PDC: Plant Dynamics Code for Design and Transient Analysis of Supercritical Brayton Cycles

Nuclear Science and Engineering Division
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PDC: Plant Dynamics Code for Design and Transient Analysis of Supercritical Brayton Cycles

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September 27, 2018
ABSTRACT

The current report documents the Plant Dynamics Code developed at the Argonne National Laboratory for steady-state and transient analysis of supercritical Brayton cycles. The report consists of three major parts.

*Code Overview* provides the general description of the code, including the purpose of the code development and the code’s main features.

*User’s Guide* explains how to work with the code, including its user interface.

*Code Manual* provides the detailed description of the code, including modeling, assumptions, and the solution schemes.
# Table of Contents

List of Figures ................................................................................................................................. vi
List of Tables ....................................................................................................................................... ix
Nomenclature ......................................................................................................................................... x

1 Code Overview .............................................................................................................................. 1
2 User’s Guide ...................................................................................................................................... 4
  2.1 Introduction and Definitions ........................................................................................................ 5
  2.2 Code File Structure .................................................................................................................... 11
  2.3 Graphical User Interface ............................................................................................................ 12
    2.3.1 GUI Main Form .................................................................................................................... 12
    2.3.2 GUI Interactive Features ................................................................................................... 14
    2.3.3 Input for PDC Steady-State Part ......................................................................................... 16
      2.3.3.1 Cycle Configuration for PDC ....................................................................................... 18
      2.3.3.2 Cycle operating conditions ......................................................................................... 21
      2.3.3.3 Turbomachinery Calculation Modes ........................................................................... 24
      2.3.3.4 Heat Addition Mode ..................................................................................................... 25
      2.3.3.5 Component Input ........................................................................................................... 25
      2.3.3.6 Turbomachinery Shafts ................................................................................................. 36
    2.3.4 Input for PDC Transient Calculations .................................................................................. 37
      2.3.4.1 General Input ................................................................................................................. 38
      2.3.4.2 Cycle Control ................................................................................................................ 39
      2.3.4.3 Heat Addition ............................................................................................................... 42
      2.3.4.4 Heat Removal ................................................................................................................. 49
      2.3.4.5 Turbomachinery Maps ................................................................................................. 50
    2.3.5 Transient Definitions ............................................................................................................ 54
      2.3.5.1 Change in Boundary Conditions ................................................................................. 54
      2.3.5.2 Load Following .............................................................................................................. 54
      2.3.5.3 Grid Disconnection/Loss of Load ................................................................................. 54
      2.3.5.4 Pipe Break .................................................................................................................... 55
      2.3.5.5 Control Action ................................................................................................................. 55
    2.3.6 Executing the PDC code ....................................................................................................... 55
    2.3.7 Viewing PDC Results .......................................................................................................... 58
      2.3.7.1 Steady-State Results .................................................................................................... 58
      2.3.7.2 Dynamic Results ......................................................................................................... 62
  2.4 Working with Text Files Directly ............................................................................................... 68
    2.4.1 PDC Input Files .................................................................................................................. 68
    2.4.2 PDC Output Files ............................................................................................................... 70
    2.4.3 Turbomachinery Map Files ................................................................................................. 71
    2.4.4 Executing the Code from Command Line ........................................................................... 72
  2.5 PDC Restart Capability ............................................................................................................ 73
  2.6 Coupling with SAS4A/SASSYS-1 Code .................................................................................... 76
    2.6.1 Coupling Approach ............................................................................................................. 76
    2.6.2 Accuracy of the Coupling Scheme ..................................................................................... 78
    2.6.3 Using Coupling with SAS4A/SASSYS-1 ........................................................................... 79
2.6.4 Transient Definition with PDC-SAS4A/SASSYS-1 Coupling ........................................ 80

3 Code Manual .................................................................................................................. 81

3.1 Steady-State Models .................................................................................................... 83

3.1.1 Cycle Calculations .................................................................................................. 84

3.1.1.1 Cycle Solution Scheme ...................................................................................... 84

3.1.1.2 Iterations in Turbomachinery Design Mode ....................................................... 87

3.1.1.3 Iterations in Turbomachinery Performance Mode .............................................. 88

3.1.2 Heat Exchangers ...................................................................................................... 90

3.1.2.1 General HX (Effectiveness Method) .................................................................. 90

3.1.2.2 Realistic HX – Solution Scheme ........................................................................ 92

3.1.2.3 Shell and Tube Heat Exchanger ......................................................................... 94

3.1.2.4 Printed Circuit Heat Exchanger (PCHE) ............................................................. 96

3.1.2.5 Cooler ................................................................................................................ 104

3.1.2.6 Crossflow Heat Exchangers for Cooler ............................................................... 105

3.1.3 Electrical Heater ...................................................................................................... 116

3.1.4 Turbomachinery ...................................................................................................... 117

3.1.4.1 Axial Compressor .............................................................................................. 123

3.1.4.2 Centrifugal Compressor .................................................................................... 134

3.1.4.3 Axial Turbine .................................................................................................... 139

3.1.4.4 Radial Turbine ................................................................................................ 148

3.1.5 Flow Splits ............................................................................................................... 154

3.1.6 Mixers ....................................................................................................................... 155

3.1.7 Valves ....................................................................................................................... 155

3.1.8 Pipes ........................................................................................................................ 156

3.1.8.1 Heat Transfer in Pipes ...................................................................................... 156

3.1.8.2 Pipe Pressure Drop .......................................................................................... 158

3.2 Dynamic Models ......................................................................................................... 160

3.2.1 General Formulation of Dynamic Equations in PDC ............................................ 160

3.2.2 Flow Branches and Reverse Flow ......................................................................... 164

3.2.3 Valves ....................................................................................................................... 168

3.2.4 Critical Flow Limitation ......................................................................................... 169

3.2.5 Pipes ........................................................................................................................ 173

3.2.6 Heat Exchangers .................................................................................................... 173

3.2.6.1 Counter-Flow Heat Exchangers ....................................................................... 173

3.2.6.2 Cross-Flow Heat Exchangers for the Cooler ..................................................... 174

3.2.6.3 Incompressible Flow Equations for Fluids outside the Cycle ......................... 176

3.2.7 Electrical Heater ..................................................................................................... 177

3.2.8 Turbomachinery ..................................................................................................... 178

3.2.8.1 Turbomachinery Maps ...................................................................................... 178

3.2.8.2 Turbomachinery Shaft Dynamics .................................................................... 180

3.2.8.3 Grid Connection Modes .................................................................................. 182

3.2.9 Incompressible Flow Treatment Option .............................................................. 183

3.2.10 Solution Algorithm ............................................................................................... 186

3.2.10.1 Numerical Solution of Differential Equations .................................................. 186

3.2.10.2 Convergence Criteria and Accuracy Control ................................................... 188

3.2.10.3 Dynamic Time Step Control ......................................................................... 190

ANL-ART-154 iv
3.2.10.4 Separate air side cooler calculations ............................................. 191
3.2.11 Initial and Boundary Conditions for Transient Calculations ............... 192
3.2.12 Transient Definitions ...................................................................... 193
  3.2.12.1 Change in Boundary Conditions .................................................. 193
  3.2.12.2 Load Following ........................................................................... 193
  3.2.12.3 Grid Disconnection/Loss of Load ................................................. 193
  3.2.12.4 Pipe Break ................................................................................ 193
  3.2.12.5 Control Action ........................................................................... 194

3.3 Plant Control System ............................................................................. 195
  3.3.1 Cycle Controls ................................................................................ 196
    3.3.1.1 Options for Scaling of Control PID Coefficients ......................... 197
    3.3.1.2 Manual Control Overwrite .......................................................... 198
    3.3.1.3 Turbine Bypass Control .............................................................. 198
    3.3.1.4 Inventory Control ...................................................................... 199
    3.3.1.5 Turbine Inlet (Throttle) Valve Control ......................................... 200
    3.3.1.6 Compressor Outlet (Throttling) Valve .......................................... 201
    3.3.1.7 Cooler Bypass Control .............................................................. 201
    3.3.1.8 Recuperator Bypass Control ....................................................... 202
    3.3.1.9 Compressor Surge Control ......................................................... 203
  3.3.2 Cooler Cold-Side Flow Rate and Pump Head Control ......................... 205
  3.3.3 Heat Addition Control ..................................................................... 206
    3.3.3.1 Control with HAHX User Input Tables ........................................ 206
    3.3.3.2 Control with Electrical Heater ................................................... 207
    3.3.3.3 Reactor Controls with SAS4A/SASSYS-1 Coupling .................... 207

3.4 Materials, Properties, and Correlations .................................................. 210
  3.4.1 Heat Transfer and Pressure Drop Correlations .................................... 210
    3.4.1.1 Straight Channels ..................................................................... 211
    3.4.1.2 PCHE Channels ......................................................................... 212
    3.4.1.3 Cross-Flow Cooler .................................................................... 214
  3.4.2 Fluid Properties ................................................................................. 216
    3.4.2.1 Cycle Working Fluid .................................................................. 216
    3.4.2.2 HAHX Hot-Side Fluids ............................................................... 216
    3.4.2.3 Cooler Cold-Side Fluids ............................................................... 217
  3.4.3 Structural Materials .......................................................................... 217

Acknowledgements ...................................................................................... 219
References .................................................................................................. 220
Appendix A: PDC Verification and Validation References ............................ 224
Appendix B: Example Problem ................................................................... 225
  B.1. Steady-State Model Setup Input Files ............................................... 227
  B.2. Steady-State Results ......................................................................... 247
  B.3. Transient Definition and Input .............................................................. 262
  B.4. Transient Results .............................................................................. 270
Appendix C: PDC Modules, Functions, Subroutines, and Call Diagrams ....... 279
List of Figures

Figure 2-1. Simple Brayton Cycle. ................................................................. 5
Figure 2-2. Recuperated Brayton Cycle. ......................................................... 7
Figure 2-3. Temperature-Entropy Diagram for Carbon Dioxide. ....................... 8
Figure 2-4. Examples of Carbon Dioxide Property Variation near the Critical Point. 9
Figure 2-5. Recompression Brayton Cycle. ..................................................... 10
Figure 2-6. PDC Directory Structure. ............................................................ 11
Figure 2-7. PDC Graphical User Interface Main Form. ...................................... 12
Figure 2-8. PDC GUI Interactive Features. ..................................................... 15
Figure 2-9. PDC GUI Form for Cycle Configuration. ....................................... 17
Figure 2-10. Cycle Configuration in the Example Input. .................................... 21
Figure 2-11. Enthalpy Reduction during Acceleration at Compressor Inlet........... 23
Figure 2-12. PDC GUI Form for Recuperator Input. ....................................... 26
Figure 2-13. PDC GUI Input Form for Recuperator: General Type. ................. 27
Figure 2-14. PDC GUI Input Form for Recuperator: Shell-and-Tube Type............ 28
Figure 2-15. Platelet PCHE. ....................................................................... 29
Figure 2-16. PDC GUI Input Form for Recuperator: Z/I PCHE. ....................... 29
Figure 2-17. PDC GUI Input Form for HAXH ................................................. 31
Figure 2-18. PDC GUI Input Form for Electrical Heater. ............................... 32
Figure 2-19. PDC GUI Input Form for Cooler. .............................................. 33
Figure 2-20. PDC GUI Input Form for Turbine. ............................................. 34
Figure 2-21. PDC GUI Input Form for Compressor. ....................................... 35
Figure 2-22. PDC GUI Input Form for Turbomachinery Shaft. ....................... 36
Figure 2-23. PDC GUI Input Form for Dynamics: General. ........................... 39
Figure 2-24. PDC GUI Input Form for Dynamics: Cycle Control. .................... 41
Figure 2-25. PDC GUI Input Form for Dynamics: Heat Addition – User Input. 43
Figure 2-26. PDC Table Input in Text Format. .............................................. 44
Figure 2-27. PDC GUI Input Form for Dynamics: Heat Addition – Automatic Control. 45
Figure 2-28. PDC GUI Input Form for Dynamics: Heat Addition – Automatic Control with Electrical Heater. .......................................................... 46
Figure 2-29. PDC GUI Input Form for Dynamics: Heat Addition – User Input with Electrical Heater ............................................................... 47
Figure 2-30. PDC GUI Input Form for Dynamics: Heat Addition – SAS4A/SASSYS-1 Coupling. ................................................................. 48
Figure 2-31. PDC GUI Input Form for Dynamics: Heat Removal. .................... 49
Figure 2-32. PDC GUI Input Form for Dynamics: Turbomachinery Maps. .......... 50
Figure 2-33. PDC Maps Folders. ................................................................. 52
Figure 2-34. PDC Maps Conversion Form. .................................................... 53
Figure 2-35. PDC Execution Windows – Steady-State Calculations. .................. 56
Figure 2-36. PDC Execution Windows – Dynamic Calculations. ..................... 57
Figure 2-37. PDC GUI Results Form: Cycle. ............................................... 59
Figure 2-38. PDC Cycle Results in Excel. ..................................................... 60
Figure 2-39. PDC GUI Results Form: Component Design. ............................. 61
Figure 2-40. PDC GUI Results Form: Component Details. ............................. 62
Figure 2-41. PDC Dynamic Results in Excel: Update Tab. ............................... 63
Figure 2-42. PDC Dynamic Results in Excel: Example of General Results Plots ........................................ 64
Figure 2-43. PDC Dynamic Results in Excel: Example of Cycle Results Plots ........................................ 66
Figure 2-44. PDC Dynamic Results in Excel: Viewing Results for Components ...................................... 67
Figure 2-45. PDC Input for Restart ............................................................................................................. 73
Figure 2-46. PDC-SAS4A/SASSYS-1 Coupling Approach ........................................................................ 77
Figure 2-47. Sodium RHX Temperature Change Prediction Error ......................................................... 78
Figure 3-1. Example of PDC Steady-State Results for Advanced Fast Reactor (AFR)-100 sCO₂ Cycle ........ 83
Figure 3-2. Flow Rate and Pressure Ratio in Turbomachinery Performance Mode ................................ 89
Figure 3-3. Heat Exchanger Effectiveness ................................................................................................. 91
Figure 3-4. Multi-Node Solution Approach for Heat Exchangers ........................................................... 92
Figure 3-5. Fins and Their Efficiency in Shell-and-Tube Heat Exchanger ................................................ 95
Figure 3-6. Shell-and-Tube Heat Exchanger Baffle Plates ...................................................................... 96
Figure 3-7. Printed Circuit Heat Exchanger ............................................................................................... 97
Figure 3-8. PCHE Zigzagged Channel ..................................................................................................... 98
Figure 3-9. PCHE HX Model with Fins ..................................................................................................... 98
Figure 3-10. Platelet PCHE ..................................................................................................................... 100
Figure 3-11. PCHE Z/I Configuration ...................................................................................................... 100
Figure 3-12. Z/I PCHE Flow Paths and Dimensions ................................................................................ 101
Figure 3-13. PCHE and Formed Plate Design and PDC Inputs ............................................................... 104
Figure 3-14. Temperature Field in a Crossflow Heat Exchanger ............................................................. 106
Figure 3-15. Finned Tube Crossflow Heat Exchanger ............................................................................. 109
Figure 3-16. Tube Lattices: Triangular (Left) and Square (Right) .............................................................. 110
Figure 3-17. Treatment of Multi-Pass HX with Separate HXs ................................................................. 111
Figure 3-18. Concept of Crossflow PCHE ............................................................................................... 115
Figure 3-19. Turbomachinery Stage Velocity Triangles for Rotor Inlet and Outlet ................................. 117
Figure 3-20. Total and Static Conditions in Turbomachinery ................................................................. 118
Figure 3-21. Concept of Pressure Loss and Increase in Entropy ............................................................. 120
Figure 3-22. Enthalpy-Entropy Diagram of Expansion in Turbine (Left) and Compression in Compressor (Right). .................................................................................................................. 121
Figure 3-23. Compressor Stage Velocity Triangles .................................................................................. 125
Figure 3-24. Blade Profile Angles .......................................................................................................... 128
Figure 3-25. Illustration of a Two-Stage Centrifugal Compressor Design ............................................... 135
Figure 3-26. Centrifugal Compressor Impeller Passage (Left) and Blade Geometry (Right) .................. 136
Figure 3-27. Centrifugal Compressor Diffuser Geometry ....................................................................... 137
Figure 3-28. Axial Turbine Stages .......................................................................................................... 140
Figure 3-29. Axial Turbine Stage Dimensions ......................................................................................... 140
Figure 3-30. Gas Velocities in a Turbine Stage ....................................................................................... 141
Figure 3-31. Stalling Incidence Plot Fitting ............................................................................................. 143
Figure 3-32. Incidence Loss Coefficient Plot Fitting ............................................................................... 144
Figure 3-33. Type 316 Stainless Steel Polished Surface Emissivity Fit ................................................. 158
Figure 3-34. Flow in a Channel ............................................................................................................... 160
Figure 3-35. Regions for Temperature, Density, and Flow Rate Calculations ...................................... 162
Figure 3-36. Flow Splits and Mixers in Dynamics .................................................................................... 166
Figure 3-37. Flow Through a Valve Opening ......................................................................................... 170
Figure 3-38. Two-Dimensional Temperature Field in a Cross-Flow Heat Exchanger ......................... 175
Figure 3-39. Compressor Stage for Moment of Inertia Calculations ................................................. 182
Figure 3-40. CO₂ Compressibility in the sCO₂ Cycle ................................................................. 184
Figure 3-41. Cycle Control Mechanisms Supported by the PDC .................................................. 197
Figure 3-42. Example of Recuperator Bypass/Throttling Control Action ..................................... 203
Figure 3-43. Compressor Surge Control ....................................................................................... 204
Figure 3-44. Reactor with Primary and Intermediate Coolant Loops .............................................. 208
List of Tables

Table 2-1. Available Ports for Components................................................................. 19
Table 2-2. CO₂ Properties Variations Near the Compressor Inlet Location .................. 23
Table 2-3. Turbomachinery Calculation Modes ............................................................ 25
Table 2-4. Summary of Heat Addition Calculation Modes in Dynamics ....................... 42
Table 2-5. Variables Available in the PDC Dynamic Output.......................................... 65
Table 2-6. Variable Types Available in the PDC Cycle Output ...................................... 66
Table 2-7. PDC Input Files ............................................................................................. 69
Table 2-8. PDC Output Files ......................................................................................... 70
Table 3-1. Heat Exchangers in PDC ............................................................................. 90
Table 3-2. Turbomachinery Efficiency Definitions in the PDC .................................... 122
Table 3-3. Relationship between IGV Angle and Maximum Deflection for 50%-Reaction Stage ........................................................................................................ 125
Table 3-4. Example of Scaling with Idea Gas Law ....................................................... 179
Table 3-5. Effect of the Incompressible Flow Treatment for sCO₂ Cycle ....................... 186
Table 3-6. Automatic Control with Coupled PDC-SAS4A/SASSYS-1 Codes ................ 208
Table 3-7. Heat Transfer and Pressure Drop Correlations in the PDC ............................ 210
Table 3-8. Structural Materials Supported by PDC ....................................................... 218
Abbreviations:

- AFR = Advanced Fast Reactor
- CBP = Cooler bypass control
- CIT = Compressor inlet temperature
- GUI = Graphical User Interface
- HAHX = Heat addition heat exchanger
- HTR = High temperature recuperator
- HX = Heat exchanger
- IHTS = Intermediate heat transport system
- IHX = Intermediate heat exchanger
- LTR = Low temperature recuperator
- PCHE = Printed Circuit Heat Exchanger
- PDC = Plant Dynamics Code
- PID = Proportional, Integral, and Differential controls
- RBP = Recuperator bypass control
- RHX = Reactor heat exchanger
- sCO₂ = Supercritical carbon dioxide (Brayton cycle)
- SFR = Sodium-cooled fast reactor
- TBP = Turbine bypass control
- TM = Turbomachinery

Variables in equations (unless noted otherwise):

- \( A \) = Area [m²]
- \( C \) = Speed [m/s]
- \( d \) = Diameter [m]
- \( h \) = Enthalpy [J/kg]
- \( k \) = Thermal conductivity [W/m-K]
- \( l, L \) = Length [m]
- \( \dot{m} \) = Mass flow rate [kg/s]
- \( M \) = Mass [kg]
\[ p = \text{Pressure [Pa]} \]
\[ Q = \text{Heat transfer rate [W]} \]
\[ r = \text{Radius [m]} \]
\[ s = \text{Entropy [J/kg-K]} \]
\[ t = \text{Time [s]} \]
\[ T = \text{Temperature [°C]} \]
\[ u = \text{Blade speed [m/s]} \]
\[ V = \text{Velocity [m/s]} \]
\[ W = \text{Work [W]} \]
\[ \Delta = \text{Difference or change [-]} \]
\[ \epsilon = \text{Efficiency or effectiveness [- or %]} \]
\[ \eta = \text{Cycle efficiency [- or %]} \]
\[ \mu = \text{Viscosity [Pa-s]} \]
\[ \rho = \text{Density [kg/m}^3] \]
\[ \omega = \text{Rotational speed [rad/s]} \]
\[ \left( \frac{\partial y}{\partial x} \right)_Z = \text{Derivative of property } Y \text{ with respect to } X \text{ along constant } Z, \]
\[ \text{for example, } C_p = \left( \frac{\partial h}{\partial T} \right)_p \]

Subscripts (unless noted otherwise):

\[ c = \text{cold side} \]
\[ h = \text{hot side} \]
\[ i, j = \text{node indices} \]
\[ in = \text{inlet} \]
\[ out = \text{outlet} \]
\[ w = \text{wall} \]
\[ wf = \text{working fluid} \]
1 CODE OVERVIEW
The Plant Dynamics Code (PDC) has been developed at Argonne National Laboratory for design and transient analysis of supercritical carbon dioxide (sCO₂) Brayton cycle energy conversion at the system level. The sCO₂ cycles take advantage of CO₂ properties variations near its critical point to reduce the compression work and thus increase cycle efficiency, compared to ideal-gas Brayton cycles operating in the same pressure and temperature range. For this reason, it is always desirable to operate the compressor as close as possible to the critical point, yet the CO₂ conditions need to remain above critical to preclude formation of two-phase flow, which could damage the compressor blades. Because of this specific feature of sCO₂ cycles, the philosophy for PDC creation and development has always been a requirement to: 1) accurately calculate the CO₂ properties everywhere in the cycle and, specifically, close to the critical point, which is usually approached at the main compressor inlet; and 2) calculate the effect of those properties variations on the performance of the cycle components, such as compressors and coolers, as well as on the integrated performance of the entire cycle. There is another consequence of the CO₂ properties variations in that the cycle layout is often different from traditional (e.g., ideal gas) Brayton cycles and specific sCO₂ cycle configurations, such as recompression and partial cooling, are used with sCO₂ in order to increase overall plant efficiency. Therefore, the PDC formulations have always been flexible enough to facilitate investigation of various alternate cycle configurations and operating conditions.

In order to further characterize the sCO₂ cycle performance near the critical point, special attention was always paid in the PDC to component design and cycle control for the conditions near the critical point. One of the unique PDC features is the distinction of where the closest approach to the critical point is occurring in the cycle. It was realized early on in the code development that as the CO₂ flow accelerates at the compressor inlet, the difference between the total and static conditions becomes very important to accurately calculate the fluid properties and their effect on the compressor performance. Likewise, special attention is paid in the cycle control system development and analysis to where the closest approach to the critical point is occurring at any specific state of the cycle and how to control that approach effectively and efficiently.

The Plant Dynamics Code effectively consists of two parts: steady-state and transient. The steady-state part of the code includes design analysis of turbomachinery components (turbines and compressors), performance analysis of heat exchangers, and integrated performance of the entire cycle. The transient part of the code solves compressible flow and energy transfer differential equations to characterize the time-dependent cycle performance. It too includes performance analysis of turbomachinery and heat exchangers. Equation formulation and solution schemes for both the steady-state and transient parts are always performed in the PDC to address the special feature of sCO₂ cycles – properties variations near the critical point. In addition, the code includes simulation of control mechanisms and control valves.

The PDC has been used extensively to optimize sCO₂ cycles, carry out analysis of nominal operating (e.g., load following) and postulated accident (pipe breaks, thermal shocks, etc.) transients, and to develop sCO₂ cycle control strategies. Most of these analyses have been done for sCO₂ cycle applications such as design and optimization of energy conversion systems for advanced nuclear reactors. For this purpose, the PDC has been coupled to the SAS4A/SASSYS-1 code for the coupled analysis of nuclear reactors with sCO₂ cycles. Still, the PDC provides
another option of defining heat addition conditions through time-dependent tables for transient analysis at the system level without the use of the SAS4A/SASSYS-1 code.

The code has been validated against separate-effects experiments, such as heat exchanger and compressor tests, as well as against integral sCO₂ test loops. The list of the code validation references is provided in Appendix A at the end of this report.

The Plant Dynamics Code has been written in Fortran code using the Fortran 90 convention. This choice was made for several reasons. First, it provided flexibility to build and extend the code’s modules and features as the analysis of sCO₂ cycle progressed from component-level design to cycle steady-state analysis to transient and control analysis of individual components and the entire system. Using Fortran 90 code optimization and acceleration features allowed detailed and accurate calculations (for example, the code uses a 42-term expansion of CO₂ properties) and still have a fast-running code to analyze many design variations as well as run transient simulations at reasonable speed. Lastly, relying on the Fortran language allowed utilization of Argonne’s vast experience in developing computer codes and to facilitate coupling of the PDC to other Argonne codes.

Even though the Plant Dynamics Code was developed for analysis of sCO₂ cycles, the code formulations are general enough to allow calculations of any Brayton cycle system and other working fluids. All that is needed is a formulation of real-gas properties for those other working fluids. Some of these properties, such as for air and nitrogen, are already included in the code. The only significant limitation is that the code was designed for analysis of a supercritical system with a single-phase properties formulation and is not intended for the analysis of two-phase flows, such as for Rankine cycles. However, a limited two-phase treatment is still included in the code for the analysis of conditions and flows that may exist in supercritical cycles, such as a critical flow through a break or a valve. It also needs to be noted that although the code can be readily applied to purely ideal-gas Brayton cycles, analyzing such systems with the PDC may not represent the optimal numerical solution, since the code would not take advantage of ideal gas laws, which can greatly simplify equation formulations and solution schemes.

The Plant Dynamics Code is designed to interact with the user through text files. The text input files serve to define the cycle configuration and operating conditions, provide the design information for cycle components, specify control targets and mechanisms, and define the transient conditions. During the calculations, the code will create other text files to report the results to the user. To facilitate working with the code’s input and output files, a Graphical User Interface (GUI) has been created for the PDC. That interface is described in the User’s Guide chapter of this report.

The Code Manual chapter provides the detailed description of the code models, assumptions, and solution techniques.
2 USER’S GUIDE
2.1 Introduction and Definitions

The Plant Dynamics Code has been developed for analysis of supercritical Brayton cycle energy conversion systems. An energy conversion cycle is a system that takes thermal energy (from a nuclear reactor, fossil plant, or another source) and converts it into electrical energy to be delivered to the electrical grid. Brayton cycles are a subset of energy conversion systems that work with gasses (or supercritical fluids), as opposed to boiling liquids. Because an energy conversion system needs to convert thermal energy into electricity, the following components are required for each Brayton cycle:

- A heat addition heat exchanger (HAHX) to deliver heat to the cycle,
- A turbine to convert internal energy and pressure of the cycle working fluid into rotational energy of the shaft,
- A generator connected to the turbine to produce electricity from the shaft rotational energy,
- A compressor to circulate the working fluid and increase its pressure, and
- A heat removal heat exchanger (cooler) to remove any heat from the cycle which could not be utilized by the turbine.

Figure 2-1 shows the configuration and components of a simple Brayton cycle. The working fluid is heated in the HAHX, expands in the turbine, which drives the generator, is cooled in the cooler, is compressed in the compressor, and returns to the HAHX.

![Simple Brayton Cycle Diagram](image)

The global cycle performance is usually measured in terms of the cycle efficiency, which defines the fraction of the heat provided to the cycle in the HAHX that is transformed into the electricity by the turbine and generator:

\[
\eta_{cycle} = \frac{W_{gen}}{Q_{HAHX}}.
\]  (2.1)
Depending on the meaning of the generator output, gross and net cycle efficiencies can be defined by Equation (2.1). In the PDC, the gross generator output is the actual power at the generator terminals, while the net generator (cycle) output subtracts off the power requirements for other cycle equipment, such as the cooling medium pump in the cooler loop. In addition, the net plant efficiency can be defined if all other power requirements and heat losses, outside the cycle, are included in Equation (2.1). For example, for a nuclear reactor, the net plant efficiency would include heat losses on the reactor side (such that $Q_{HAHX}$ is replaced by $Q_{Reactor}$) and all power requirements for coolant pumps and all other equipment on the reactor side.

To model an energy conversion cycle in the PDC, the user first needs to “build” the cycle from the components and pipes connecting the components. For the example in Figure 2-1, the following components need to be defined in the PDC input files or user interface forms (note that the actual component names “in quotation marks” can be arbitrarily selected by the user):

- Heat addition heat exchanger(s): “HAHX”,
- Generator(s): “Generator”
- Turbine(s): “Turbine”,
- Compressor(s): “Compressor”,
- Cooler(s): “Cooler”
- Turbomachinery shaft(s): “Shaft”, connecting “Turbine”, “Compressor”, and “Generator” (if all of these components are on common shaft).

The user must then “connect” all of the components with pipes. For example, Pipe #1 could connect the outlet of the “HAHX” with the inlet of the Turbine, Pipe #2: “turbine” outlet to the “Cooler” inlet, and so on.

After the cycle is defined, the user needs to provide the required input for each component, plus, if needed, define the transient to be analyzed, including input for control actions. Once all input is provided, the code can be executed. It will first do the steady-state calculations, with the main goal of calculating the cycle efficiency, followed by the dynamic calculations, if those are requested, to perform calculations that characterize the cycle behavior in the transient.

Figure 2-1 shows the simplest Brayton cycle configuration. Other components, such as recuperative heat exchangers (called “recuperators”) and flow split/merges, as well as more than one of the components shown in Figure 2-1, can be added to the PDC model of this cycle to simulate more complex cycle configurations. Figure 2-2 shows an example of a recuperated Brayton cycle, where part of the available energy from the turbine outlet is used in the recuperator to preheat the flow before it enters the HAHX. This arrangement allows for better utilization of the available heat in the cycle thus increasing the cycle efficiency but at the cost of adding another heat exchanger that increases the capital cost of the power converter.
Figure 2-2. Recuperated Brayton Cycle.

Other examples of more complex Brayton cycle include the: Interheated cycle, where one or several heat exchangers are added between the turbine stages; and Intercooled cycle, where one of several coolers are added between compressor stages. In addition, any combination of recuperated, interheated, and intercooled cycles can be simulated to basically model a cycle of any complexity. One particular variation of a recuperated Brayton cycle, - a recompression Brayton cycle, - has been of interest for supercritical fluids. This cycle configuration along with the reasons for adopting it are described below.

The Plant Dynamics Code has been designed to analyze supercritical Brayton cycles. A supercritical region is defined (see Figure 2-3 for carbon dioxide fluid) as the region above the critical pressure and/or temperature. The critical point is the point where the difference between the liquid and gas behavior of a fluid disappears and the fluid behaves like a single “supercritical” fluid. The critical point in Figure 2-3 is the top-most point of the red two-phase “dome.” The supercritical region is located above the critical temperature, $T_{\text{crit}}$, and the critical pressure, $p_{\text{crit}}$. 
Supercritical cycles are often designed to take advantage of the fluid properties variations near the critical point. If the compression (see Figure 2-1) is carried out close to, but still above, the critical point, the compression work (i.e., PdV work), which can be visualized by the distance between the equal-pressure lines (isobars) in Figure 2-3, is reduced significantly, compared to the expansion work between the same pressure limits away from the critical point. That difference increases the useful work available from the turbine, thus increasing the cycle efficiency. If the compression is done above the critical point in the “Supercritical” region in Figure 2-3 and the entire cycle stays in that region, there is no phase change in the working fluid anywhere in the cycle. Such single-phase operation benefits component design by eliminating the provisions for phase change inside of the components. It also simplifies the analysis of such cycles because the equations only need to be formulated for a single phase of the fluid. On the other hand, both the component design and the code formulations need to take into account the strong properties variations near the critical point. Figure 2-4 shows examples of such properties variations for carbon dioxide: the specific heat can experience orders-of-magnitude increases while the density can double in a span of less than 1 °C in temperature. In addition, to take full advantage of the properties variations it is beneficial to perform the compression work as close to the critical point as possible, often within 1 °C and less than 0.1 MPa of the critical conditions while remaining above them, which could present challenges for cycle control. The equation and fluid properties formulations in the PDC described in this report are specifically designed to account for such
changes in fluid properties and their effects on the design and performance of each component and the entire cycle, including dynamic behavior and cycle control.

Figure 2-4. Examples of Carbon Dioxide Property Variation near the Critical Point.

Aside from the potential for cycle efficiency increase, there is another implication of the fluid properties variations near the critical point. Due to the strong dependence of the specific heat on pressure, there arises a significant difference in the specific heats for the two sides (i.e., the high
and low pressure sides) in the recuperated Brayton cycle in Figure 2-2. This difference results in different temperature changes on the two sides of the recuperator, such that the heat recuperation is less effective than for ideal-gas cycles. To overcome this behavior, a recompression cycle configuration is often used for supercritical fluids. In this configuration (Figure 2-5), the recuperator is split into two parts – high- and low-temperature recuperators (HTR and LTR, respectively). The flow is arranged in such a way that only part of the main cycle flow goes through the cold side of the LTR. This compensates for the differences in the specific heats in the LTR, such that the temperature changes on the two sides of this heat exchanger are close to each other. Because of the better temperature match, overall heat recuperation in the cycle increases also increasing the cycle efficiency. The flow reduction on the cold side of the LTR is achieved by sending part of the main flow to bypass the cooler and the main compressor, but instead directly compressing that flow in the so-called “recompression” compressor. The flows from the recompression compressor and the LTR merge back to the full cycle flow before it enters the high-temperature recuperator. Since this heat exchanger operates at higher temperatures further from the critical point than the LTR does, the difference in specific heats is not that large in the HTR, so no flow splitting is required. Since the recompression flow is not being cooled in a cooler, the recompression compressor is less effective than the main compressor (i.e., it requires more work input per unit mass flow due to the higher temperature at the compressor inlet). However, this disadvantage is usually surpassed by the benefits of better recuperation. As a result, the cycle efficiency of the recompression cycle is usually higher than that of the recuperated cycle for supercritical cycles. For this reason, the recompression cycle configuration in Figure 2-5 is usually selected for supercritical Brayton cycles, such as supercritical carbon dioxide (sCO₂) energy conversion systems.

Figure 2-5. Recompression Brayton Cycle.
2.2 Code File Structure

The Plant Dynamics Code does not require installation. Instead, all of the files supplied with the code should simply be copied into a directory.

The PDC directory structure is shown in Figure 2-6. With the exception of the main directory name, that structure should not be changed and directories cannot be renamed since the code will look for specific files in pre-defined locations. For example, the input files for dynamic calculations need to be in the “Code\Data\DY\Input” folder.

Figure 2-6. PDC Directory Structure.

The user interface is started by executing the “PDC_GUI.exe” file. The code itself will be executed from the interface. There is also an option to run the code from a command line. It is done by executing the “PDC.exe” file in the “Project” directory.
2.3 Graphical User Interface

A form-based user interface has been created for the Plant Dynamics Code to guide the user in preparation of the PDC input files, to execute the code, and to display the code’s results. The interface is launched by executing the “PDC_GUI.exe” file in the main code directory.

2.3.1 GUI Main Form

The main form of the PDC Graphical User Interface (GUI) is shown in Figure 2-7. First, the location of the PDC executable file needs to be defined. Refer to the PDC directory structure in Figure 2-6 to define the path to the file. The path can be either typed in the text field or located by clicking on the “Find” button. Once the PDC executable file is located, the rest of the form will become active. Also, the location of the executable file will only need to be defined once – the location will be saved for the next time that the GUI is started.

The GUI main form serves to define the type of calculations the user wants to perform, to view or edit the input files, execute the code, and view the code’s result. These actions are defined in the corresponding areas of the main form. Some of the areas, buttons, or checkboxes may become unavailable, depending on the other choices made. For example, the code could not be executed until the path is specified and the input is provided.
Model Selection

Defines if a New or the Existing model is to be used. If “Existing” model is selected (default choice), the user will be offered to modify the current input files. For “New” model, all of the GUI input forms will be opened with blank fields, which will need to be filled. Also in this case, viewing the results will not be available until the code is run.

Calculations

Defines if steady-state or dynamic calculations are requested. Note that steady-state calculations are always required: even for a dynamic calculation, the steady-state solution serves as a starting point for a transient. That option cannot be unchecked. If only steady-state calculations are selected (“Dynamic” is unchecked), then dynamic input editing and results viewing become unavailable.

View/Edit Input

Clicking on the buttons in this section will open the GUI forms for steady-state and dynamic input, respectively. These buttons may become unavailable depending on other choices made on this form. For example, if “New” model is selected, the “Dynamic” input button is disabled until the input for the steady-state model is provided. The GUI input forms are described in detail further in this chapter.

Execute the Code

This button executes the PDC file defined in the Path file. It too may become unavailable until the required input is provided.

View Results

Clicking on the “Steady-State” button will open the GUI form which will display the code’s results related to the steady-state calculation. Clicking on the “Dynamic” button opens the Excel file to view the transient results. Both these features are described further in this document.

Close

Closes the PDC user interface.

When the “New” model is selected, the GUI will delete all of the input files and they will need to be reconstructed by using all the GUI input forms. Before the files are deleted, the GUI will display a corresponding warning message and will advise the user to create a copy of all files in the steady-state and dynamic input folders. Those copies could be later used for populating the input forms by clicking on the load button, 📂, which will appear, if the GUI could not locate the PDC input file in the directories in Figure 2-6. In addition to the new model, the load button could be used to copy input for new components added to the model. For example, if the user adds a new recuperator for which the input has not been created yet, the input can be copied from another recuperator input file using the load button and later modified for the new component. Once the external file is loaded, the load button will disappear from the forms to avoid double-filling the form’s fields.
Also, when “new” model is selected, providing input for dynamic calculations will not be available until the steady-state model is created. This is done because the PDC dynamic input uses component names, for example, valve names for control, defined in the cycle configuration file.

