	using 120 cells; each is 40 cm wide and 5.33 cm long.
	All nodes cell-centered.
Cavity condition	Dry
Upper atmosphere temperature	300 K
Upper atmosphere emissivity	
Ambient pressure	
Melt/substrate heat transfer coefficient model	film heat transfer coefficients
Melt/substrate interfacial heat transfer	0
resistance	
Constant in Ramacciotti correlation	7.26 (Average for oxide type [15])
Solid-fraction variation	See Figure C-23
Timestep	0.025 seconds

Table C-34 INPUT FILE DATA SHEET FOR THE COMAS 5A TEST WITH CONCRETE CHANNEL



Figure C-111 Leading edge penetration comparison for COMAS-5a core oxide spreading test with concrete channel



Figure C-112 Posttest debris profile prediction for the COMAS 5a core oxide spreading test with concrete channel

Test parameter	Value
Test name	Comas 5a, steel channel
Melt composition (wt %)	29 UO ₂ , 12 ZrO ₂ 18 FeO, 2 Cr ₂ O ₃ , 39 Fe
Melt delivery technique	Melt poured into an accumulator box that was 40 cm
	wide (per channel), 25 cm long, and 5 cm deep relative
	to spreading surface. Pour initiated by opening a plug
	device at the bottom of the accumulator.
Melt temperature	2173 К
Total pour mass	333.3 kg (assumes 1000 kg pour uniformly
	distributed between the 3 channels)
Substrate material	Steel
Spreading geometry	1-D channel, 6.4 m long by 40 cm wide
Code input parameter(s)	Value(s)
Melt composition (wt %)	29 UO ₂ , 12 ZrO ₂ 18 FeO, 2 Cr ₂ O ₃ , 39 Fe
Melt pour temperature	2173 К
Melt oxide phase solidus – liquidus	1598 К – 2223 К
Melt metal phase solidus – liquidus	1810 K – 1820 K
Melt pour rate and duration	3333.3 kg/sec over a 0.1 sec (simulating
	instantaneous deposition in the accumulator,
	followed by initiation of spreading)
Melt material property evaluation	Code subroutines
Substrate composition	Steel (code default composition)
Substrate initial temperature	300 K
Substrate material properties evaluation	Code subroutines
Substrate solidus - liquidus temperatures	1810 K – 1811 K (code default values)
Substrate nodalization	At each substrate nodal location, six 5.0 mm cells,
	followed by six 10 mm cells. All nodes cell-centered.
Spreading cavity nodalization	Accumulator: modeled as a single cell that is 40 cm
	wide, 25 cm long, and 5 cm deep. Channel: modeled
	using 120 cells; each is 40 cm wide and 5.33 cm long.
	All nodes cell-centered.
Cavity condition	Dry
Upper atmosphere temperature	300 K
Upper atmosphere emissivity	1.0
Ambient pressure	0.1 MPa
Melt/substrate heat transfer coefficient model	Dittus – Boelter
Melt/substrate interfacial heat transfer	0
resistance	
Constant in Ramacciotti correlation	7.26 (Average for oxide type [15])
Solid-fraction variation	See Figure C-23
Timestep	0.025 seconds

Table C-35 INPUT FILE DATA SHEET FOR THE COMAS 5A TEST WITH STEEL CHANNEL






Figure C-114 Comparison of substrate thermal response predictions with COMAS 5a steel channel data 4 m from channel inlet



Figure C-115 Posttest debris profile prediction for the COMAS 5a core oxide spreading test with steel channel

Test parameter	Value	
Test name	Comas EU2b, ceramic channel	
Melt composition (wt %)	42.8 UO ₂ , 17.7 ZrO ₂ , 26.5 FeO, 3.0 Cr ₂ O ₃ , 10.0 SiO ₂	
Melt delivery technique	Melt poured into an accumulator box that was 40 cm wide (per channel), 25 cm long, and 5 cm deep relative to spreading surface. Pour initiated by opening a plug device at the bottom of the accumulator.	
Melt temperature	2343 K	
Total pour mass	210 kg (assumes 630 kg pour uniformly distributed between the 3 channels)	
Substrate material	Unspecified ceramic; assumed to be Cordierite	
Spreading geometry	1-D channel, 6.4 m long by 40 cm wide	
Code input parameter(s)	Value(s)	
Melt composition (wt %)	42.8 UO ₂ , 17.7 ZrO ₂ , 26.5 FeO, 3.0 Cr ₂ O ₃ , 10.0 SiO ₂	
Melt pour temperature	2343 К	
Melt oxide phase solidus – liquidus	1443 К – 2173 К	
Melt metal phase solidus – liquidus	1810 К – 1820 К	
Melt pour rate and duration	2100 kg/sec over a 0.1 sec (simulating instantaneous deposition in the accumulator, followed by initiation of spreading)	
Melt material property evaluation	Code subroutines	
Substrate composition	Corderite (modeled using user-specified material input properties)	
Substrate initial temperature	300 K	
Substrate material properties evaluation	$c_s = c_l = 840 \text{ J/kg-K}$, Δh _f = 1.0 MJ/kg, $\rho_s = \rho_l = 2200 \text{ kg/m}^3$, $k_s = k_l = 3.8 \text{ W/m-K}$, and $\epsilon = 0.3$	
Substrate solidus - liquidus temperatures	1893 K – 1923 K	
Substrate nodalization	At each substrate nodal location, six 5.0 mm cells, followed by six 10 mm cells. All nodes cell-centered.	
Spreading cavity nodalization	Accumulator: modeled as a single cell that is 40 cm wide, 25 cm long, and 5 cm deep. Channel: modeled using 120 cells; each is 40 cm wide and 5.33 cm long. All nodes cell-centered.	
Cavity condition	Dry	
Upper atmosphere temperature	300 K	
Upper atmosphere emissivity	1.0	
Ambient pressure	0.1 MPa	
Melt/substrate heat transfer coefficient model	Dittus - Boelter	
Melt/substrate interfacial heat transfer resistance	0	
Constant in Ramacciotti correlation	7.26 (Average for oxide type [15])	
Solid-fraction variation	See Figure C-23	
Timestep	0.025 seconds	



Figure C-116 Leading edge penetration comparison for COMAS-EU2b core oxide spreading test with ceramic channel



Figure C-117 Posttest debris profile prediction for the COMAS EU2b core oxide spreading test with ceramic channel

Table C-37 INPUT FILE DATA SHEET FOR THE COMAS EU2B TEST WITH CONCRETE CHANNEL

Test parameter	Value	
Test name	Comas EU2b, concrete channel	
Melt composition (wt %)	42.8 UO ₂ , 17.7 ZrO ₂ , 26.5 FeO, 3.0 Cr ₂ O ₃ , 10.0 SiO ₂	
Melt delivery technique	Melt poured into an accumulator box that was 40 cm wide (per channel), 25 cm long, and 5 cm deep relative to spreading surface. Pour initiated by opening a plug device at the bottom of the accumulator.	
Melt temperature	2343 K	
Total pour mass	210 kg (assumes 630 kg pour uniformly distributed between the 3 channels)	
Substrate material	Siliceous concrete	
Spreading geometry	1-D channel, 6.4 m long by 40 cm wide	
Code input parameter(s)	Value(s)	
Melt composition (wt %)	42.8 UO ₂ , 17.7 ZrO ₂ , 26.5 FeO, 3.0 Cr ₂ O ₃ , 10.0 SiO ₂	
Melt pour temperature	2343 K	
Melt oxide phase solidus – liquidus	1443 К – 2173 К	
Melt metal phase solidus – liquidus	1810 K – 1820 K	
Melt pour rate and duration	2100 kg/sec over a 0.1 sec (simulating instantaneous deposition in the accumulator, followed by initiation of spreading)	
Melt material property evaluation	Code subroutines	
Substrate composition	4.2 CO ₂ , 3.7 H ₂ O, 1.4 K ₂ O, 0.7 Na ₂ O, 0.8 TiO ₂ , 69.8 SiO ₂ , 13.7 CaO, 0.7 MgO, 4.0 Al ₂ O ₃ , 1.0 Fe ₂ O ₃	
Substrate initial temperature	300 K	
Substrate material properties evaluation	Code subroutines	
Substrate solidus - liquidus temperatures	1390 К – 1960 К	
Substrate nodalization	At each substrate nodal location, six 5.0 mm cells, followed by six 10 mm cells. All nodes cell-centered.	
Spreading cavity nodalization	Accumulator: modeled as a single cell that is 40 cm wide, 25 cm long, and 5 cm deep. Channel: modeled using 120 cells; each is 40 cm wide and 5.33 cm long. All nodes cell-centered.	
Cavity condition	Dry	
Upper atmosphere temperature	300 K	
Upper atmosphere emissivity	1.0	
Ambient pressure	0.1 MPa	
Melt/substrate heat transfer coefficient model	Locally, larger of the Dittus – Boelter and Bradley slag film heat transfer coefficient models	
Melt/substrate interfacial heat transfer resistance	0	
Constant in Ramacciotti correlation	7.26 (Average for oxide type [15])	
Solid-fraction variation	See Figure C-23	
Timestep	0.025 seconds	