The rest of this section describes the GUI features activated by selecting the corresponding actions on the main form.

2.3.2 GUI Interactive Features

All the PDC GUI forms are designed to provide additional information to the user in several ways – see Figure 2-8. ToolTips are the small pop-up banners that will be displayed as the user points the cursor on the form elements (input labels, buttons, etc.). Those banners show some short information of the element - for example, a short description of that particular input. The ToolTip banners will disappear after a short time.

If the additional information is too complex to fit in a ToolTip banner, the cursor will change to the help cursor, 📚, and clicking on this area will open a sub-form with detailed explanation.

Some of the GUI forms also include pictures to provide yet additional information of the field. For example, if the form asks the user to provide an input for the heat exchanger length, there is a picture to show what this dimension means. All of these pictures are small in the forms, but can be extended and scaled for a better view by clicking on them.
The PDC user interface also provides the choice to a user to specify the input and view the output in various units. One example of unit selection is shown in Figure 2-8. To change the units, the user needs to select the units from the list. For example, the following units are supported for the length: “m”, “cm”, “mm”, “in”, “ft”. If the field to which units are applied is not empty, then the number will be converted by the GUI to the selected units.

The PDC GUI is also built on a principle of requesting as little information from the user as possible. For example, in the heat exchanger input forms, only the input fields relevant to a selected heat exchanger type are displayed and need to be filled by the user.

Another example of the GUI interactive features is already discussed for the main GUI form and it is present in all other forms. Some of the GUI controls, such as buttons, may become disabled if user selections make those controls irrelevant. This is done to further simplify user interactions with the GUI by eliminating meaningless options.

Sometimes, a warning message will be displayed by the GUI to confirm the user’s actions. For example, if any of the fields on the input forms have been changed, the GUI will ask if the user wants to save the input before that form is closed.
### 2.3.3 Input for PDC Steady-State Part

Clicking on the “View/Edit Input” - “Steady-State” button on the main PDC GUI form opens the form for the cycle input shown in Figure 2-9. Note that the actual appearance of this and other GUI forms may be different from what is shown in this report, since all PDC GUI forms are sizeable with automatic scrolling capability, if the entire form content cannot fit into a screen.

In the steady-state input form in Figure 2-9, the general cycle input is provided, and the cycle configuration is defined.

The general input includes:

<table>
<thead>
<tr>
<th>Specification</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Working fluid</strong></td>
<td>Specifies the cycle’s working fluid. Even though several options are provided, the Plant Dynamics Code has only been tested with CO₂ working fluid.</td>
</tr>
<tr>
<td><strong>First iteration</strong></td>
<td>If “Use output file” is selected, the existing output file will be read and used to define cycle conditions for the first iteration of steady-state calculations. This is a preferred option. However, it cannot be used for the first run after the cycle configuration has been changed.</td>
</tr>
<tr>
<td><strong>Heat addition mode</strong></td>
<td>Specifies whether the heat is added to the cycle either in a heat exchanger (regular mode) or through an electrical heater (an option for test loops).</td>
</tr>
<tr>
<td><strong>Type of turbomachinery calculations</strong></td>
<td>There are two options here: “Design” and “Performance”. In “Design” mode, the turbines and compressors are designed to match the required cycle conditions. In “Performance” mode, the turbine and compressor designs are given and their performance is used to calculate cycle conditions. This mode is usually applied for test loops. More detailed description of these modes is provided below in Section 2.3.3.3.</td>
</tr>
<tr>
<td><strong>Limiting cycle pressure</strong></td>
<td>Defines the upper limit on pressure for cycle iterations. The actual pressures in the cycle are set by the compressor input described below.</td>
</tr>
<tr>
<td><strong>First guess for flow rate</strong></td>
<td>Defines the value of the working fluid flow rate for first iteration. The input is not used if “First iteration” is set to “Use output file.”</td>
</tr>
<tr>
<td><strong>Pipe material</strong></td>
<td>Defines the material for all pipes in the cycle.</td>
</tr>
<tr>
<td><strong>Ambient temperature</strong></td>
<td>Defines the ambient temperature in the building for the heat loss calculations.</td>
</tr>
</tbody>
</table>
Figure 2-9. PDC GUI Form for Cycle Configuration.
**Heat transfer correlation in pipes**
Defines the correlation to use for heat transfer between the working fluid and the pipe wall.

**Maximum number of iterations**
Defines the maximum number of cycle iterations to achieve convergence on cycle temperatures, pressures, and flow rates.

In this and other PDC input forms, the user interface tracks any user input provided to the forms. If any field is changed, that field becomes **bold** on the form to indicate where the change has been made. Also, the “Save & Close” button becomes enabled once any change is introduced to the form. If the user tries to close a form with changed fields without first saving the changes, a warning message will be displayed asking if the changes need to be saved. In the PDC GUI, form changes cannot be undone—the interface only tracks the fact of the field change, not the actual values. The changes can be ignored though by closing the form without saving. Note that changing the units on the input forms does not change the actual value of the input (all the inputs are converted to default PDC inputs before save). So, even though the value in the field will change when units are changed, selecting different units will not trigger indicators for the input change described above.

### 2.3.3.1 Cycle Configuration for PDC

The PDC user interface does not provide a graphical capability to construct the cycle by placing and connecting the component’s icons. Instead, the PDC utilizes the definition of the cycle configuration in a text format or its equivalent in the GUI cycle input form. The main idea of this input is this: the user provides the list of the components and then lists the pipes connecting those components.

The Components area in the cycle input form (Figure 2-9) defines which cycle components are supported in the PDC. To create a component, the user simply writes its name in a corresponding box. If multiple components of the same type are needed, then they should be listed one per line in that box. The component names are arbitrary, but are limited to 5 characters. Also, the names should be unique for each component in the cycle.

When all the component names are entered, they need to be connected by pipes to complete the definition of the cycle layout. The pipe connections are defined in the Pipes area of the form. For each pipe, the following input should be provided:

<table>
<thead>
<tr>
<th><strong>Index</strong></th>
<th>Pipe index; should be unique and consequent.</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>From/To Components and Ports</strong></td>
<td>Defines which components and ports the pipe connects. Component is selected from the list of the provided components. Port is selected from the list of the available ports for that component. The ports by component type are defined in Table 2-1.</td>
</tr>
<tr>
<td><strong>Count</strong></td>
<td>Number of parallel runs of the pipe section. It is assumed that all parallel pipes are identical.</td>
</tr>
</tbody>
</table>
Length  
Pipe length.

Diameter  
Inner pipe diameter.

Thickness  
Pipe thickness.

Bends  
Number of pipe bends. Each bend is assumed to be 90°.

Rbend/D  
Bend radius, relative to the pipe inner diameter.

k_HL  
Pipe heat loss multiplication factor. k_HL=0 means perfectly insulated pipes (note: such input is required for pipes that do not see flow at steady-state, such as those with fully closed valves). k_HL=1 means that the heat loss will be calculated by the PDC based on the pipe wall temperature, its surface area, and natural circulation of air around it (for that, a horizontal pipe orientation is assumed). A user can provide other values for this input. Values between 0 and 1 would represent less-than-perfect insulation, while values greater than 1 would mean heat loss enhancement.

<table>
<thead>
<tr>
<th>Component Type</th>
<th>Ports</th>
</tr>
</thead>
<tbody>
<tr>
<td>Heat Addition</td>
<td></td>
</tr>
<tr>
<td>Heat Exchanger</td>
<td>CI (cold inlet)</td>
</tr>
<tr>
<td></td>
<td>CO (cold outlet)</td>
</tr>
<tr>
<td>Turbine</td>
<td>I (inlet)</td>
</tr>
<tr>
<td></td>
<td>O (outlet)</td>
</tr>
<tr>
<td>Compressor</td>
<td>I (inlet)</td>
</tr>
<tr>
<td></td>
<td>O (outlet)</td>
</tr>
<tr>
<td>Cooler</td>
<td>HI (hot inlet)</td>
</tr>
<tr>
<td></td>
<td>HO (hot outlet)</td>
</tr>
<tr>
<td>Recuperator</td>
<td>CI (cold inlet)</td>
</tr>
<tr>
<td></td>
<td>CO (cold outlet)</td>
</tr>
<tr>
<td></td>
<td>HI (hot inlet)</td>
</tr>
<tr>
<td></td>
<td>HO (hot outlet)</td>
</tr>
<tr>
<td>Mixer</td>
<td>II (primary inlet)</td>
</tr>
<tr>
<td></td>
<td>I2 (secondary inlet)</td>
</tr>
<tr>
<td></td>
<td>O (outlet)</td>
</tr>
<tr>
<td>Split</td>
<td>I (inlet)</td>
</tr>
<tr>
<td></td>
<td>O1 (primary outlet)</td>
</tr>
<tr>
<td></td>
<td>O2 (secondary inlet)</td>
</tr>
<tr>
<td>Tank</td>
<td>I (inlet)</td>
</tr>
<tr>
<td></td>
<td>O (outlet)</td>
</tr>
</tbody>
</table>

Valves, Generators, and Shafts are not connected by pipes.
The cycle configuration in Figure 2-9, for example, defines that Pipe#1 connects the cold outlet port of RHX (which is a heat addition HX) to the inlet port of Turb (a turbine). It consists of a single parallel pipe, has a length of 20 m, inner diameter of 0.683 m, and has four 90° bends with each bend radius equal to the pipe diameter. Note that for the results reporting the node numbers will be defined by the pipe index:

Inlet node number = 2 x (pipe index) - 1

Outlet node number = 2 x (pipe index).

For example, Pipe#1 will have inlet and outlet nodes, 1 and 2, respectively, Pipe#5 – nodes 9 and 10, and so on.

Figure 2-10 shows the cycle configuration modeled with the input in Figure 2-9. Because the GUI form has limited space, not all pipes and valves are shown in Figure 2-9; a user needs to scroll the pipe input section of the form to see and modify the input for all pipes. The same cycle configuration is also provided in Figure 2-10. The figure shows all the cycle components, connecting pipes, and valves. It also shows the pipe indices and the node numbers.

When the cycle configuration is complete, no unconnected ports should remain for any of the components. The GUI will not check for unconnected ports. However, when the code is executed, an error message will be generated if an error is detected, such as an unconnected or double-connected port.

For all Flow Splits, the flow fraction at the primary port (I1) needs to be specified. This is done in the “Flow Splits” table of the cycle input form.

The Valves are assumed to be located in the middle of the pipe, rather than at the end of a pipe. As such, there are no connecting ports for the valves. Instead, the pipe index on which each pipe is located needs to be specified in the “Valves” tables of the form. Also, the table provides the design resistance of the valve. In this column, “0” means no resistance from the valve (i.e., “fully open valve”), a value greater than zero means the flow resistance in MPa, and “-1” means that the resistance will be calculated by the code (this input includes fully closed valves).

The input for the pipes, valves, and splits can be modified directly in the cycle input form. To add or delete rows in the corresponding tables, the + and - buttons below the tables should be used, respectively. The Pipes table can also be sorted in accessing order by clicking on the sort button.

The input for the cycle components is accessed by double-clicking on the component name in the corresponding component type box. The GUI will open the input form corresponding to the component type.

No input for Generators and Turbomachinery Shafts need to be provided in the cycle input form. Those inputs are provided in the separate TM Shaft input form and are discussed below.
2.3.3.2 Cycle operating conditions

As can be noticed from Figure 2-9, the cycle input form does not define the cycle operating conditions, in terms of minimum and maximum temperatures and pressures (the “Limiting cycle pressure” input is simply a limit for iterations). Those conditions are provided in other input forms described below.

The Heat Addition Heat Exchanger input includes the conditions on the hot side of the heat exchanger, including the inlet and outlet temperatures. That input, together with the calculated HX performance will define the maximum temperature in the cycle. Also, the hot side input
includes the total heat addition to the cycle, which defines the “size” of the cycle, in terms of the supplied heat addition rate.

The cycle minimum temperature and pressure, as well as the maximum pressure, are all provided in the compressor input. As will be described below, each compressor input form includes the flags to define those conditions for the cycle. These flags need to be turned on and the corresponding values need to be provided in at least one of the compressor’s input (although, not necessary in the same component). The minimum temperature can only be set for a compressor which is connected to a cooler.

For supercritical cycles, it is important to precisely define the temperatures of interest at the low-temperature end of the cycle. This is due to operation near the critical point. For an ideal gas cycle, such as a helium gas Brayton cycle, the distinction between cooler-outlet and compressor-inlet total and static temperatures is not important because the helium properties, such as specific heat and compressibility, are not strong functions of the temperature. For cycles operating close to the critical point, such as the sCO2 cycle, the properties could differ significantly depending on what temperature they are calculated at. Even though the difference between, for example, total and static temperatures at the compressor inlet could be only of the order of 1 °C, the properties variation is significant, as demonstrated below.

In the case where any kind of flow mixing at the compressor inlet is used for temperature control, there will be a difference between the cooler-outlet and compressor-inlet temperatures. An example would be a cooler bypass flow where part of the flow (i.e., hotter flow) bypasses the cooler to mix with the flow from the cooler (cooler flow) in the proportion determined to provide just the right temperature desired at the compressor inlet (see Figure 2-10 above for an example of such a configuration). Unless this bypass flow fraction is significant, the difference between the cooler-outlet and compressor-inlet temperatures is small. For the bypass fraction of 5%, this difference is only a few tenths of a degree Celsius. Still, even this small variation is important near the critical point and should be taken into account. In the case where the pressure drop in a pipe connecting the cooler with the compressor is not ignored, the resulting change in pressure may also affect the properties. Again, even though the pressure difference is expected to be small, the effect on the properties could be significant.

The difference between compressor inlet and the compressor first stage inlet conditions is illustrated in Figure 2-11. The flow needs to be accelerated to the design speed before entering the first stage. During this acceleration, a portion of the internal energy is transformed into kinetic energy such that the total energy is conserved. As a result, the enthalpy and temperature decrease as the speed increases during acceleration. The total enthalpy (= static enthalpy + C^2/2) is conserved. If there were no losses during the acceleration, the process would be isentropic and the total temperature would be the same before and after acceleration (the total temperature is defined as the temperature at the total enthalpy and given entropy, as illustrated in Figure 2-11). If the process is not ideal, then the total temperature at the end of acceleration would be smaller than that at the beginning of the acceleration. In any case, due to the decrease in static enthalpy, the static temperature at the first stage inlet is lower than at the compressor inlet. Since the properties of a fluid are defined by the static temperature, the properties would be different at the compressor inlet and the first stage inlet.
Figure 2-11. Enthalpy Reduction during Acceleration at Compressor Inlet.

Table 2-2 demonstrates the differences between the temperatures and pressures at the cooler-outlet, compressor-inlet, and first stage inlet for an example of a sCO₂ cycle. It also shows how significant the properties variations close to the critical point are even for small changes in temperature and pressure. It follows from the previous discussion that if two-phase flow is to be avoided in the compressor and in the cycle, one needs to ensure that the temperature at the first-stage inlet stays above the critical value (i.e., not at the compressor-inlet or cooler-outlet). For these reasons, 31.25 °C and 7.4 MPa were selected for the first-stage inlet for the example in Table 2-2 to maintain some margin above the onset of two-phase flow (for CO₂, T\text{crit}=30.98 °C, p\text{crit}=7.377 MPa); all other temperatures are calculated based on this temperature. The minimum cycle temperature control discussed in Sections 3.3.1.7 and 3.3.2 of this report refers to adjusting the control mechanisms in order to maintain this first stage inlet temperature above the critical temperature (even though it is sometimes called the “compressor-inlet temperature” for simplicity).

Table 2-2. CO₂ Properties Variations Near the Compressor Inlet Location

<table>
<thead>
<tr>
<th>Location</th>
<th>T, °C (static)</th>
<th>p, MPa (static)</th>
<th>C, m/s</th>
<th>ρ, kg/m³</th>
<th>c_p, kJ/kg-K</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cooler outlet</td>
<td>33.66</td>
<td>7.781</td>
<td>7.8(^1)</td>
<td>406.7</td>
<td>39.75</td>
</tr>
<tr>
<td>Compressor inlet</td>
<td>33.85</td>
<td>7.775</td>
<td>8.8(^1,2)</td>
<td>381.1</td>
<td>27.68</td>
</tr>
<tr>
<td>First stage inlet</td>
<td>31.25</td>
<td>7.400</td>
<td>42.4</td>
<td>368.6</td>
<td>58.54</td>
</tr>
</tbody>
</table>

\(^1\)Speed is calculated in pipes for a presumed flow rate and pipe diameter; properties are based on the calculated static conditions such that the speed does not affect the properties.

\(^2\)Coolant speed is ignored at the compressor-inlet for a conservative compressor design approach; thus, it is assumed that the total and static conditions are identical.
For the reasons discussed above, the PDC input for the minimum cycle pressures and temperatures are specified for the location of the compressor first stage inlet. That input is provided on the compressor input forms described below. The maximum pressure input is also provided on the compressor input form since the compressor inlet pressure is the highest pressure in the cycle.

### 2.3.3.3 Turbomachinery Calculation Modes

The PDC supports two calculation modes for turbomachinery at steady-state: design and performance. This is one of the general cycle inputs in Figure 2-9. The main differences between these two modes are described in Table 2-3.

In the “Design” mode, the cycle conditions, including turbomachinery inlet and outlet temperatures and pressures and flow rates are first calculated from the cycle conditions. The turbines and compressors are designed to match these conditions. Those design subroutines calculate the physical dimensions of the turbomachinery components (blade heights and angles, flow areas, radii, etc.). In addition, they calculate the component performance in terms of efficiency. This efficiency is supplied back for the cycle calculations to calculate new cycle conditions and flow rates. The process is repeated until convergence on the cycle conditions and turbomachinery efficiencies is achieved. This mode should be used when the cycle is designed to meet external conditions, such as heat duty and hot side temperatures in a Heat Addition Heat Exchanger(s). Note from Table 2-3 that this mode cannot be used with Electrical heaters (see Section 2.3.3.4 below), since in that case there would not be conditions on the hot side of a HAHX to match to obtain a working fluid flow rate in the cycle.

In the “Performance” mode, the turbomachinery designs are given and provided to the PDC as input. This mode is used when the cycle is already designed, such as for simulation of experiment loops. In this mode, the PDC will calculate the working fluid flow rate in the cycle based on the performance (pressure ratios) of the compressors and pressure drop characteristics of the rest of the cycle, including pressure drops in components and pipes and pressure ratio in the turbines. The same turbomachinery performance subroutines will calculate the turbine and compressor efficiencies, which will be provided to the cycle calculations for iterations.

Note that the turbomachinery calculation mode only applies to the steady-state calculations in the PDC. In the dynamic part, the performance subroutines (or turbomachinery maps) will always be applied either to a given design of turbines and compressors or the designs calculated at steady-state.