Figure C-118 Leading edge penetration comparison for COMAS-EU2b core oxide spreading test with concrete channel



Figure C-119 Posttest debris profile prediction for the COMAS EU2b core oxide spreading test with concrete channel

Test parameter	Value
Test name	Comas EU2b, steel channel
Melt composition (wt %)	42.8 UO ₂ , 17.7 ZrO ₂ , 26.5 FeO, 3.0 Cr ₂ O ₃ , 10.0 SiO ₂
Melt delivery technique	Melt poured into an accumulator box that was 40 cm wide (per channel), 25 cm long, and 5 cm deep relative to spreading surface. Pour initiated by opening a plug device at the bottom of the accumulator.
Melt temperature	2343 K
Total pour mass	210 kg (assumes 630 kg pour uniformly distributed between the 3 channels)
Substrate material	Steel
Spreading geometry	1-D channel, 6.4 m long by 40 cm wide
Code input parameter(s)	Value(s)
Melt composition (wt %)	42.8 UO ₂ , 17.7 ZrO ₂ , 26.5 FeO, 3.0 Cr ₂ O ₃ , 10.0 SiO ₂
Melt pour temperature	2343 К
Melt oxide phase solidus – liquidus	1443 К – 2173 К
Melt metal phase solidus – liquidus	1810 К – 1820 К
Melt pour rate and duration	2100 kg/sec over a 0.1 sec (simulating instantaneous deposition in the accumulator, followed by initiation of spreading)
Melt material property evaluation	Code subroutines
Substrate composition	Steel (code default composition)
Substrate initial temperature	300 K
Substrate material properties evaluation	Code subroutines
Substrate solidus - liquidus temperatures	1810 K – 1811 K (code default values)
Substrate nodalization	At each substrate nodal location, six 5.0 mm cells, followed by six 10 mm cells. All nodes cell-centered.
Spreading cavity nodalization	Accumulator: modeled as a single cell that is 40 cm wide, 25 cm long, and 5 cm deep. Channel: modeled using 120 cells; each is 40 cm wide and 5.33 cm long. All nodes cell-centered.
Cavity condition	Dry
Upper atmosphere temperature	300 K
Upper atmosphere emissivity	1.0
Ambient pressure	0.1 MPa
Melt/substrate heat transfer coefficient model	Dittus – Boelter
Melt/substrate interfacial heat transfer resistance	0
Constant in Ramacciotti correlation	7.26 (Average for oxide type [15])
Solid-fraction variation	See Figure C-23
Timestep	0.025 seconds

Table C-38 INPUT FILE DATA SHEET FOR THE COMAS EU2B TEST WITH STEEL CHANNEL



Figure C-120 Leading edge penetration comparison for COMAS-EU2b core oxide spreading test with steel channel



Figure C-121 Posttest debris profile prediction for the COMAS EU2b core oxide spreading test with steel channel

Test parameter	Value
Test name	Comas EU-4
Melt composition (wt %)	29 UO ₂ , 12 ZrO ₂ 18 FeO, 2 Cr ₂ O ₃ , 39 Fe
Melt delivery technique	Melt poured into an accumulator box that was 40 cm wide (per channel), 25 cm long, and 5 cm deep relative to spreading surface. Pour initiated by opening a plug device at the bottom of the accumulator.
Melt temperature	2323 К
Total pour mass	2000 kg
Substrate material	Steel
Spreading geometry	1-D channel, 2.5 m long, followed by a 45° sector with an effective radius of 6.0 m.