The detailed description of the cycle and turbomachinery calculations in different modes are provided in the Code Manual part of this document, in Section 3.1.1.
### Table 2-3. Turbomachinery Calculation Modes

<table>
<thead>
<tr>
<th>Mode</th>
<th>Design</th>
<th>Performance</th>
</tr>
</thead>
<tbody>
<tr>
<td>Turbine and compressor designs</td>
<td>Calculated by PDC</td>
<td>Given</td>
</tr>
<tr>
<td>PDC turbomachinery subroutines</td>
<td>Design</td>
<td>Performance</td>
</tr>
<tr>
<td>Working fluid flow rate</td>
<td>Calculated to match hot side conditions of Heat Addition Heat Exchanger</td>
<td>Calculated to match the pressure rise in the compressor(s) to the pressures in the turbine(s) and the rest of the loop</td>
</tr>
<tr>
<td>Flow rate iterated parameter</td>
<td>HAHX hot side outlet temperature</td>
<td>Turbine outlet pressure</td>
</tr>
<tr>
<td>Allowable heat addition modes</td>
<td>Heat exchanger</td>
<td>Heat exchanger or Electrical heater</td>
</tr>
<tr>
<td>Turbomachinery input files read</td>
<td>&lt;Name&gt;_dat.txt</td>
<td>&lt;Name&gt;_des_dat.txt</td>
</tr>
</tbody>
</table>

#### 2.3.3.4 Heat Addition Mode

The PDC supports two modes for heat addition to the cycle: heat exchanger and electrical heater. In the Heat Exchanger mode, the heat is added to the cycle by means a fluid on the hot side of a Heat Addition Heat Exchanger. The hot-side fluid and its inlet/outlet temperatures and pressures are specified in the input as described in the HAHX input in the next section. For the Electrical Heater mode, the heat is added directly from the heater tubes to the cycle working fluid.

In addition to the steady-state input described in the next section, there would be differences in the dynamic input, in particular with respect to the HAHX/heater control. Those differences and the corresponding GUI forms are described in Section 2.3.4.3 below.

#### 2.3.3.5 Component Input

The input for each component can be viewed and modified by double-clicking on the component name in the cycle configuration form. Depending on the component type (turbine, recuperator, etc.), the GUI will open the corresponding form to provide the input for that component. All of these forms are similar, but have a different field specific to that component type. If “Existing” model was selected on the main GUI form or the input was previously provided and saved, then each form will be populated with the values from the corresponding input file. Otherwise, an empty form will be opened and the user will need to fill out the entire form.

Figure 2-12 shows the form for recuperator input. The component name, as it was clicked on in the cycle input form, is displayed on the top. In the top-right corner of the form, there are Save, Save&Close, and Close buttons. The Save button saves the current information on the form in the PDC input file. The Close button closes the form and returns back to the cycle input form.
Save&Close does a combination of these two actions. This button only becomes available after any field in the form has been changed. The rest of the form is devoted to the recuperator input required by the PDC. In the example in Figure 2-12, the form is filled with the input data stored in the PDC input file for the component “HTR.”

![Figure 2-12. PDC GUI Form for Recuperator Input.](image)

There are four types of recuperator that the user can choose from: General, Shell-and-Tube, Platelet Printed Circuit Heat Exchanger (PCHE), and Z/I PCHE. Figure 2-12 above shows the recuperator input form view for a Platelet PCHE. For the General type, only efficiency and pressure drops on two sides need to be provided. Note that this type is intended for steady-state calculations only and is not supported in dynamics. A corresponding message will be displayed on the form. Since no other input is needed for the General recuperator type, it will not be displayed on the form, as shown in Figure 2-13.
Figure 2-13. PDC GUI Input Form for Recuperator: General Type.

The required input and the recuperator form appearance for the Shell-and-Tube type are shown in Figure 2-14.
The difference between the platelet PCHE and Z/I PCHE is that the former utilizes headers incorporated in the plates, as shown in Figure 2-15. The Z/I configuration assumes that the headers are outside of the HX core. This configuration includes the regions of cross-flow on two sides of each plate. The steady-state subroutine accounts for this region, but it is not currently supported in dynamic calculations, which assume that the flow is purely counter-current. Therefore, if the Z/I PCHE type is selected, a message is displayed that this type is not supported in transients and an equivalent Platelet configuration needs to be used.
The required input for the Platelet PCHE is shown in Figure 2-12 above. The input for the Z/I PCHE is demonstrated in Figure 2-16. The only difference between the two for the PDC input is that the Z/I PCHE input does not require internal header length input.
The input forms for other components are similar to that of the recuperator form described above. In most cases, the user needs to select the component type and provide the input needed for that type. The input form for each component type may also request other information specific to that type.

The GUI form for the heat addition heat exchanger (HAHX) input is shown in Figure 2-17. The majority of the form is similar to the recuperator form. However, this form also asks for the input for the hot side of the HAHX, including the hot side fluid (selected from the list of fluids supported by the PDC), inlet/outlet temperatures, pressure, and total power. If multiple HAHXs are used, the user also needs to provide the input for the hot side fluid flow fractions for each HX starting from HX #2 in the component list. The PDC assumes that the HAHXs are arranged in parallel with respect to the hot side flow. If a single HAHX is used, that particular input is ignored. The power input is for the total power provided to the cycle. If a single HAHX is used, then it is equal to the heat duty of that heat exchanger; otherwise, it will be scaled with flow fractions to calculate the heat duty for each HX.
Figure 2-17. PDC GUI Input Form for HAXH.

The PDC input form for an electrical heater is shown in Figure 2-18. The form is similar to that of other shell-and-tube heat exchanger forms. However, the heater form includes a field on the Steady-state solution mode. The user can specify either “Given outlet temperature” or “Given power” for this field. The actual value for either of these options is provided in the second input field on the form.
The selection of which heat addition form to open (HAHX or heater) is defined by the “Heat addition mode” field in the cycle input form in Figure 2-9.

![Figure 2-18. PDC GUI Input Form for Electrical Heater.](image)

The input form for a cooler (Figure 2-19) is similar to that of the HAHX with the difference that the conditions on the cold side (cooling medium) need to be provided for the cooler. The PDC supports the choice of either water or air for the cooling medium.
As shown in Figure 2-19, the general input for a cooler includes the “Iteration option” field. Since the purpose of the cooler is to meet the requested conditions at the compressor inlet, the PDC steady-state solution algorithm iterates on the cooler conditions to match the requested conditions at the compressor inlet. The “Iteration option” field defines which parameter will be iterated on to match the compressor-inlet conditions. The choices supported by the PDC are: Cooling fluid flow rate, Number of units, and (cooler) Length. There is also a “No iteration” option which can be used to test the performance of a particular cooler design, but this option should not be used for cycle calculations, since there would be a mismatch between the cooler-outlet and compressor-inlet conditions.
The PDC cooler subroutines support two additional types of the heat exchangers: a cross-flow PCHE and cross-flow finned tubes. The input for the cross-flow PCHE is the same as for other types of PCHE. The required input for the cross-flow finned tubes is demonstrated in Figure 2-19.

The PDC GUI form for the turbine input is shown in Figure 2-20. The code currently supports the design of an axial turbine only, so there is no selection of a turbine type.

![Figure 2-20. PDC GUI Input Form for Turbine.](image-url)
The GUI form for the compressor input is shown in Figure 2-21. There are two types of compressors supported by the code: axial and centrifugal. In addition, the input for the compressor has flags to set the minimum temperature, minimum pressure, and outlet pressure. If flags are selected, then the corresponding values need to be provided.
2.3.3.6 Turbomachinery Shafts

The turbomachinery shafts are defined in the PDC in a way somewhat similar to the cycle components and pipes. First, the turbomachinery components need to be listed in the cycle input (Figure 2-9), then the input need to be provided to specify how the components are connected by the shafts. The PDC shaft input, however, is much simpler than the pipe input – for each shaft, only the list of the turbomachinery components (turbines, compressors, and generators) located on that shaft is needed.

Figure 2-22 shows an example of the turbomachinery shaft input form. This form is opened by clicking on the shaft name (“Shaft” in the case for Figure 2-22) in the “Shafts” box of the “Components” region on the cycle configuration form (see Figure 2-9). The form defines the components located on this shaft, which could be either typed in, one-per-line, or selected from the drop box below and clicking on the “Add” button. Only turbomachinery components, i.e., turbines, compressors, and generators, can be connected by a shaft. In the A PDC, only one generator can be connected to a particular shaft.

![Figure 2-22. PDC GUI Input Form for Turbomachinery Shaft.](image)

The rest of the form provides other input for the shaft.

- **Generator’s moment of inertia**
  - Combined inertia of the generator and the shaft itself. This input is used in dynamic calculations only.

- **Generator efficiency**
  - Fraction of the generator power delivered to the grid.

- **Mechanical loss**
  - Fraction of power loss in other turbomachinery components – turbines and compressors. The turbine useful work is reduced by the amount of mechanical loss, while the compressor power requirement is increased by that amount.
There are three Shaft connection modes to the grid that are supported in the PDC, as described below. Those connection modes are only used in transient calculations. In steady-state, the net generator power is simply calculated from the shaft power balance (with losses described above) and is reported as the PDC output. The shaft connection modes for dynamic calculations are:

**Synchronous**

Shaft speed is fixed by the grid. A shaft power balance determines the generator power supplied to the grid, but does not affect the shaft speed. Input for the generator moment of inertia is not used. Shaft speed can still be changed from the user-specified table-versus-time (see cycle control input in Section 2.3.4.2).

**Asynchronous**

The shaft is connected to the grid, but the shaft speed is not dictated by the grid. Instead, the shaft speed is calculated using the shaft dynamic equations (see Section 3.2.8.2) based on the difference between the net generator output and grid demand, with account for the total inertia of the shaft. The user input for the shaft speed versus time (see cycle control input in Section 2.3.4.2) provides the target speed that the cycle controls will try to match.

**Not connected**

No grid connection. Effectively, this mode is equivalent to the asynchronous mode with the grid demand equal to zero. Shaft speed is calculated dynamically using the net generator output and total inertia of the shaft. To avoid a sudden jump in the shaft speed at the start of the transient calculations, it is recommended to change the shaft speed input to obtain zero net generator output at steady-state.

### 2.3.4 Input for PDC Transient Calculations

The PDC input for transient calculations is provided for five areas: general input, cycle control, heat addition, heat removal, and turbomachinery maps. The detailed description of the input for these areas is provided in sub-sections below. When the GUI form for the dynamic input is opened by clicking on the “Dynamic” button in the “View/Edit Input” section of the GUI Main form (see Figure 2-7), the names of these five areas will be displayed on the top of the form (see figures below). The user can click on an area name to navigate to that area. In addition, the areas can be visited consequently by clicking on the “Previous” and “Next” buttons at the bottom of the dynamic input form. The GUI will track which areas have been visited (viewed) by showing the checkboxes next to each area name at the top of the form – with a checked box indicating the visited area.

Some of the transient input is provided in a value-versus-time table (see, for example, the Grid demand input in Figure 2-23 below). For these tables in the PDC, linear interpolation is used between the table points. If a table does not cover the entire transient simulation time, the first value in the table is maintained for times prior to the first time entry, while the last value is maintained for times after the last entry. A maximum of 100 entries can be used for the PDC.
input tables. To enter/modify such tables in a GUI form, the field for the number of table points needs to be changed first. The interface will then update the table to reflect that number of points. After that, the table entries can be modified. For some tables, the GUI provides selection of units.

2.3.4.1 General Input

The GUI form for PDC general transient input is shown in Figure 2-23. This form defines the transient input such as transient simulation time, time step and convergence criteria, compressible/incompressible treatment, and file access. The ToolTips are shown for each field to give a user brief description of the input. For a more detailed description, refer to the Code Manual section of this report.

The general transient input form also allows the user to specify and use the PDC restart files. That capability of the code and how to use it is described in Section 2.5 below.

The general input form includes the tabular input for grid demand versus time. This table should be used to define the grid demand for load following transients. Also, the loss-of-load (grid disconnection) transient is triggered by entering a grid demand of less than or equal to -100 at the corresponding time.

Finally, the form for general input can be used to simulate a postulated pipe break accident. For this transient, the required input is the equivalent break diameter and the break location (specified as the pipe number and inlet/outlet location). The pipe break is assume to occur at time=0. If “0” is provided for the break size, no pipe break is simulated and the input for the break location is ignored by the code.

Navigation to other areas of the dynamic input can be done using the area names on the top of the form or by clicking the “Next” button at the bottom of the form (the “Previous” button is disabled in this form, since this is the first area of dynamic input). The “Save” button is used to save any changes introduced in the form. The “Save & Next” button saves the results and advances to the next area of dynamic input. It becomes available after any form field has been changed. Clicking on the “Done” button closes the dynamic input form and returns the interface to the main form.

Similar to other input forms, any changes made on the dynamic input form will be shown in bold font. If the user tries to close the form or tries to navigate to another area before first saving the changes, a warning message will be displayed asking if the changes need to be saved.
2.3.4.2 Cycle Control

The PDC GUI form for the cycle control input is shown in Figure 2-24. The form includes several tabs (listed on the top of the form) for each of the control mechanisms supported by the PDC. Each tab includes the fields relevant to the PDC input specific for that control. The example in Figure 2-24 shows the content for the “Minimum Temperature” control tab.
The detailed description of the PDC control mechanisms along with the required input is provided in the Code Manual portion of this report.

The GUI form for the control input tracks which tabs have been visited by displaying unvisited tabs in a bold font. It also tracks any changes introduced in the form. The tabs where the changes are made will be shown with a “*” symbol in the tab name. The actual changed fields will be highlighted with bond font.
Figure 2-24. PDC GUI Input Form for Dynamics: Cycle Control.
2.3.4.3 Heat Addition

There are three options in the PDC to define the conditions on the hot side of a HAHX in a transient: direct user input, SAS4A/SASSYS-1 coupling, and automatic control. This selection is done by the “Heat Addition calculations in dynamics” input at the top of the dynamic Heat Addition form. The form also shows the selected heat addition mode in steady-state (see Figure 2-9), since this mode defines what options and inputs will be available for dynamic calculations. Table 2-4 summarizes the available modes for dynamic calculations as a function of the heat addition mode selected for the steady-state (HAHX or electrical heater in Figure 2-9). Because of the different input requirements, the PDC GUI form for heat addition in dynamics will look differently for the four cases in Table 2-4.

Table 2-4. Summary of Heat Addition Calculation Modes in Dynamics

<table>
<thead>
<tr>
<th>Dynamic Mode</th>
<th>User Input</th>
<th>Automatic Control</th>
</tr>
</thead>
</table>
| **Heat Addition Heat Exchanger (HAHX)** | Input: hot-side fluid conditions at the HX inlet, as a function of time | Input:  
|                                      |                                                                  | - target working fluid temperature at the HX outlet, as a function of time        |
|                                     |                                                                  | - hot-side fluid pressure and flow rate at the HX inlet, as a function of time   |
|                                     |                                                                  | **Controlled parameter: hot-side fluid temperature at the HX inlet**            |
| **Electrical Heater**               | Input: heater power as a function of time                       | Input:  
|                                     |                                                                  | - target working fluid temperature at the HX outlet, as a function of time        |
|                                     |                                                                  | **Controlled parameter: heater power**                                          |

Figure 2-25 shows the GUI form for the user input with a heat addition heat exchanger. For this option, the user needs to specify the time-dependent values for the hot side fluid’s mass flow rate, temperature, and pressure at the HAHX inlet. These inputs are provided in the value-versus time tables, with the value being normalized (except for the temperature table) to the corresponding steady-state (design) value. For temperature, normalization is done assuming Kelvin units. The example in Figure 2-25 shows that since “1” is input for the pressure table, the steady-state value for the inlet pressure will be maintained through the entire transient (for times beyond those specified in tables, t>1000 s in this case, the last value is maintained in the PDC tables). For the
inlet temperature, 528 °C is set to be maintained during the entire transient. For the flow rate, a reduction from 100% to 60% is implemented from 120 s to 600 s.

![PDC GUI Input Form for Dynamics: Heat Addition – User Input.](image)

In addition to the tabular input in the form, there is also an option to provide the same input in a text format. This option is initiated by clicking on the corresponding “Table Input” button located below the tables in Figure 2-25. A table input form (Figure 2-26) will be opened and filled with the current table in the input field. That table can be edited as any text document. The only
requirement is that the table should have two numbers per line, time and value, separated by either a space (or a number of spaces) or tab(s). This text input is convenient if the hot side conditions are calculated in another program. The tables can be copied and pasted here from another text editor or Excel.

To accept changes, the “Done” button should be used. Clicking on the “Cancel” button will disregard any changes in the field.

Notice that the number of table entries does not need to be specified in the text input form. That number will be calculated by the GUI once the text input form is closed and input is converted to the PDC input table in Figure 2-25.

As shown in Table 2-4, the PDC also supports automatic control of the cycle’s fluid temperature at the HAHX (or heater) outlet. This option is triggered by selecting “Automatic control” for the HAHX calculation mode at the top of the form. In this mode, which is shown in Figure 2-27, the user needs to provide the target outlet temperature and any limiting conditions on the control, such as total power and rate of change. When the heat exchanger is selected for the heat addition
mode (on the steady-state input form), the working fluid outlet temperatures will be matched by adjusting the hot-side fluid temperature at the HAHX inlet. The hot fluid’s flow rate and pressures need to be provided in the table forms, as shown in Figure 2-27.

![Figure 2-27. PDC GUI Input Form for Dynamics: Heat Addition – Automatic Control.](image)

If the “Electrical heater” heat addition mode was selected for steady-state and the Automatic control option is selected for dynamic calculations, then the working fluid outlet temperature will
be matched by automatic control of the heater power. The required input for this mode is shown in Figure 2-28.

![PDC GUI Input Form for Dynamics: Heat Addition – Automatic Control with Electrical Heater.](image)

If automatic control is not needed for the electrical heater, then the “User input tables” mode needs to be selected. In this case, only heater power as a function of time needs to be provided for dynamic calculations as shown in Figure 2-29.
In addition to the heat addition modes described above, the PDC also supports coupling to the SAS4A/SASSYS-1 code to calculate the hot-side fluid conditions at the HAHX inlet. The appearance of the heat addition input form when the SAS4A/SASSYS-1 coupling option is selected is shown in Figure 2-30. The detailed description of the PDC input for coupled PDC-SAS4A/SASSYS-1 calculations is provided in Section 2.6 below.
Figure 2-30. PDC GUI Input Form for Dynamics: Heat Addition – SAS4A/SASSYS-1 Coupling.
2.3.4.4 Heat Removal

The only PDC input required for the transient heat removal conditions is the temperature of the cooling fluid at the cooler inlet (i.e., ambient temperature). The required flow rate will be calculated by the control system. It is assumed that the ambient pressure is fixed in transients. Figure 2-31 shows the GUI form for the heat removal input with the table for the ambient temperature. The table is similar to that in the heat addition form, except the temperature input is not normalized and is the actual temperature.

![Figure 2-31. PDC GUI Input Form for Dynamics: Heat Removal.](image-url)
2.3.4.5 Turbomachinery Maps

Figure 2-32 shows the GUI form to provide PDC input for the turbomachinery treatment in dynamics. At the top of the form, the list of all turbines and compressors from the cycle configuration (Figure 2-9) is displayed. The map input needs to be provided for each component. The user needs to click on each component’s name to view/edit input for that component.