Code input parameter(s)	Value(s)	
Melt composition (wt %)	29 UO ₂ , 12 ZrO ₂ 18 FeO, 2 Cr ₂ O ₃ , 39 Fe	
Melt pour temperature	2323 K	
Melt oxide phase solidus – liquidus	1598 К – 2233 К	
Melt metal phase solidus – liquidus	1810 K – 1820 K	
Melt pour rate and duration	2.0.10 ⁴ kg/sec over a 0.1 sec (simulating	
	instantaneous deposition in the accumulator,	
	followed by initiation of spreading)	
Melt material property evaluation	Code subroutines	
Substrate composition	Steel (code default composition)	
Substrate initial temperature	300 K	
Substrate material properties evaluation	Code subroutines	
Substrate solidus - liquidus temperatures	1810 K – 1811 K (code default values)	
Substrate nodalization	At each substrate nodal location, six 5.0 mm cells,	
	followed by six 10 mm cells. All nodes cell-centered.	
Spreading cavity nodalization	Accumulator: modeled as single 40 cm wide, 25 cm	
	long, and 5 cm deep cell. Channel: modeled with 50	
	cells that are 40 cm wide and 5.33 cm long. 2-D	
	spreading area: modeled as 45° sector with 110 cells	
	with a radial length of 5.33 cm. All nodes cell-	
	centered.	
Cavity condition	Dry	
Upper atmosphere temperature	300 K	
Upper atmosphere emissivity	1.0	
Ambient pressure	0.1 MPa	
Melt/substrate heat transfer coefficient model	Dittus – Boelter	
Melt/substrate interfacial heat transfer	0	
resistance		
Constant in Ramacciotti correlation	7.26 (Average for oxide type [15])	
Solid-fraction variation	See Figure C-23	
Timestep	0.025 seconds	



Figure C-122 Leading edge penetration comparison for COMAS-EU4 core oxide spreading test in 2-D geometry with steel channel



Figure C-123 Posttest debris profile prediction for the COMAS EU4 core oxide spreading test in 2-D geometry with steel channel

Appendix D

SUMMARY OF POST PROCESSING TO PRODUCE CORQUENCH-COMPATIBLE INPUT BASED ON MELTSPREAD OUTPUT

At the end of the calculation, subroutine CQSTART within MELTPSPREAD generates the output data file 'cqinput.dat' that documents the cavity geometry, ablation, core debris temperature, and core debris composition profiles within the spreading domain at the end of the transient. Although this information is embedded in various other MELTSPREAD output files, the intent of cqinput is to compile in a single file the specific information that is needed to generate an input file for CORQUENCH which can then be run to examine longer term debris coolability and water management issues once spreading is complete.

To help automate the process, a small piece of fortran software called '*cqprocess2.f*' has been developed to process data from *cqinput* which, along with user-supplied modeling assumptions and information defined in the data file '*cqassume.dat*,' then produces an output data file called '*cqpasteme.dat*.' The text in this file can then be inserted directly into the CORQUENCH input file that is needed to execute CORQUENCH. In particular, *cqpastme* can be inserted as Lines 46-49 of the CORQUENCH input file '*quenchin.dat*;' see Tables 3-1 and 3-2 in the CORQUENCH User's Manual.^[9] This process is illustrated in the flow diagram that is shown in Figure D-1. This capability has been developed for two reasons, both of which are based on a desire to reduce the amount of effort required to prepare a CORQUENCH input file, as well as the possibility of making mistakes if this process is done manually. The two reasons are:

- 1) Constituent indexing schemes used in MELTSPREAD and CORQUENCH are not the same, thus requiring tedious but straightforward manipulation of the output that is best done with software, and
- 2) MELTSPREAD runs may include hundreds of nodes, but this level of fidelity is not needed for a CORQUENCH simulation. Moreover, a CORQUENCH simulation may need to cover many hours to days of real time, thus requiring fewer nodes to reduce computational time. Thus an automated process is needed to logically collapse the MELTSPREAD output into CORQUENCH input based on user-supplied guidance.