Figure 2-32. PDC GUI Input Form for Dynamics: Turbomachinery Maps.
The PDC transient simulation with turbomachinery maps is described in detail in the Code Manual portion of this report. Here, only a brief information on the required input is provided. The turbomachinery maps need to be generated for each turbine and compressor. Once generated, the maps can simply be read from the file and used in transient calculations. There are, however, several options as to how the maps can be used.

The majority of the fields on the map form are related to generation of turbomachinery maps. If the map has already been generated and only needs to be read from a file (as is the case for the majority of the transient calculations with the PDC), only two top fields in the GUI maps form in Figure 2-32 are relevant and are displayed to the user.

The “Map option” field specifies if the map needs to be generated or used. The choices for this field are:

**Use**
Read the turbomachinery map from the map file. The only other input needed is for the verification field (see below). This option is to be used for majority, if not all, transient calculations.

**Generate**
Generate (calculate) the map. Refer to the Code Manual section for more details. The input on the GUI form needs to be provided to define the range of the map parameters (e.g., minimum and maximum rotational speed for this map), etc. Typically, a map needs to be generated only once. However, if the component design changes significantly, or the intended transient simulation may extend beyond the range of the existing map, a new map will need to be generated (in both cases, though, a map verification option described below can be used as an alternative).

**Skip**
No action on that particular map will be taken by the PDC, meaning that the map will not be generated or read. This option is intended to be used in the map generation calculations. For example, if map generation for a compressor is requested, reading or generation of a turbine map can be skipped. If this option is used, no transient calculation can be performed. This input will need to be changed to “use” for the transient calculations.

The PDC folder structure for turbomachinery maps is shown in Figure 2-33. The PDC allows the user to create and use two types of maps: general and synchronous. Synchronous maps are used when the shaft speed in the transient is fixed at the design value. For these maps, only one value for the shaft speed (=1) is needed. Therefore, a more detailed computational grid for other variables (inlet pressure, inlet temperature, and outlet pressure) can be used to improve the accuracy of the maps with the same map size. In general maps, the shaft speed is not fixed, so less points are left for other parameters. At the beginning of each transient, the PDC reads input related to the shaft connection mode and shaft speed control, and determines what type of maps (i.e., from what folder) to read.
When map generation is requested, the maps are generated in the “Data\DY\Maps” folder as “Map_<component-name>.txt” files. These files then need to be moved to the corresponding General or Synchronous folder. Even though it is perfectly acceptable to generate only general maps with a wide range of shaft speeds (and copy those files to both folders), it is recommended to utilize the two-type capability of the PDC and generate two sets of the maps to improve code accuracy. This is especially important for the compressor operating close to the critical point, where very high resolution of the inlet temperature (and pressure) is needed not only to improve accuracy but also to avoid instabilities.

It is expected that for supercritical cycles, an accurate solution is needed in the vicinity of the critical point. Therefore, it is recommended to use as many points as possible to generate the turbomachinery maps. As shown in the example in Figure 2-32, using at least one million points total for a map has been selected as a good practice to achieve sufficient accuracy. Because calculating the maps close to the critical point can be time-consuming and challenging, the turbomachinery maps input parameters – ranges and steps – need to be selected carefully for each map.

The turbomachinery maps are originally generated by the PDC in text format to allow the user to check the maps, if needed. With so many points, the map files become very large files – around 500 MB each. To reduce the size of the map files, they need to be converted to binary format using the “Map conversion” button at the bottom of the map form. Clicking on this button will open another form, shown in Figure 2-34. In this form, the map text file to be converted needs to be selected first, then the type of the component (turbine or compressor) and the type of the map (general or synchronous) need to be specified. There is also an option to delete the original text file after the conversion is completed. The conversion process is initiated by clicking on the “Convert” button. Note that once the turbomachinery maps are converted to binary format, they cannot be opened and checked in a text editor. However, the PDC is also supplied with a reverse conversion utility, which can convert the binary TM map files back to text files. That utility is described in Section 2.4.3 below.
The “Map verification” option on the PDC TM maps form appears when the “Use” option is selected for a particular component. This input defines if the turbomachinery maps need to be verified with the actual performance subroutines. In this case, the maps will be used to provide the first guess for the turbomachinery solution at each time step, but the performance subroutines will be used to obtain more accurate solution. Using maps verification improves accuracy but increases computational time since the performance subroutines require several layers of iterations on the working fluid properties and conditions. For example, the cycle conditions in a transient define the inlet and outlet pressures for a turbine or compressor, but the fluid flow rate needs to be iterated on, at each time step, to match these pressures. The following options for map verification are supported in the PDC:

- **No**
  No map verification. The turbomachinery maps define the solution for this component in a transient. This is the fastest option.

- **Always**
  Always use performance subroutines to improve the solution obtained with the maps. This is the most accurate but the slowest option.

- **Active shaft speed control**
  Use performance subroutines only when the shaft speed is changing. This option is useful for a multi-stage transient involving different operating regimes – for example, load following with subsequent separation from the grid and/or plant shutdown.
The PDC stores the turbomachinery map input in a separate file for each component. Therefore, if any changes on the map form are made, these changes need to be saved before another component can be selected. If the user switches to another component without saving the changes, a warning message will be displayed asking if the changes need to be saved.

The turbomachinery map GUI form also tracks for which components the input has been viewed. This is reflected by the check marks next to the component names. If the turbomachinery input form is closed before all components are viewed, the GUI will ask if the user really wants to proceed without visiting all the input.

2.3.5 Transient Definitions

In general, a transient in the PDC is initiated by any entry in the PDC input which is different from the steady-state value. Below are listed some of the most common transient initiators for the PDC. There is no requirement that a single transient initiator should be used, such that any reasonable combination of the examples listed below can be used in the PDC.

2.3.5.1 Change in Boundary Conditions

A transient can be initiated by any change in the boundary conditions. This includes the conditions for the HAHX hot-side fluid, including those calculated by external code, as well as cooling fluid cooler-inlet temperature. These inputs are provided in the Heat Addition and Heat Removal sections of the PDC dynamic input.

2.3.5.2 Load Following

The PDC automatic control system (Section 3.3) is set up to match the generator output to the grid demand. The grid demand table, in terms of values normalized to the steady-state cycle output, is provided by the user in the General section of the PDC dynamic input. This table should be used to specify the load following transient.

2.3.5.3 Grid Disconnection/Loss of Load

As a variant of load following, a complete disconnection from an electrical grid (loss of electrical load) can be simulated using the grid demand table. To start such a transient, an entry of “-100” needs to be provided in the table. The grid disconnection transient can be started at any time. When it is initiated, the grid demand will be set equal to zero. In addition, if synchronous mode with fixed shaft speed is used for a shaft, the shaft will be switched to asynchronous mode with the variable shaft speed.
2.3.5.4 Pipe Break

The General section of the PDC dynamic input includes the input for simulating a pipe break. The input includes the equivalent break diameter (for a circular break) and the break location. If any positive value for the break diameter is entered, the PDC will simulate the pipe break at the corresponding location. The break is assumed to happen instantaneously at time=0.

If zero break diameter is entered, there is no break and the break location input is ignored.

2.3.5.5 Control Action

The plant control system described in Section 3.3 can be used to initiate a transient. A transient can be initiated by a manual control action (see Section 3.3.1.2). In addition, any entry in the target tables for any of the controls which is different from the corresponding steady-state value will automatically initiate a transient.

2.3.6 Executing the PDC code

The Plant Dynamics Code is executed from the user interface by clicking on the “Run” button on the main form (Figure 2-7). A new command-line window is opened where the code reports on its progress. Unless the restart capability is used, the code always starts from finding the steady-state solution. Figure 2-35 shows a typical view of the PDC code window in steady-state mode with a brief description of the main elements in the window. A set of iterations are run until convergence is achieved. For more information on the steady-state solution algorithm, refer to the Code Manual section of this report.
Once the steady-state calculations are completed, the PDC automatically proceeds to transient calculations, if those are requested in the input. Figure 2-36 shows a typical view of the PDC execution window for the transient part.
The dynamic time step is automatically adjusted by the PDC (see the Code Manual part). It is displayed in the code window as a negative power of 10, in seconds. For example, “2” in Figure 2-36 means that the time step is $10^{-2}$ seconds. The window also shows the number of sub-steps for the cycle and cooling sides. This is the number of steps in which the main time step is divided to solve the differential equations.

The PDC supports execution of up to eight instances of a code (in dynamic calculations only, not in steady-state). If more than one instance of the code is executed, the results for runs from the second one on are written to files with “2”, etc. at the end of their names. This feature is useful on multi-core machines, for instance, to investigate the plant response to variations of a control setup.

The code also reports when a restart file is written. The times at which those files are created are defined in the general part of dynamic input (Figure 2-23). In addition, a restart file is created at the end of the code’s simulation. The restart file name includes the file set number and time (e.g., “r1_t30” means the file is created with code run #1 at 30 seconds into transient). The restart files are binary and could only be used to restart the PDC.

Figure 2-36. PDC Execution Windows – Dynamic Calculations.
2.3.7 Viewing PDC Results

Once the code is executed, the results can be viewed in the user interface by clicking on the “Steady-state” or “Dynamic” buttons in the “View Results” section of the main GUI form (Figure 2-7).

2.3.7.1 Steady-State Results

During the steady-state calculations, the PDC creates the results files for the entire cycle and for each of the components. Clicking on the “Steady-State” results button in the GUI opens the form which shows the PDC results for the cycle (Figure 2-37). On this form, several tables show the PDC results, such as heat/power balance and cycle efficiency, working fluid conditions along the cycle points, results for the pipes and flows, working fluid inventory, and general results for components. All of these tables can be copied-and-pasted for reporting or plotting, if needed. The units for heat duty, pressure, and temperature may be changed in this form.
The cycle results form in Figure 2-37 also has a “Scheme” button that opens an Excel file where the cycle results can be displayed graphically. The interface will transfer all of the information from the form to the Excel file. The data is automatically used to update the cycle schematic. However, neither the user interface nor the Excel file draws the cycle schematic. That drawing needs to be updated manually by the user, if the cycle layout changes. The Excel file also allows the user to change the units in the legend; the values on the diagram will be updated automatically to reflect new units. The detailed instructions for how to use this Excel file are provided in the file (and also in Figure 2-37). The cycle schematic can be copied and pasted to other applications, such as to Word for reporting.
After changes are made to the file, it can be saved as a regular Excel file. Notice that unless the file name or location is modified using the “Save As” menu, the Excel will override the file supplied with the code. It is recommended to create and keep a copy of the original file, “SS – results.xlsx” in an “Excel” folder (see Figure 2-6), for backup purposes.

In the top-right corner of the cycle results form in Figure 2-37, there are two buttons to display the detailed results for components. The “Design” button opens another form which displays a table with the design information for each cycle component (Figure 2-39). That information is useful, for example, to define the design parameters for requesting heat exchanger manufacturer quote. This table can be copied either by selecting text in the window or using the “Copy” button to copy the entire table.
The other button for component results, “Details” in Figure 2-37, opens a form (Figure 2-40) which displays the detailed results for the cycle components. In the top-left corner of this form, a list of the available output files for components is provided. Selecting one of those files displays the file content on the form. Similar to the component design form, the information can be copied, as needed, for reporting or plotting.
2.3.7.2 Dynamic Results

The PDC transient results are viewed in another Excel file, which is opened by the GUI when the user clicks on the “Dynamic” button in the results section of the main form. The main control “Update” tab of the file is shown in Figure 2-41. This sheet has two control buttons: “Update” and “Update Graphs”. The “Update” button is used to automatically update the contents of the Excel file (“Data” and “BC Data” sheets) from the PDC output files. The user needs to specify the Output, File Set, and Restart cells first. The Output cell contains the path to the PDC dynamic output files. That cell is updated by the GUI automatically. The File Set is the PDC run number as displayed in the PDC run window in Figure 2-36 (“1” should be used, unless multiple parallel code executions were initiated). The Restart cell needs to be updated (set to “Yes”) only if the PDC restart capability is used. The description of how to use the Excel file in that case is provided below. For normal transient calculations, the Restart cell should be “No”.

The PDC results transfer is initiated by clicking on the “Update” button. An Excel script\(^1\) will be executed which will open the PDC output files, and copy their contents to the “Data” and “BC Data” sheets of the file, for general and cycle results, respectively. Then, the general and cycle result plots can be viewed in “Graphs” (see an example in Figure 2-42) and “BC Graphs” (Figure 2-43), respectively. The script will automatically switch to the “Graphs” tab at the end of its execution.

---

\(^1\) Excel scripts should be allowed by security settings for this file to function properly.
Changing the value of the “Restart?” cell to “Yes” allows the user to update only a portion of the plots and can be used if the PDC restart capability was utilized. If the value is set to “Yes,” then the Excel script will only update values in the “Data” and “BC Data” sheets for the times after the restart time. All of the values prior to that time will remain unchanged. Notice though that the Excel file supplied with the code contains the results of a sample problem. To properly use the restart capability, the PDC code needs to be executed first from beginning of the transient (from time=0). Then, the Excel file should be opened, updated with the transient data and saved (it is recommended to create a copy of the file supplied with the code prior to this action). Then, when the PDC is run from a restart, the “Restart?” cell need to be changed to “Yes” prior to clicking on the “Update” button. The script will then update only the results for the times starting at the restart time.

The “Update” tab of the Excel file in Figure 2-41 also has capability to change the time scale on all plots. To do that, the user needs to change Graphs Scale cells (min, max, and major units – highlighted in dark green) and click on the “Update Graphs” button. Another Excel script will be executed which will change the time axes on all plots in the “Graphs” and “BC Graphs” sheets.

Similar to the steady-state Excel file, the file can be saved after changes are made. So, it is recommended to create and keep a copy of the original file, “PDC Dynamic Results.xlsm” in an “Excel” folder (see Figure 2-6), for backup purposes.

The “Update” sheet also contains instructions on how to use the file. This file can be used to update and view the code results as the code is still being executed. However, caution should be
exercised to avoid the file access violation with the code, which will result in code termination. To update the Excel file when the code is running, the code execution first needs to be paused. This is achieved by going to the code execution window (Figure 2-36) and pressing the “Pause” button on the keyboard. Make sure that the code is really paused before proceeding to the next step – this will be evident by the fact that the Time counter in the code window has stopped advancing. Then, return to the Excel file and click on the “Update” button. After the files are loaded (and the Excel file switches to the “Graphs” sheet), the code execution can be resumed. Go back to the code window and press any key on the keyboard. The Time counter should start changing again.

The results plots can be viewed on the “Graphs” tab. This sheet contains a number of plots, such as the one shown in Figure 2-42. In each plot, up to five different curves can be shown. The variables for each curve are selected at the top row. The cells in that row are color-coded according to the curves. For example, in Figure 2-42, Q_RHX_Rx is selected in the blue cell in the top row and is shown in a blue line on the plot. Once a variable is selected, its units are shown in the second row. It is up to the user to make sure that the correct variables are selected and the correct curves are plotted on each graph. The user also needs to manually change the plot title and the vertical axis title, if necessary.

The selection of the variables to plot on each graph is made from all of the variables from the PDC dynamic output file. Table 2-5 lists all of the available variables in the order they appear in the list.
Table 2-5. Variables Available in the PDC Dynamic Output

<table>
<thead>
<tr>
<th>Variable</th>
<th>Description</th>
<th>Units</th>
<th>Range</th>
</tr>
</thead>
<tbody>
<tr>
<td>Time</td>
<td>Current time</td>
<td>s</td>
<td></td>
</tr>
<tr>
<td>d_Time</td>
<td>Time step</td>
<td>s</td>
<td></td>
</tr>
<tr>
<td>Get_SS</td>
<td>1 = Calculations prior to actual transient 0 = Actual transient</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Q_RHX_Rx</td>
<td>Heat transfer rate on HAHX hot side</td>
<td>MW</td>
<td></td>
</tr>
<tr>
<td>m_RPF</td>
<td>HAHX hot side fluid flow rate</td>
<td>kg/s</td>
<td></td>
</tr>
<tr>
<td>T_in_RHX</td>
<td>HAHX hot side fluid inlet temperature</td>
<td>°C</td>
<td></td>
</tr>
<tr>
<td>T_out_RHX</td>
<td>HAHX hot side fluid outlet temperature</td>
<td>°C</td>
<td></td>
</tr>
<tr>
<td>Q_RHX_CO2</td>
<td>Heat transfer rate on HAHX cold side</td>
<td>MW</td>
<td></td>
</tr>
<tr>
<td>Q_&lt;Cool&gt;</td>
<td>Heat transfer rate in cooler, hot side</td>
<td>MW</td>
<td>All coolers</td>
</tr>
<tr>
<td>W_&lt;Turb&gt;</td>
<td>Turbine power</td>
<td>MW</td>
<td>All turbines</td>
</tr>
<tr>
<td>W_&lt;Comp&gt;</td>
<td>Compressor power</td>
<td>MW</td>
<td>All compressors</td>
</tr>
<tr>
<td>W_2_grid</td>
<td>Power-to-grid</td>
<td>MW</td>
<td></td>
</tr>
<tr>
<td>W_grid</td>
<td>Grid power demand</td>
<td>MW</td>
<td></td>
</tr>
<tr>
<td>Eff_cyc</td>
<td>Cycle efficiency</td>
<td>%</td>
<td></td>
</tr>
<tr>
<td>Eff_sys</td>
<td>System efficiency</td>
<td>%</td>
<td></td>
</tr>
<tr>
<td>Nr_&lt;Shaft&gt;</td>
<td>Shaft rotational speed</td>
<td>%</td>
<td>All shafts</td>
</tr>
<tr>
<td>MTank</td>
<td>Mass in inventory tank</td>
<td>kg</td>
<td></td>
</tr>
<tr>
<td>dM_tank</td>
<td>Change in mass in inventory tank from t=0</td>
<td>kg</td>
<td></td>
</tr>
<tr>
<td>f_st_&lt;Comp&gt;</td>
<td>Compressor stall margin</td>
<td>-</td>
<td>All compressors</td>
</tr>
<tr>
<td>f_ch_&lt;Comp&gt;</td>
<td>Compressor choke margin</td>
<td>-</td>
<td>All compressors</td>
</tr>
<tr>
<td>f_ch_&lt;Turb&gt;</td>
<td>Turbine choke margin</td>
<td>-</td>
<td>All turbines</td>
</tr>
<tr>
<td>f_op_&lt;Valve&gt;</td>
<td>Valve open fraction</td>
<td>%</td>
<td>All valves</td>
</tr>
<tr>
<td>f_sc_&lt;Split&gt;</td>
<td>Secondary flow fraction</td>
<td>%</td>
<td>All splits</td>
</tr>
<tr>
<td>T_min_&lt;Split&gt;</td>
<td>Minimum temperature inside compressor</td>
<td>°C</td>
<td>All compressors</td>
</tr>
<tr>
<td>p_min_&lt;Comp&gt;</td>
<td>Minimum pressure inside compressor</td>
<td>MPa</td>
<td>All compressors</td>
</tr>
<tr>
<td>m_sec_&lt;Cool&gt;</td>
<td>Cooling fluid flow rate in cooler</td>
<td>kg/s</td>
<td>All coolers</td>
</tr>
<tr>
<td>dp_sc_&lt;Cool&gt;</td>
<td>Pressure drop on cold side of cooler</td>
<td>Pa</td>
<td>All coolers</td>
</tr>
<tr>
<td>W_pmp_&lt;Cool&gt;</td>
<td>Cooling fluid pumping power in cooler</td>
<td>MW</td>
<td>All coolers</td>
</tr>
</tbody>
</table>

The “BC Graphs” and “BC Data” tabs contain the PDC transient results related to the cycle, such as state points and pipe flow rates. Figure 2-43 shows an example of a cycle results plot on the “BC Graphs” sheet. The approach to plotting variables is similar to that for the general results in Figure 2-42. Each plot can contain up to five curves which can be selected by the user. However, as shown in Figure 2-43, the selection process is somewhat different for the cycle plots. First, the variable type needs to be selected according to those listed in Table 2-6. Then, the node index for which the value is to be plotted needs to be specified in the second row. The third row is reserved for the name of the curve that the user wants to appear in the plot’s legend. These names need to be changed manually by the user.
The dynamic results Excel file also contains the “Input” sheet which keeps a copy of all of the transient PDC input to preserve the definition of the transient for which the results are obtained. The contents of this sheet are also automatically updated when the PDC dynamic results are loaded by the script.