Additional detail regarding these various files and how they are used is provided below.

STRUCTURE AND CONTENT OF MELTSPREAD OUTPUT FILE 'cqinput'

The MELTSPREAD file *cqinput* is generated to document the cavity geometry, ablation, core debris temperature, and core debris composition profiles within the spreading domain at the end of the transient. Specifics are summarized in Table D-1.





Table D-1 'cqinput' FILE DESCRIPTION

Line	Variable	Definition/Function
No.	Name(s)	
	NUMNOD	Total number of spreading nodes in MELTSPREAD analysis
	TMSTOP	Minimum melt temperature allowed at any node site. Set to large
		value if it is desired to use the average calculated melt temperature.
	KP	Spreading node number
	NAC(KP)	NAC(KP)=0 if the node is inactive (i.e., does not contain core debris),
		or NAC(KP)=1 if core debris is present at the node site
	RAD(KP)	Radial location (i.e. distance along spreading path) within the
		cell at which the node is located
	ARC(KP)	Width of spreading channel perpendicular to spreading direction
	AREA(KP)	Surface area of node
	DXN(KP)	Overall length of the node parallel to the flow direction
	EL(KP)	Elevation of concrete surface remaining at node location
	TMP(KP),	For KP-th node, TMP=average temperature, CMP=specific heat, and
3	CMP(KP),	XMT=total mass of core debris at node site.
	XMT(KP)	<i>Note</i> : Lines 3 and 4 are omitted if the node is inactive (i.e. NAC=0)
	YM(K,KP),	For the KP-th node, this is the mass of K-th corium constituent
4	YC(K,KP),	in the melt, crust, and particle bed regions, respectively $(1 \le K \le M)$
	YB(K,KP)	22; see Table D-2). Note : Line 4 is repeated 22 times.

Index	Constituent	Notes
1	Na ₂ O	
2	TiO ₂	
3	SiO_2	1
4	CaO	7
5	MgO	7
6	Al ₂ O ₃	
7	FeO	7
8	Fe ₂ O ₃	
9	Fe ₃ O ₄	
10	Fe	7
11	Cr	
12	Ni	1
13	Zr	1
14	ZrO ₂	1
15	B ₂ O ₃	7
16	U	
17	B ₄ C	1
18	Si	7
19	SiC	7
20	Cr_2O_3	7
21	NiO]
22	UO ₂	

Table D-2 SUMMARY OF INDICIAL SCHEME FOR MELT-CONCRETE CONSTITUENTS IN CORQUENCH4^[9]

The first line documents the total number of spreading nodes NUMNOD used in the MELTSPREAD run, as well as the time TMSTOP (in seconds) at the end of the run. Line 2 defines geometric characteristics of each spreading node; this line is repeated NUMNOD times. For each node, NAC=0 if the node is inactive (i.e., does not contain core debris), or NAC=1 if core debris is present at the node site. RAD is the radial location (i.e., distance along spreading path) within the cell at which the node is located, while ARC is the channel width perpendicular to spreading direction. AREA is the surface of the node, and DXN is the overall length of the node parallel to the flow direction. Finally, EL is the elevation of the concrete surface remaining at the node site.

For cases in which the node is active (i.e., NAC=1), Lines 3 and 4 define the core debris conditions at each node site. Note that both of these lines are omitted for inactive nodes (NAC=0). For active nodes, TMP on Line 3 is the average temperature of the core debris, CMP is the specific heat of the debris, and XMT is the total mass of debris. Note that if there is no previously frozen

material at the node site, then TMP corresponds to the melt temperature. However, if material has been previously frozen at the node site, then TMP corresponds to the thermal equilibrium temperature of the combined debris regions, both liquid and solid.

Finally, Line 4 defines the mass of the K-th corium constituent in the melt, crust, and particle bed regions, respectively (1 < K < 22) at each active node site; see Table D-2 for the index assigned to each debris constituent. Line 4 is repeated 22 times, which corresponds to the total number of debris constituents treated in CORQUENCH. Note that if particle bed formation by melt jet fragmentation is **not** modeled (i.e., NJET=0; see Table 4-1), then all core debris at the node site is assigned to the 'melt' matrix, YCM. However, if particle bed formation is modeled (i.e., NJET=2; see Table 4-1) and the user desires to treat this material as discrete input in the CORQUENCH simulation¹, then an equivalent top crust thickness is calculated based on the reasoning that a crust must exist to support the overlying particle bed. The crust thickness is evaluated based on the local upwards heat flux from the debris to overlying atmosphere at the end of the simulation, the debris freezing temperature and thermal conductivity, and the 'crust' upper surface temperature that is taken to be water saturation temperature if water is present, or the overlying structure temperature if water is absent. With the crust thickness known, the corresponding crust mass is then calculated and the 'melt' mass is deficited by that amount so that mass is conserved.

STRUCTURE AND CONTENT OF INPUT FILE 'cqassume'

cqassume is a user-supplied file defining modeling assumptions and other information that is needed to guide the mapping of the MELTSPREAD debris distribution data written to *cqinput* into text that can be directly imported into the CORQUENCH input file *quenchin*. Specifics are provided in Table D-3. NUMCQ on Line 1 defines the total number of nodes into which the MELTSPREAD results are to be collapsed for input into the CORQUENCH analysis. Note that NUMCQ must be less than or equal to the total number of nodes used in the MELTSPREAD analysis, NUMNOD. Also on Line 1, TMINCQ is the minimum allowed melt temperature to be written to the output file *cqpasteme*. The background for this parameter is that CORQUENCH requires that the debris be at least partially molten at the start of the simulation; i.e., the initial temperature must be above the solidus temperature of either the

¹ The decision on whether or not the particle bed is retained as a discrete zone in the MELTSPREAD output to *cqinput* is determined by the setting of NBEDCQ; see Line 65 in Table 4-1. If NEBDCQ=1, then the bed is combined with the underlying melt and/or solidified debris and thermally equilibrated with that material.

metal or oxide phase, if both phases are present. If only one phase is present, then the same requirement is applied to that single phase. In some MELTSPREAD calculations in which thin debris layers' form, the material can be completely solidified. Thus, TMINCQ is provided as a check against the MELTSPREAD output temperature TMP (see Table D-1). If TMP is less than TMINCQ, then TMP is set equal to TIMINCQ. If the user desires to override this option, then simply set TMINCQ to an artificially high number. Note that even if this is done, at startup of the CORQUENCH calculation the initial melt temperature is checked against the freezing temperature calculated for the particular debris composition; if it is less than the freezing temperature, a note is written to the CORQUENCH diagnostics file to that effect, and the run is terminated. At that point, the user can manually increase the melt temperature setting in *quenchin* and restart the run.

Line	Variable	Definition/Function
No.	Name(s)	
	NUMCQ	Total number of nodes into which the MELTSPREAD results are to be collapsed for input into the CORQUENCH analysis. Note: NUMCQ must be < NUMNOD.
	TMINCQ	Minimum allowed melt temperature at any given node site
2	NST(K), NSTP(K), N2DC(K), NSMP(K), IFLG(K), XL2D(K)	 For the K-th collapsed node: NST(K) and NSTP(K) are the first and last nodes from the MELTPSPREAD analysis that are to be collapsed into a single node for the CORQUENCH analysis. N2DC(K) defines the cavity geometry and ablation modeling assumptions for the collapsed node; corresponds to N2DCALCC(K) in the CORQUENCH input file (see Table 3-2, Line 46 in [9]). NSMP(K)=0 if the collapsed node is not considered to be a sump, or NSMP(K)>1 if the node is considered to be a sump with preexisting elevation difference(s) between adjacent node(s); see discussion in text for appropriate settings. If a melt pour occurs over the course of the calculation, set IFLG(K)=0 if the collapsed node is not a receptor of relocating melt, or set IFLG(K)=1 if it is. For cases in which N2DC=3 or 4 (see definition in the text), then XL2D is the distance between the ablating wall(s) for the 2-D rectilinear cavity modeling assumption cases.
		Mole. Life 2 is repeated nonicy liftes.