The dynamic results Excel file also contains the “Component” sheet to display the transient results for individual components. The view of this sheet is provided in Figure 2-44. To view the
results, the user first selects the component name from the drop-down list in cell A2 and then clicks on the “Get Results” button. The Excel file will show the results for that component as recorded by the PDC. When the file is opened from the GUI, the list of the components for which the transient results are available is automatically updated.

Since the data format is different for different component types (e.g., heat exchangers or turbines), no plots are shown on this sheet. However, since the results are displayed in a standard Excel format, those plots can easily be created in the file. Notice, however, that the component results will be erased the next time the file is opened by the GUI, or if another component is selected. Therefore, it is recommended to copy the component data to another sheet (or another file or application) for plotting. The same method can be used for any data in the Excel file.

Figure 2-44. PDC Dynamic Results in Excel: Viewing Results for Components.
2.4 Working with Text Files Directly

The user interface described in the previous section is the recommended way to interact with the Plant Dynamics Code. However, there is also an option to work with the PDC input/output files directly. Those files are the text files and can be viewed or modified in any text editor.

The PDC input and output files are located in the “Data” folder of the code (see Figure 2-6). The files are organized by the calculation type: “SS” for steady-state and “DY” for dynamics, as well as by the purpose of the file: Input or Output.

2.4.1 PDC Input Files

The PDC input files are distinguished by a “_dat” string at the end of the file name. In general, the following concept is adopted for all PDC input files. Two lines are devoted for each input in the files. The first line gives the description of that input and, where applicable, the units. This line is for user information only, its content is ignored by the code. The second line includes the numeric values read by the code. If multiple values are requested, they should be separated by a space or a tab. The required units are provided in the description line and could not be changed. Here is an example of a portion of the input file requesting the recuperator length:

Unit length, m
0.6

Since the description lines are ignored by the code, the input file lines could not be moved around or deleted. For example, the code assumes that the first input for a recuperator is always the recuperator type, followed by given efficiency, etc. The input files can also contain additional lines, such as a title line or sections headers (e.g., recuperator type). Those lines are usually designated by strings of “*” or “-” characters. The code expects those lines to be there, so they too cannot be deleted.

Most of the input files for cycle components provide the choice of the component type. For example, a PCHE or Shell-and-tube HX for recuperator. The code will use the input only applicable to the selected type. However, the input lines for another available type (or types) should not be deleted since the code expects those lines to be there.

The value lines are the only ones that can be modified. When the code reads the value (or values), it only reads the number of the inputs specified by the description. In the example above, the code will only read one number for the unit length. Everything written beyond that in the value line is not read by the code and can be used to provide comments, store variations of the input, or for any other purpose.

Since the structure of the PDC input files is fixed and cannot be modified, it is recommended to modify the existing files rather than creating new ones. For example, if a new component is introduced, it is recommended to create a copy of the file which already exists for the same component type, rename it, and modify the value lines.
Table 2-7 provides the list and description of the PDC input files for both steady-state and dynamic calculations. With the exception of the files containing the component names, the file names of the PDC input files cannot be changed.

### Table 2-7. PDC Input Files

<table>
<thead>
<tr>
<th>File Name</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Steady-State (“Data\SS\Input” folder)</strong></td>
<td></td>
</tr>
<tr>
<td>Cycle_dat.txt</td>
<td>Main cycle input and cycle configuration.</td>
</tr>
<tr>
<td><code>&lt;Component-name&gt;_dat.txt</code></td>
<td>Input files for each component. The PDC will look for the input files with the first part of the file name matching the component name <em>exactly</em>, as defined in Cycle_dat.txt. For example, “HTR_dat.txt” for component named “HTR”. The file structure and content depends on the component type. This file is required for the following component types: HAXH, recuperator, cooler, turbine, compressor, and shaft.</td>
</tr>
<tr>
<td><code>&lt;Component-name&gt;_des_dat.txt</code></td>
<td>Input files for turbomachinery components (turbine and compressor) with given (known) design. Same naming convention as above applies.</td>
</tr>
<tr>
<td>RHX_HS_dat.txt</td>
<td>Hot side conditions for a heat addition heat exchanger. These conditions are common for all HAXHs, if multiple HXs are used in the model.</td>
</tr>
<tr>
<td><strong>Dynamic (“Data\DY\Input” folder)</strong></td>
<td></td>
</tr>
<tr>
<td>Dynamic_dat.txt</td>
<td>General input for transient calculations.</td>
</tr>
<tr>
<td>BCcontrol_dat.txt</td>
<td>Input for the Brayton Cycle control in transient.</td>
</tr>
<tr>
<td>HAcontrol_dat.txt</td>
<td>Input for the heat addition control in transient.</td>
</tr>
<tr>
<td>SAS_dat.txt</td>
<td>Input for SAS4A/SASSYS-1 coupling, if used. If coupling is not used, the first input in this file should be set to 0.</td>
</tr>
<tr>
<td>RPF_MFR_dat.txt</td>
<td>Table for the HAHX hot side fluid (historically, Reactor Primary Fluid) mass flow rate as a function of time. Flow rate values are provided as relative to the design (steady-state) value.</td>
</tr>
</tbody>
</table>
### PDC: Plant Dynamics Code for Design and Transient Analysis of Supercritical Brayton Cycles
#### September 27, 2018

<table>
<thead>
<tr>
<th>File Name</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>RPF_T_in_dat.txt</td>
<td>Table for the HAHX hot side fluid temperature at the HAHX inlet as a function of time. Temperature values are provided as relative (based on Kelvin units) to the design (steady-state) value.</td>
</tr>
<tr>
<td>RPF_p_in_dat.txt</td>
<td>Table for the HAHX hot side fluid pressure at the HAHX inlet as a function of time. Pressure values are provided as relative to the design (steady-state) value.</td>
</tr>
<tr>
<td>H2O_T_in_dat.txt</td>
<td>Table for the cold side fluid (historically, water) temperature at the cooler inlet (same as ambient temperature) as a function of time. Temperature values are provided as absolute temperatures in °C units.</td>
</tr>
<tr>
<td>Map_&lt;Comp.-name&gt;_dat.txt</td>
<td>Input files for map generation/usage of turbomachinery components. The PDC will look for the input files with the middle part of the file name matching the component name exactly, as defined in Cycle_dat.txt. For example, “Map_Turb_dat.txt” for a component named “Turb.” These files are required for all turbomachinery components: turbines and compressors.</td>
</tr>
</tbody>
</table>

#### 2.4.2 PDC Output Files

Table 2-8 shows the list of the PDC output files for the steady-state and dynamic calculations. If several parallel runs of the code are initiated, the code runs starting from the second one on will have the corresponding number added to the end of the dynamic output files (e.g., T_BC_res2.txt).

**Table 2-8. PDC Output Files**

<table>
<thead>
<tr>
<th>File Name</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cycle_res.txt</td>
<td>Main cycle results.</td>
</tr>
<tr>
<td>SS_des.txt</td>
<td>Cycle results in tabular form.</td>
</tr>
<tr>
<td>BC_des.txt</td>
<td>Design information on cycle components.</td>
</tr>
</tbody>
</table>
Temperature and properties distribution for heat exchangers (HAHXs, recuperators, and coolers). `<Comp.-name>` is replaced with component name (e.g., HTRDistTXT.txt).

Results of design calculations for turbomachinery components.

Results of design calculations for turbomachinery components in tabular form.

Dynamic ("Data\DY\Output" folder)

Repeat of all dynamic input files.

Initial conditions for dynamic calculations for Brayton cycle.

General results of dynamic calculations.

Results for Brayton Cycle temperatures, pressures, densities, and flow rates.

Transient results for components.

Map extrapolation warnings.

Binary restart files.

Input for SAS4A/SASSYS-1 related to the HAHX design.

### 2.4.3 Turbomachinery Map Files

The turbomachinery map files are located in the “Data\DY\Maps” folders “General” and “Synchronous.” The map files are created by the PDC as text files that can be viewed by the user. However, the map files should not be modified since the code requires these file to be of a certain format.

The PDC uses map files as binary files, which are about 1/3 the size of the text files. There are two utilities supplied with the PDC, `Map2bin.exe` and `Map2txt.exe`, located in the code’s `Utilities` folder which can be used to convert the turbomachinery map files to binary and text format respectively. Conversion to binary format is required for the code to use the maps. Conversion to the text format is only provided for user’s convenience so one can check the maps when needed. That conversion is not required by the code.
The map conversion utilities need to be called from the command line. The following call format is applied to both utilities:

```
Map2bin.exe -f "Path\File.txt"
Map2txt.exe -f "Path\File.bin"
```

where “-f” should be replaced with either “-t” for the turbine map or “-c” for the compressor map. The “Path” is the path to the map file, either absolute or relative to the utility location.

Both utilities will create the corresponding file which will be added to the folder where the original file exists. If the original file is no longer required, it needs to be manually deleted by the user.

### 2.4.4 Executing the Code from Command Line

If the user interface is not used, the Plant Dynamics Code can be run either from a command line or from the file explorer by executing the “PDC.exe” file in the “Code\Project” directory. If the code is run from the file explorer, it is recommended to lunch the PDC.bat batch file instead of PDC.exe since it will keep the code window open in case the code is terminated due to an error.
2.5 PDC Restart Capability

The Plant Dynamics Code’s restart capability allows the user to save the progress of a transient simulation and later restart the simulation from that point. The restart feature saves all of the variables used in dynamic calculations to a binary file. This file can later be read by the code and the calculations can be continued (“restarted”) from the time at which the restart file was created.

The restart files can be created at several time points during a transient run. A user input in the General area of the PDC dynamic input (Figure 2-45), or in the “Dynamic_dat.txt” file, specifies at what times the restart files are created. The binary restart files are saved in a “Data\DY\Output\” folder and their names include the time at which the files were created. For example, restart files “Restart_r1_t150.bin” and “Restart_r1_t1600.bin” are created at 50 s and 1,600 s into a transient, respectively. A user can choose to start the dynamic calculations from any of those points in time. To do that, a user needs to copy the corresponding restart file into the “Data\DY\Input\” directory and provide the restart file name in the “Dynamic_dat.txt” input file. Alternatively, these steps can be accomplished using the GUI interface as shown in Figure 2-45. At the top of the form, there is a flag to use the restart feature and to specify the restart files. Then, clicking on the “Copy files” button will copy the specified restart files from the “Output” to the “Input” folder. A standard Windows message will be displayed, if the files already exist in the destination folder presenting the user an option to override the files. Two directories where the restart files are created and are read from (Output and Input) are intentionally selected to be different to preclude accidental rewriting of a restart file by the code.

If the SAS4A/SASSYS-1 coupling is used, its restart file is saved together with the PDC restart file, so both codes can be restarted from the same time.

![Input for Dynamic Calculations](image)

Figure 2-45. PDC Input for Restart.
When the PDC code is run in coupled mode with the SAS4A/SASSYS-1 code, a restart file from SAS4A/SASSYS-1 is also saved along with the PDC restart file. The SAS4A/SASSYS-1 restart file is created automatically after each run; i.e., after each time step when SAS4A/SASSYS-1’s execution is called from the PDC in transient calculations. That SAS4A/SASSYS-1 restart file is now automatically copied into the same directory as the PDC restart file and is distinguished by the addition of “_SAS” at the end of its name. That file should also be copied by a user into the “Input” folder to be read for restart. The SAS4A/SASSYS-1 restart file needs to be specified in the GUI form too and will be copied together with the PDC restart file.

The PDC restart feature is triggered by the flag in the General dynamic input form in Figure 2-45 (or by providing “1” in the restart input in “Dynamic.dat.txt” file). If the restart box is unchecked (or “0” is entered in the “Dynamic.dat.txt” file), the rest of the restart input in this line is ignored, and the calculations proceed as before; i.e., starting from steady-state calculation followed by the full transient calculations from time=0. If the restart box is checked (or “1” is entered in “Dynamic.dat.txt” file), then the restart capability is used. In this case, the names of the restart files, for the PDC and SAS4A/SASSYS-1, respectively, should be provided. The code will bypass the steady-state calculation and instead will continue the transient calculations from the restart file time.

The other line is provided in the input (also highlighted in Figure 2-45) to specify at which times the restart files are created during the transient run. A user can specify up to 20 times; the restart files will be created with names containing “_t####”, where “####” is replaced with the time into the transient when the files are created. In addition, a restart file is automatically created at the end of the transient calculations. Note that this input is used regardless of whether the restart option is used. In other words, the restart files will be saved at the specified times even if the calculations are not proceeded from the restart.

Although the restart files can theoretically be saved after each and every time step, the file name will only include the transient time rounded up to a nearest integer. Because of that, the saved times should be at least 1 s apart. For example, a restart at 10.3 s, created as the “..._t10” file, would overwrite the file created at 9.8 s.

The restart capability in the PDC was created to allow more effective investigation of transient cycle behavior. One of the possible examples where the restart capability would help is an optimization of a control strategy toward the end of a fairly long transient. With the restart, the effect of the variation in the control system parameters can be calculated at any time in the transient without the need to repeat the entire transient history (provided that the change does not affect earlier results).

In order to provide the capability to change input parameters after a restart, the input files for the dynamic calculations, including the cycle control parameters, are read after the restart files are read. Therefore, the input parameters are naturally replaced with those provided in the input files. For example, to investigate the effect of various PID control coefficients on the transient behavior of the system, a user will change those coefficients in the input file before resuming the calculations using the restart option. (Similar modifications can be made in the SAS4A/SASSYS-1 input file, if changes in the reactor-side conditions are needed.) Similar to the input files, the
turbomachinery maps are also read after the restart files (the turbomachinery map data is not saved in the restart file). This approach, in theory, allows using different maps for various parts of a transient. However, that option should be used with caution to make sure that switching between the maps does not affect, at least to a significant degree, the transient results prior to the restart time.

In addition to more effective transient simulation, using the restart capability eliminates the need to repeat the steady-state calculation every time for each transient. If the restart file is saved at time \( t = 0 \), the full transient can still be run without any limitations on the transient itself. It is noted however, that the restart capability cannot be used to investigate the effect of design modifications (e.g., number of high temperature recuperator modules), since those changes would alter the results of the steady-state calculation. For this reason, the input files for the steady-state part of the code are not re-read after the restart.
2.6 Coupling with SAS4A/SASSYS-1 Code

The Plant Dynamics Code has two options to define the hot side fluid conditions at the Heat Addition Heat Exchanger (HAHX) in a transient. The first option defines the hot-side fluid conditions, including temperature, flow rate, and pressure, at the HAHX inlet as time-dependent tables (see Figure 2-25 in Section 2.3.4.3 above). These inputs need to be known as boundary conditions or need to be calculated by a separate code. In the case of reactor applications, the reactor-side fluid conditions need to be calculated by a separate reactor analysis code.

The second option available in the PDC is to use the SAS4A/SASSYS-1 code to calculate the hot-side HAHX conditions in a transient. The SAS4A/SASSYS-1 Liquid Metal Reactor Code System [1] is the leading capability for modeling advanced reactors at the system level. The SAS4A/SASSYS-1 code couples reactor dynamics with thermal hydraulics calculations and includes very detailed reactivity feedback models along with comprehensive thermal hydraulic models for the primary, intermediate, and decay heat liquid metal loops.

In order to use the PDC-SAS4A/SASSYS-1 coupling capability described here, the SAS4A/SASSYS-1 executable file is required. **The SAS4A/SASSYS-1 executable file is not supplied with the Plant Dynamics Code and needs to be independently obtained from Argonne National Laboratory.**

2.6.1 Coupling Approach

The main goal of the PDC-SAS4A/SASSYS-1 coupling is to implement data transfer between the two codes at each time step. The coupling approach utilizes the restart capability of SAS4A/SASSYS-1 to allow the code to be executed for some transient time, paused, and restarted later with modifications to the input files. That restart capability is used to basically implement SAS4A/SASSYS-1 calculations on a step-by-step basis, using an algorithm shown in Figure 2-46 and described below. The transient calculation is preceded by steady-state calculations in both the PDC and SAS4A/SASSYS-1.

The coupling is achieved by correlating the two codes on the conditions in the HAHX, which for reactor applications is called the reactor heat exchanger (RHX). This could be, for example, the intermediate sodium-to-CO₂ heat exchanger for sodium-cooled reactors (SFRs) with an intermediate sodium loop. Since most of the coupled PDC-SAS4A/SASSYS-1 analyses have been carried out so far for SFRs, the coupling approach is described below in terms applicable to an SFR with a sCO₂ cycle energy converter; however, the basic principles would be the same for all other reactor or cycle types.

The transient calculations at each time step start with a guess of an intermediate sodium RHX-outlet temperature. That guess is based on extrapolation of the results at a previous time step (or steady-state values). The sodium RHX-outlet temperature is selected for such an extrapolation because it is expected that it would be a slowly-changing variable due to the thermal inertia of the heat exchanger mass. No iterations are implemented to verify the extrapolated value; it is simply
compared to the actual value calculated on the next time step. As is demonstrated below, that simple extrapolation provides sufficient accuracy for the dynamic calculations.

Figure 2-46. PDC-SAS4A/SASSYS-1 Coupling Approach.
The extrapolated RHX-outlet temperature is supplied to the SAS4A/SASSYS-1 restart input file. Then, the SAS4A/SASSYS-1 code is called to calculate the reactor side parameters for one time step. After that, the SAS4A/SASSYS-1 output files are read and the data required for the PDC calculations – the intermediate sodium flow rate and its temperature at the RHX inlet – are provided as input data for the PDC calculations. Since the sCO2 cycle time step is usually smaller than a reactor time step, the PDC code is run for one or several time steps until it reaches the same transient time as that of the SAS4A/SASSYS-1 code. The PDC calculates the sCO2 cycle parameters along with the sodium temperature at the RHX outlet. The latter value is used again to calculate the next guess for the SAS4A/SASSYS-1 calculations. That process continues until the specified maximum transient time is reached.