Table D-3 'cqassume' FILE DESCRIPTION

In Line 2, which is repeated NUMCQ times, NST(K) and NSTP(K) are the first and last nodes from the MELTPSPREAD analysis that are to be collapsed into the K-th node in the CORQUENCH analysis. The axial surface area of this collapsed node is then calculated as the sum of the areas of the individual nodes. The second parameter N2DC(K) controls the cavity ablation modeling assumptions for the collapsed node. In particular, set:

- N2DC(K)=1 to perform a 1-D (axial) basemat erosion calculation;
- N2DC(K)=2 to perform a 2-D cylinder geometry (axial plus radial; right cylinder assumed) erosion calculation;
- N2DC(K)=3 to perform a 2-D notch-geometry calculation with two opposing, ablating walls;
- N2DC(K)=4 to perform a 2–D notch-geometry calculation with one wall ablating and the others inert; or
- N2DC(K)=5 to perform a 2-D cylindrical annulus (axial plus radial; right cylinder geometry assumed with inner radius fixed) erosion calculation.

For the K-th node, also set NSMP(K)=0 if the node is not considered to be a sump with a pre-existing elevation difference between adjacent node(s) that could limit sidewall ablation area relative to the pool height available for ablation. For instance, if the melt pool surface elevation at the node is greater than the sump depth, then sidewall ablation area is limited by the sump wall height as opposed to depth. If the node is considered to be a sump, then set NSMP(K)=1 if the melt surface elevation is to be compared to the concrete elevation of the node to the left (i.e., K–1) to determine the controlling sidewall height, or set NSMP(K)=2 if the comparison is made to the node to the right (i.e., K+1). Finally, if N2DC(K)=3, then set NSMP(K)=3 if both left and right walls are compared. If N2DC(I)=3 or 4, then XL2D(I) is the distance between the The corresponding width between the nonablating concrete sidewall(s). ablating walls (known as XWID2DC in the CORQUENCH input; see Line 46 in Table 3-2 of [9]) is then calculated from the total node axial surface area divided by XL2D. This same result is applied to the case in which a 1-D node is constructed (i.e. N2DC(K)=1).

STEPS CARRIED OUT BY PROGRAM 'cqprocess2'

Many of the steps and checks carried out by *cqprocess2* have already been outlined above. A few additional details are provided here.

After the input data is read from *cqinput* and *cqassume*, the first step carried out by *cqprocess2* is to combine the constituent masses for nodes that are to be collapsed into larger nodes for the CORQUENCH analysis. The axial surface areas of the collapsed nodes are also summed up to get the total axial surface area of the new node. The effective surface elevation of this new node is then found by area-weighting the elevations of the individual nodes. This approach is approximate, but conserves mass and energy based on the MELTSPREAD analysis results. For collapsed nodes that are found to contain core debris, these nodes are declared to be 'active' by setting NACTIV=1 as part of the CORQUENCH input.

With these steps completed, the characteristics of the new mesh are then calculated based on the geometry assumptions defined in *cqassume*. The overall approach is to conserve spreading length (needed for the detailed water inventory analysis) and axial surface area. The combined node incremental distance DX is found as the sum of the individual node DX's. The channel width ARC at the end of each collapsed node is set equal to the width of the last node that is included as part of the summation. The average melt temperature for the collapsed node is then calculated by thermally equilibrating the core debris in the combined nodes based on the individual debris temperatures (TMP), effective specific heats (CMP), and debris masses (XMP) in each individual node; see Table D-1.

With the above steps completed, the output data file *cqpasteme* is then created. This file contains the all the information needed as input in Lines 46 to 49 of the CORQUENCH input file in the proper format. Thus, *cqpasteme* can simply be inserted into *quenchin* and the file is then problem is ready to run once the other input data is provided.



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