### 2.6.2 Accuracy of the Coupling Scheme

As discussed above, the coupling scheme relies on the extrapolation of the sodium temperature change in RHX. Figure 2-47 shows an example of the calculated error in the prediction of the sodium temperature change in the RHX. The plotted value in Figure 2-47 is:

\[
\text{Prediction Error} = \left| \frac{\Delta T_{\text{actual}} - \Delta T_{\text{predicted}}}{\Delta T_{\text{actual}}} \right|
\]

(2.2)

![Figure 2-47. Sodium RHX Temperature Change Prediction Error.](image-url)
The prediction error in Figure 2-47 is plotted as a function of time for a transient that simulated linear grid load reduction from 100% to 0% in 1200 s. The maximum error in the sodium temperature change is calculated at the very beginning of the transient. This is due to the fact that at those earlier times no transient information is available and the prediction could only be made based on the steady-state value. Once the temperature change starts varying, the accuracy of the prediction increases significantly. The prediction error also increases when significant changes are introduced to the system. For example, the error shows an increase at the start and stop of the inventory control action (between 200 and 600 s) and at the transition to steady-state operation at zero power at 1200 s. In any case, the prediction error does not exceed $10^{-4}$ and stays well below that value for most of the transient. Since the transient calculations on sCO$_2$ side were performed with a convergence criteria of $10^{-5}$, the simple extrapolation described above provides sufficient accuracy for the dynamic calculations and no iterations are needed.

2.6.3 Using Coupling with SAS4A/SASSYS-1

The SAS4A/SASSYS-1 coupling is triggered by setting a corresponding flag in the Heat Addition transient input form in Figure 2-30 (or in “SAS.dat.txt” file). The figure also lists all other input needed for the coupling. The input specifies the location of the SAS4A/SASSYS-1 folder, which needs to contain the SAS4A/SASSYS-1 executable file, SAS4A/SASSYS-1 model input file, and SAS4A/SASSYS-1 restart file (the latter will be replaced by the PDC as calculations progress). The path input for the SAS4A/SASSYS-1 folder can be either the full path or relative to the PDC executable file. The file names for the executable and input files are also provided in the input.

The PDC input in the form in Figure 2-30 also includes the input for active reactor control. The description of how the reactor control is implemented in the PDC is provided in the control section of the Code Manual part of this report in Section 3.3.3.3).

In addition to the PDC input, the following modifications need to be made to the SAS4A/SASSYS-1 input file to make the SAS4A/SASSYS-1 model compatible with the PDC coupling:

- The RHX needs to be represented by a steam generator with a table look-up option of temperature change versus time. This table should have zeros in all value entries, except the first two, which should be set to “1” for steady-state (the actual values will be re-written by the PDC during the transient).

- The input for the element representing that steam generator – length, flow area, and hydraulic diameter – needs to be consistent with the PDC input for the RHX. These values are calculated by the PDC in the steady-state calculation and are reported in the “\Daily\Output\SAS_input.txt” file.

- The SAS4A/SASSYS-1 steady-state results should be consistent with the PDC input for the HAHX hot side (inlet/outlet temperatures and heat duty – in Figure 2-17 or in the “RHX_HS_dat.txt” file). If necessary, the SAS4A/SASSYS-1 model input needs to be adjusted to achieve the agreement on the reactor side (intermediate loop) temperatures (for example, by changing the IHX tube perimeter).
- Maximum problem time should be set to 0 to run steady-state calculations only. The problem time will be updated by the PDC in the SAS4A/SASSYS-1 restart file as needed.
- Maximum number of time steps should be set to a very large number since the transient time will be defined by the PDC.
- SAS4A/SASSYS-1 plotting data output frequency should be set to each time step.
- The following variables, in that order, need to be specified in the front of the PRIMAR output file:
  - Next PRIMAR time step,
  - Flow rate at steam generator inlet,
  - Inlet temperature for the steam generator element,
  - Outlet temperature for the steam generator outlet,
  - Core-outlet temperature,
  - IHX-outlet temperature on primary side,
  - Core flow rate, and
  - Core flow rate times outlet temperature.

2.6.4 Transient Definition with PDC-SAS4A/SASSYS-1 Coupling

When the SAS4A/SASSYS-1 coupling is used, the transient can be defined in the PDC input, in the SAS4A/SASSYS-1 input, or in both. For example, the SAS4A/SASSYS-1 input file needs to be used to set reactor scram as a transient initiating event. Depending on the desired transient definition, a corresponding input may be provided for the PDC, for example, if the transient assumes simultaneous turbine trip. It is the user’s responsibility to make sure that the input is consistent between the PDC and SAS4A/SASSYS-1 and actually simulates the intended transient.

Caution also needs to be exercised defining transients when active reactor control is implemented. For example, if the PDC input is set to use active control for the reactor power, any input in the SAS4A/SASSYS-1 file for the reactor reactivity will be overwritten by that active control.
3 CODE MANUAL
The primary purpose of the Plant Dynamics Code is the transient analysis of supercritical Brayton cycles. At the same time, the PDC includes the steady-state part, which is designed to accomplish two goals. First, the steady-state solution serves as the starting point for any transient calculations and thus is required by the code. Second, the steady-state part can be used independently of the dynamic part to carry out cycle design calculations, such as finding the optimal cycle configuration, for example.

In this chapter of the report, the PDC steady-state (in Section 3.1) and dynamic (in Section 3.2) models are described in detail, including assumption, formulation of the equations, and solution approaches.
3.1 Steady-State Models

The primary goal of the PDC steady-state models is to calculate the working fluid's pressure and temperature distribution around the cycle, plus the flow rates. From that information, all other cycle and component performance metrics can be calculated, including cycle efficiency, turbine power and efficiency, heat exchanger heat transfer rate, effectiveness, and pressure drop, and so on. Figure 3-1 shows typical PDC steady-state results, including pressure and temperature distributions throughout the cycle and some component performance results.

In the process of obtaining the steady-state solution for the cycle, other results are obtained by the code and are reported to the user in the output files. These results include, for example, the detailed temperature distribution inside the heat exchanger, loss contributions in the turbomachinery, and piping wall temperature and the heat loss. The general rule for reporting the PDC steady-state results is that every value calculated by the code will be reported in one of the PDC output files.

Figure 3-1. Example of PDC Steady-State Results for Advanced Fast Reactor (AFR)-100 sCO2 Cycle.
3.1.1 Cycle Calculations

The steady-state results are calculated in the PDC by going through the cycle and combining the performance of each component with boundary conditions and other inputs, such as the flow split requirement in a recompression closed Brayton cycle incorporating two compressors. This process usually requires an iterative solution since the boundary conditions for one component (e.g., heat exchanger) are defined in part by the performance of other components, such as turbines, compressors, and other heat exchangers. The detailed description of how the PDC obtains the steady-state solution is provided below, followed by detailed descriptions of the component models, including flow splits, mixers, valves, heat exchangers, turbomachinery, and pipes.

3.1.1.1 Cycle Solution Scheme

Before the cycle calculations start, the PDC checks if all components ports (e.g., hot/cold inlet/outlet for a recuperator) are connected to another component by a pipe. If an open (unused) connection is detected, an error message is displayed by the PDC saying which component is missing a connection.

Next, the PDC fills the flow fraction array for each pipe. This is done by going around the cycle, possibly several times until all pipes are filled. First, a flow fraction of “1” is assigned to all pipes. The PDC also keeps in a separate array flags that specify whether or not the flow fraction for that pipe has been defined. Those flags are initially set to “not filled” for all pipes. Then, the PDC goes around the cycle starting from the HAHX outlet, modifies the flow fractions, if necessary, and sets the flag to “filled” for the current pipe. If a flow splitter is encountered, then the code proceeds to the primary outlet port of that split. The flow fraction is set to that on the inlet port multiplied by the primary flow fraction specified for that split in the input. The code continues until another flow split or flow merge point is encountered. For a flow merge, the flow fraction at the outlet is set to the sum of those at two inlet ports. Next, the code starts from the secondary outlet ports for each flow split and fills the flow fraction array downstream of those ports. Lastly, the code checks if any of the pipe flow fractions remain unfilled. If so, an error message is provided to the user indicating that the code could not calculate all of the flow fractions, possibly resulting from a wrong assignment of pipe connections in the input (for example, if there is a closed loop not connected to the main cycle).

All of these checks and the flow fractions array fill are done in the read_data_CO2 subroutine following the reading of the input files for the cycle and all components. The flow fractions set here are fixed for the entire steady-state calculations, although the actual values for the flow rates will be changing during the iterations.

Next, the iterations on the working fluid conditions are carried out. These calculations are performed in the CO2_cycle subroutine. For these calculations, the flow rate in the system is known (the iterations on the flow rate are described in the next sections) and the performance of each component, in terms of the pressure drop (change) and temperature change (heat transfer) is either known from the previous iteration or is obtained from a first guess.
The Plant Dynamics Code has been developed for the analysis of supercritical cycles. These cycles usually operate with their cold end close to a critical point. Due to significant properties variations near the critical point, a special solution technique, described below, was developed to avoid as much as possible iterations on conditions close to those at the critical point. For this reason, the general approach in the PDC for cycle iterations is to start such iterations at the components located close to the critical point and then extend the solution to other cycle components.

The steady-state solver fills the pressure and temperature arrays in the following steps. For both pressure and temperature, each step progresses through the pipes and components and updates the pressure or temperature on the other end based on the current value and the known pressure or temperature change for that component or pipe from the previous iteration. The process continues unless a component specific to that particular step is encountered. Each step below is performed for all components meeting the criteria. For example, Step 1a is carried out for all compressors for which a minimum temperature is set in the input.

1a. **Pressures upstream from the compressors for which the minimum pressure was set in the input file** (see minimum pressure flag in Figure 2-21). This minimum pressure is usually set for the compressor operating closest to the critical point, so going upstream ensures that the pressure increases and moves away from the critical point. The process continues until a compressor or turbine is reached.

1b. **Pressures downstream from the compressors.** This step is carried out starting from the compressors for which the outlet pressure was specified in the input file and when the outlet pressure was not set in step 1a. The process continues until a turbine is reached. The compressor outlet pressure is usually far enough from the critical point so going downstream (in the direction of decreasing pressure) is not a concern from the point of view of maintaining supercritical conditions.

1c. **Pressures downstream from the turbines.** This step only fills the pressure points between turbines located in series. Otherwise, the turbine pressures are filled in steps 1a and 1b. The process starts from a turbine for which the outlet pressure is not set (if there is one) and continues until another turbine is reached.

1d. **Pressures downstream from the secondary outlet for splitters.** This process continues until a turbine, compressor, mixer, or another splitter is reached.

1e. **Pressures upstream from the secondary inlet for mixers.** This step is only performed if that pressure is not filled in any of the previous steps. The process continues until a turbine, compressor, or secondary outlet port for a splitter is reached.

After these steps are completed, it is checked that all pressures in the cycle are filled. If not, then the PDC will try to repeat Steps 1a-1e several times to see if that would resolve the issue. If that attempt is unsuccessful, a message “**Not all pressure nodes are filled**” will be displayed by the code and the execution will stop. If this happens, the user is advised to check the cycle
configuration and that all of the inputs, such as minimum pressure flags for compressors, are provided.

When the pressure array is completely filled, the code proceeds to filling out the temperature array. Again a step-wise approach is implemented with the following steps.

2a. *Temperatures upstream from the compressors for which the minimum temperature was set in the input file* (see minimum temperature flag in Figure 2-21). These compressors are required to have a cooler upstream which is used to meet this required minimum temperature. This process will continue until a cooler is reached and will set the target cooler-outlet temperature. The code will also check if any major component – turbine, compressor, or a heat exchanger – is reached before the cooler and will stop execution and provide a corresponding error message in this case. This means that only mixers and splits are allowed between a cooler and a compressor if the compressor’s minimum temperature is defined in the input. Again, this step will work in the direction of increasing temperature (either from pressure drop in a pipe or from hotter cooler bypass flow, if any is used) and thus will go away from the critical point.

2b. *Temperatures downstream from other components – HAHXs, turbines, compressors, recuperators, splits, mixers, and tanks*. For each component, the outlet temperature is calculated as described below which is then used to calculate the pressure at the other end of the connected pipe, from the pipe pressure drop and the heat loss. For heat exchangers, the outlet temperature is directly calculated by the HX performance subroutine. For turbines and compressors, the definition of the component efficiency is used to calculate outlet temperature. For splits and tanks, the outlet conditions are set to be equal to that at the inlet. And for a mixer, the outlet enthalpy is calculated based on the inlet enthalpies and flow fractions at the two inlet ports, while the pressure at the outlet port is equal to that at the primary inlet port. The outlet temperature is then calculated from pressure and enthalpy. More detailed descriptions of each component modeling is provided in the following sections of this chapter.

The pressure, temperatures, and flow rates for pipes are then used to calculate the pressure drop, heat loss, and wall temperatures for each pipe. In addition, if a specific pressure drop is set in the input for a valve, it is also added to the total pressure drop for the corresponding pipes.

When all temperatures and pressures in the cycle are calculated, the PDC checks if any of them exhibit a difference from the previous iteration larger than the required accuracy and repeats all the above steps until convergence is achieved.

After that, all other component performance characteristics are calculated, including heat transfer in the heat exchangers, turbines and compressors work, working fluid inventory, and so on. The turbomachinery power values are used then to calculate the net available power for each shaft, which are then added together to obtain the net power available from the cycle and the cycle efficiency.
As mentioned in the description of Step 2b, the PDC uses a turbomachinery efficiency value to calculate the component’s outlet temperature in cycle iterations. That efficiency value is obtained from either the design or performance subroutines described below. These subroutines usually require several layers of iterations on fluid properties, often close to the critical point. Therefore, these subroutines are relatively slow and for this reason calling these subroutines is not integrated in the cycle iteration to improve computational speed. Rather, the cycle-turbomachinery iterations are performed in two layers. First, the cycle conditions are calculated as described above using the value for the turbine or compressor efficiency. These calculations will define the conditions for turbomachinery design or performance. Then, the turbomachinery design or performance subroutines are used to re-calculate the efficiency of those components, and the iterations are continued in this fashion until convergence on turbine and compressor efficiencies is achieved.

The solution method described above is used by the PDC to obtain the working fluid conditions in the cycle, such as pressures and temperatures. For these calculations, the working fluid flow rate is assumed to be known. The solution approach to finding the flow rate depends on the input parameter “Type of turbomachinery calculations” defined in Figure 2-9 and described in Section 2.3.3.3. The detailed approach for finding the working fluid flow rate depending on the turbomachinery mode is described in the following two sections.

3.1.1.2 Iterations in Turbomachinery Design Mode

In the turbomachinery design mode, the PDC will “design” the turbines and compressors, meaning that it will calculate the required blade dimensions, angles, flow areas, etc. As part of these calculations, the turbine and compressor efficiencies are also calculated. The detailed description of the turbomachinery design approach in the PDC is provided in Section 3.1.4. The PDC designs the components to match the required conditions, including inlet and outlet pressures, inlet temperature, flow rate, and rotational speed, to obtain the dimensions and the working fluid speed. The rotational speed is defined in the input for the turbomachinery shaft. The inlet and outlet conditions are obtained from the PDC cycle calculations.

To obtain the flow rate for the cycle and turbomachinery design calculations, the PDC uses the HAHX performance subroutines. The HAHX hot side conditions, including the inlet/outlet temperatures and pressures and heat duty are provided in the input, along with the heat exchanger dimensions and design. From the inlet and outlet enthalpies and heat duty, the flow rate for the hot side fluid is calculated and is fixed for all further steady-state calculations. From the previous iteration of the cycle, the working (cold side) fluid conditions (temperature and pressure) at the HAHX inlet are known. The PDC then calls the HAHX performance subroutines and adjusts the working fluid flow rate to match the required hot-side HAHX-outlet temperature and, thus, heat duty of the HAHX (which is also the heat addition rate to the cycle).

In the process of the HAHX calculations, the working fluid outlet temperature and pressure drop are known. Those and the working fluid flow rate are supplied to the cycle calculation, which will again calculate the HAHX inlet conditions. This process is repeated until convergence on the HAHX conditions and the flow rate is obtained.
Once the cycle and flow rate iterations are completed, the PDC will call the turbomachinery design subroutines. These subroutines will calculate the outlet temperatures for turbines and compressors and their efficiencies. If needed, iteration on those and the cycle conditions are carried out until the entire system converges. The results from the final iteration are the PDC steady-state results reported to the user in the output files. These results also includes the design and performance at the design point of the cycle’s turbines and compressors.

Note that since in this mode the working fluid flow rate is calculated to match the conditions on the HAHX hot side, this mode requires a HAHX to be present and thus cannot be used with an electrical heater. For that component, the turbomachinery performance mode is required.

The turbomachinery design mode is recommended for the design and analysis of systems with known boundary conditions but some flexibility in the design. For example, it should be used for cycle design for the power conversion system for a nuclear power plant.

3.1.1.3 Iterations in Turbomachinery Performance Mode

In the turbomachinery performance mode, the turbine and compressor designs are given, i.e., provided in the input files. This means that the outlet conditions, including the outlet pressure, have to be calculated using the turbomachinery performance subroutines and therefore cannot be selected arbitrarily. Moreover, the flow rate in the system is established based on the head-flow characteristics of both the turbine and compressor and the pressure drops in other components and piping. When the designs of all components are defined, the flow rate in the system is found at the conditions such that the pressure ratio delivered by the compressor matches that of the rest of the cycle including the turbine. Those equilibrium conditions are schematically illustrated in Figure 3-2. The compressor pressure ratio decreases with increasing flow rate. For the turbine and the rest of the cycle, the pressure ratio is increasing with the flow rate. For example, the pressure drop in pipes and heat exchangers is roughly proportional to the square of the flow rate. The closed system will eventually find an equilibrium solution with the flow rate and pressure ratio matching both the compressor and system curves, as shown in Figure 3-2.
The internal cycle iterations described in Section 3.1.1.1 are repeated in this mode too with the turbomachinery efficiencies obtained from the performance (rather than design) subroutines. In the cycle calculation, the turbine-outlet pressure will be calculated from calculating the pressures upstream of the compressors. At the same time, the turbine-outlet pressure will also be calculated by the turbine performance subroutine. These two pressures, which should be equal, are reported to the PDC and are used to carry out iterations on the working fluid flow rate. The flow rate is changed until the difference between the two pressures is within the required convergence criteria. Effectively, this solution approach ensures that the cycle characteristics (including the turbine pressure ratio) matches the compressor characteristic in Figure 3-2.

Note that in this mode, the working fluid conditions at the HAHX or a heater, including inlet temperature and flow rate are calculated in the cycle. If the electrical heater option is used, the heater power will be used to calculate the heater-outlet temperature. Thus, the required heater power will automatically be preserved. However, if the HAHX option is used, the HX performance subroutine will calculate the working fluid outlet temperature. Since the flow rate and temperatures are already defined in the cycle, there is no guarantee that the heat addition rate will be preserved in these calculations. So, it is up to the user to monitor the results of the PDC calculations in this mode and adjust input parameters (e.g., HAHX hot-side conditions) to ensure that the required heat addition rate is preserved.

The turbomachinery performance mode is recommended for the systems with known design of all components, such as analysis of experiment loops.
3.1.2 Heat Exchangers

A heat exchanger is a component where heat is transferred from one fluid (hot side) to another fluid (cold side). In the PDC, there are three heat exchanger component classes, as presented in Table 3-1.

<table>
<thead>
<tr>
<th>Component Class</th>
<th>Heat Addition HX</th>
<th>Recuperator</th>
<th>Cooler</th>
</tr>
</thead>
<tbody>
<tr>
<td>Description</td>
<td>HX to add heat to the cycle</td>
<td>Heat transfer within the cycle</td>
<td>Heat rejection from the cycle</td>
</tr>
<tr>
<td>Hot side fluid</td>
<td>HAHX hot side fluid (user’s choice)</td>
<td>Cycle working fluid</td>
<td>Cycle working fluid</td>
</tr>
<tr>
<td>Cold side fluids</td>
<td>Cycle working fluid</td>
<td>Cycle working fluid</td>
<td>Cooling medium – water or air</td>
</tr>
<tr>
<td>Specific inputs</td>
<td>Hot side inlet/outlet conditions and heat duty</td>
<td>None</td>
<td>Cold side inlet conditions Target hot side outlet conditions are defined by cycle input</td>
</tr>
<tr>
<td>Steady-state solution</td>
<td>Cold-side fluid outlet temperature</td>
<td>Hot/cold side outlet conditions, heat transfer rate</td>
<td>Required HX size or cold side flow rate to match the target hot side outlet conditions</td>
</tr>
</tbody>
</table>

There are two major approaches to defining the heat exchangers in the PDC:

1. **General heat exchanger**, where a required heat exchanger performance in terms of the effectiveness and pressure drop is specified by the user. This type is only applicable to HAHXs and recuperators (i.e., not applicable to coolers) and is only available for the steady-state solution (i.e., cannot be used in dynamic calculations).

2. **Realistic heat exchanger**, where the user provides the heat exchanger dimensions and the code calculates the HX performance. This is the most common HX approach in the PDC and can be used for all heat exchangers in both steady-state and dynamic calculations.

The description of these two approaches is provided in the following sections.

3.1.2.1 General HX (Effectiveness Method)

For a general heat exchanger, the user only specifies the HX effectiveness and the pressure drops. The HX effectiveness definition used in the PDC is defined as the temperature change on each side as a fraction of maximum possible change, as shown in Figure 3-3. The maximum possible
temperature change is achieved when the outlet temperature on one side is equal to the inlet temperature on the other side. The effectiveness is calculated for both hot and cold sides and the maximum value is selected to represent the heat exchanger effectiveness.

When the “General” HX type is selected for a component, the input for the HX effectiveness is used by the PDC to calculate the outlet temperature for the side that limits the effectiveness. The outlet temperature on the other side is calculated to conserve the heat transfer rate on the two sides. The input for the pressure drops is used to calculate outlet pressures.

![Effectiveness formula](figure3_3.png)

Effectiveness = \( \text{max}\{\varepsilon_{\text{hot}}, \varepsilon_{\text{cold}}\} \)

For a HAHX, the user input is the HX effectiveness on the cold side (the hot side inlet/outlet temperatures are given). It is used to calculate the cold side outlet temperature. The inputs for the pressure drops are used to calculate outlet pressures on both sides. The user input for the total heat transfer rate is used to calculate flow rates on both sides. The flow rate value for the cold side is used as the working fluid flow rate in the cycle as described in Section 3.1.1.2.

For a recuperator, the effectiveness in Figure 3-3 is provided for the input. The code will calculate the outlet temperatures based on the effectiveness and the conservation of energy, while checking which side represents the limiting conditions for the effectiveness definition. The inputs for the pressure drops are used to calculate outlet pressures on both sides. The flow rates on both sides are defined by the cycle calculations. The inlet/outlet enthalpies and flow rates define the recuperator heat transfer rate.
The general heat exchanger type is not applicable to cooler, since the cooler needs to match the outlet conditions on the working fluid side, which are defined by the cycle input.

Also, this mode cannot be used in dynamic calculations since it lacks the required input needed for dynamic calculations, such as thermal inertia of the HX wall mass and the off-design performance of the HX.

3.1.2.2 Realistic HX – Solution Scheme

The realistic heat exchanger model is triggered by selecting any heat exchanger type other than General. In this model, the user selects the HX type (options are described below) and supplies the heat exchanger dimensions and internal configuration. The inlet conditions on the two sides, including temperature, pressure, and flow rate, are either supplied by the user directly in the input or obtained from the cycle calculations. The code then calculates the HX performance in terms of the outlet temperatures, outlet pressures (or pressure drops), heat transfer rate, and the HX effectiveness.

The detailed description of the PDC heat exchanger model for the steady-state calculations is provided in Reference [2] which is available on the internet. To account for the fluid properties variations, the heat exchanger is divided into multiple nodes along the heat exchanger length (Figure 3-4). The heat transfer equations are solved for each node assuming that the properties are constant in that node. A special matrix-based solution scheme for the heat exchanger was developed for the PDC [2] which simultaneously solves the equations in all nodes to find the outlet conditions and the properties distribution along the HX length. Iterations are then implemented to converge between the fluid properties, heat transfer rates, and pressure drops in all nodes.

![Figure 3-4. Multi-Node Solution Approach for Heat Exchangers.](image-url)
The general heat transfer equation in the PDC heat exchangers relates the heat transfer rate (per unit length) with the temperature difference and the total thermal resistance between the hot and the cold sides:

\[ q'(z) = \frac{T_h(z) - T_c(z)}{res_h + res_w + res_c}, \tag{3.1} \]

where \(res_h\), \(res_w\), and \(res_c\) = thermal resistances on the hot side, wall, and the cold side, respectively. These resistances are calculated based on the heat exchanger type as described in the following sections of this report.

The above equation is combined with the energy conservation equation to complete the system of equations to be solved:

\[ -\dot{m}_h dh_h = q'(z)dz = \dot{m}_c dh_c. \tag{3.2} \]

Reference [2] provides the detailed description of how the above equations are solved in the PDC to obtain the temperatures on the two sides at each node. Recently, the PDC HX equations where extended to include the effects of the pressure drop on the temperature change, which is not considered in Reference [2]. The approach is still the same, with the addition of a constant term in all of the equations, which represents the partial derivative of enthalpy with respect to pressure at constant temperature:

\[ dh = c_p dT + \left(\frac{\partial h}{\partial p}\right)_T dp. \tag{3.3} \]

That partial derivative of enthalpy with respect to pressure is calculated from the fluid properties formulation and is assumed to be fixed for each node. For some fluids, such as ideal gasses and some liquid metals the partial derivative could be zero, such that the effect of the pressure drop on the temperature equations is not needed. However, the general formulation of the heat transfer equations solved by the PDC for each heat exchanger node are:

\[
\begin{align*}
\frac{dT_h}{dz} &= -\frac{1}{\dot{m}_hc_{p,h}} \frac{T_h(z) - T_c(z)}{res_h + res_w + res_c} - \frac{\left(\frac{\partial h}{\partial p}\right)_T}{c_{p,h}} \frac{\Delta p_h}{\Delta z} \\
\frac{dT_c}{dz} &= \frac{1}{\dot{m}_cc_{p,c}} \frac{T_h(z) - T_c(z)}{res_h + res_w + res_c} - \frac{\left(\frac{\partial h}{\partial p}\right)_T}{c_{p,c}} \frac{\Delta p_c}{\Delta z};
\end{align*} \tag{3.4}
\]

where \(\Delta p_h\) and \(\Delta p_c\)= pressure drop over region of node length, \(\Delta z\), on hot and cold sides, respectively.

The wall temperature in each node is calculated as the mid-wall temperature based on the conservation of the heat transfer rate between hot side and the wall and the wall and the cold side:
\[
\frac{\bar{T}_h - T_w}{\text{res}_h + \text{res}_w/2} = \frac{T_w - \bar{T}_c}{\text{res}_w/2 + \text{res}_c},
\] 

(3.5)

where \(\bar{T}_h\) and \(\bar{T}_c\) = node-average temperatures on the hot and cold sides, respectively.

The number of the axial nodes for the HX solution is a user choice provided in the input. More nodes increase the accuracy of the solution by more accurately accounting for the properties variations, but increase the computational time, especially for the dynamic calculations. At least several nodes are required for heat exchangers operating close to the critical point to avoid issues such as the development of a pinch point inside the heat exchanger.

### 3.1.2.3 Shell and Tube Heat Exchanger

The shell-and-tube heat exchanger consists of a cylindrical vessel (shell) and straight tubes inside it. One flow is inside of the tubes, while the other flow is outside the tubes on the shell side. Which flow is on the tube side is a user input in the PDC. The flow is assumed to be counter-flow, meaning that the flows on the tube and shell sides go in opposite directions.

The tube can have longitudinal fins (i.e., fins along the tube length) on the inside or outside tube surface to increase the heat transfer area. The number of fins on each side and the fin dimensions are a user input. The fins increase the surface area. However, since the fin temperature is usually less than that of the tube, a concept of the fin and total surface area efficiency \[3\] is used to account for how effective the fins are in increasing the heat transfer to/from the tube. The fin efficiency equations along with the fin dimensions are provided in Figure 3-5.

For the shell-and-tube heat exchanger, the thermal resistances on the tube and shell sides and the tube wall for the heat transfer equations in Section 3.1.2.2 are defined as:

\[
\text{res}_\text{fluid} = \frac{1}{h \cdot \text{WP} \cdot \eta};
\] 

(3.6)

\[
\text{res}_w = \frac{\ln(D_o/D_i)}{2\pi k_w};
\] 

(3.7)

where

- \(h\) = heat transfer coefficient = \(Nu \frac{D}{k_{\text{fluid}}}\),
- \(\text{WP}\) = wetted perimeter (surface area per unit length),
- \(\eta\) = total surface efficiency from Figure 3-5,
- \(D_o, D_i\) = outer and inner tube diameters, respectively,
- \(k_w\) = tube wall thermal conductivity,
- \(Nu\) = Nusselt number,
- \(D\) = corresponding diameter,
- \(k_{\text{fluid}}\) = fluid thermal conductivity.
Figure 3-5. Fins and Their Efficiency in Shell-and-Tube Heat Exchanger.

Total surface efficiency
\[ \eta = 1 - \frac{a_f}{a} \left( 1 - \eta_f \right) \]

Fin efficiency
\[ \eta_f = \frac{\tanh(ml)}{ml} \]

\[ a_f = N_f (2l + \delta)L \]

\[ a = a_f + (\pi D - N_f \delta)L \]

\[ m = \frac{hP}{kA} \]

\[ P = 2(L + \delta) \quad A = L\delta \]

\[ \frac{a_f}{a} = \frac{N_f (2l + \delta)}{\pi D + N_f 2l} \]

\[ \frac{P}{A} = \frac{2(L + \delta)}{L\delta} = \frac{2}{\delta} + \frac{2}{L} \approx \frac{2}{\delta} \quad (\delta \ll L) \]

\[ D = \begin{cases} D_o & \text{for outer surface} \\ D_i & \text{for inner surface} \end{cases} \]

\[ m = \frac{2h}{k\delta} \]
In the PDC shell-and-tube heat exchanger model, there is no heat transfer between the shell side fluid and the shell. The active tube length for the heat transfer is assumed to be equal to the total length of the heat exchanger.

The shell side of a heat exchanger can contain baffle plates as shown in Figure 3-6. The plates can cover the full or a fraction of the shell cross-sectional area, as defined by the baffle cut input. The baffle plates can also have flow holes.

In the PDC heat exchanger model, the baffle plates are assumed to affect the pressure drop (friction factor) only and have no effect on the heat transfer. In particular, a purely counter-flow configuration is still modeled even in the presence of the baffle plates. A model previously developed by ANL [4] for the analysis of sodium heat exchangers was adopted in PDC to include the effects of the baffle plates on the shell side pressure drop.

![Figure 3-6. Shell-and-Tube Heat Exchanger Baffle Plates.](image)

3.1.2.4 Printed Circuit Heat Exchanger (PCHE)

The Printed Circuit Heat Exchanger (PCHE) model in the PDC simulates a compact diffusion-bonded heat exchanger. This heat exchanger was originally developed by Heatric Division of Meggitt (UK), Ltd. [5] under the PCHE name. Since then, several other manufacturers have developed their own versions of diffusion-bonded heat exchangers with various names. Since the designs of these heat exchangers are similar, they can all be modeled with the PDC model described in this section. However, for historical reasons, this model still uses the “PCHE” name in the PDC and thus will be used in this report.

A PCHE is fabricated from a stack of several or more metallic plates. Each plate has semicircular channels chemically etched on one side. The plates are bonded together, forming a metal cube with semicircular channels inside it. The hot and cold-side fluids flow inside these channels in counter-current directions (Figure 3-7). This technology makes it possible to have very small channels (as small as 0.5 mm in diameter) to increase the heat transfer area making these heat exchangers much more compact than shell-and-tube HXs.
The PCHE channels can be either straight or zigzagged. A zigzagged channel configuration with the definition of the channel angle ($\alpha$) used in the PDC is shown in Figure 3-8. The figure also shows the ratio between the channel length and the HX heat transfer section length. For a straight channel, the zigzag angle is zero and the channel and heat transfer region lengths are identical. PCHE technology allows different channel angles on the two sides of the HX, including any combination of zigzagged and straight channels. Also, the plate thicknesses, channel dimensions, and channel pitches can be different on the two sides. That means that the number of channels on the two sides is not necessarily the same and the individual channels on the hot and cold sides do not necessarily align with each other.
To account for the zigzagged geometry and different number of channels on both sides, the following approach is implemented in the PDC for the PCHE model. The model solves the heat transfer equations on a whole-plate basis. That is, the heat transfer region is divided into several regions along its length and the solution is obtained for the total flow through the whole plate (instead of the flow through each individual channel). This way there is always one hot channel (hot plate) per one cold channel (cold plate). The plates are considered as flat plates with zigzagged fins between them. Figure 3-9 demonstrates how the plates with etched channels are represented by flat plates with fins to be used in the model.

The interpretation of the geometry as plates with fins requires utilization of a fin efficiency for heat transfer. According to Figure 3-9, the fins have a cross section that is variable with height such that the exact calculation of their efficiency is complicated. Instead, the fin efficiency is an input parameter for the PCHE HX type as shown in Figure 2-12, for example.
The heat transfer rate per HX unit length for the plate geometry with fins is defined as:

\[
q' = \frac{T_{\text{hot}} - T_{\text{cold}}}{1 + \frac{1}{t} \left( \frac{h_{\text{hot}} HTP_{\text{hot}} \eta_{\text{hot}}}{k_w HTP_{w}^{+}} + \frac{1}{h_{\text{cold}} HTP_{\text{cold}} \eta_{\text{cold}}} \right)}, \tag{3.8}
\]

where

- \( h \) = heat transfer coefficient,
- \( HTP \) = heat transfer perimeter (see below),
- \( \eta \) = heat transfer surface (fin) efficiency,
- \( t \) = (flat) plate thickness,
- \( k_w \) = plate thermal conductivity.

The heat transfer perimeter is a heat transfer surface area per unit length. Since the solution is obtained per HX unit length for the whole plate, the heat transfer perimeter accounts for channel length and the number of channels per plate (Figure 3-8):

\[
HTP = \frac{A}{L} = \frac{P_{ch} \cdot 2l \cdot N_{ch}^{nl}}{\lambda} = \frac{(\pi/2 + 1) \cdot d \cdot N_{ch}^{nl}}{\cos(\alpha/2)}. \tag{3.9}
\]

The flow parameters, like Reynolds number, are still calculated based on the flow through an individual channel.

The PDC supports two PCHE configurations: platelet and Z/I configuration.

**Platelet PCHE**

In the platelet configuration, shown in Figure 3-10, the flow distribution and collection headers are integrated within the plates. This design allows for a relatively short flow distribution region, such that more heat exchanger length is available for the counter-flow channel region. Because of this feature, this PCHE configuration tends to produces higher-effectiveness heat exchangers than other configurations. Since the flow distribution regions are relatively short, they are ignored in the PDC heat transfer calculations, which allows application of purely counter-flow equations to the entire heat exchanger. The pressure drop in the distribution regions and the headers is accounted for through a user input parameter that specifies what fraction of the total heat exchanger pressure drop comes from the channels.

To account for the headers and flow distribution regions within the plates, one of the PDC inputs for the platelet PCHE is the “header length,” which, is shown in Figure 3-10 as \( L_h \), actually combines all the regions other than the flow channel on one side of the heat exchanger. The active heat transfer region length is then calculated in the PDC as the total HX length minus two times that input for header length.
Z/I PCHE

The other option for the PCHE in the PDC is the Z/I configuration. That PCHE configuration employs a Z-shaped flow path on one side and an I-shaped path on the other side, as shown in Figure 3-11. On the “I” side of the HX, the flow channels start on one end of the plates and end on the opposite end. On the “Z” side, the channels start on a side of the heat exchanger, go first perpendicular to the channels on the other side, then make a turn to form the counter-flow region, then turn again to end on the other side of the plate. This configuration simplifies the plate design by allowing the headers to be external to the fabricated heat exchanger core block. At the same time, it requires a relatively large area of cross-flow, which is less effective in heat transfer than the counter-flow configuration.

The main difference between the PDC’s Z/I PCHE model and the previously described PCHE model is the effect of the crossflow region. The flow configuration and major dimensions of the Z/I configuration are shown in Figure 3-12. Note that the flow lines in Figure 3-12 represent generally zigzagged channels. Away from the crossflow regions at each end of the heat
exchanger, the configuration is purely counter-flow such that the PCHE model described above for counter-flow heat transfer is still applicable.

![Figure 3-12. Z/I PCHE Flow Paths and Dimensions.](image)

For the counter-flow region, an analysis is carried out based upon an average channel. The average channels are those in the middle of the heat exchanger (marked by thick arrows in Figure 3-12). It follows from the geometric considerations in Figure 3-12 that the crossflow region length based on the average channel is

\[ L_{cf} = \frac{W_{HX} - w_{land}}{2}, \]  

(3.10)

where

- \( W_{HX} \) = width of the block,
- \( w_{land} \) = thickness of “land”, i.e. the region at the edges without channels.

The length of the counter-flow region is equal to \( L_{HX} - 2L_{cf} \).

Note that the length of the crossflow region is the same on both Z and I sides.

To account for heat transfer in the crossflow region, an effectiveness number of transfer units (\( \varepsilon \)-Ntu) approach is implemented [6]. Under this approach, both fluids are assumed to have constant thermophysical and transport properties. Thus, the heat transfer properties (i.e., thermal resistances) for the two fluids and the wall are constant for the entire crossflow region. The heat transfer in the cross flow region is calculated as follows,

\[ Q = \varepsilon \cdot Q_{\text{max}}, \]  

(3.11)

where
\( \varepsilon = \) crossflow region effectiveness,
\( Q_{\text{max}} = \) maximum possible heat transfer rate.

The maximum heat transfer rate is calculated as

\[
Q_{\text{max}} = C_{\text{min}} (T_{h,i} - T_{c,i}),
\]

where

\[
C_{\text{min}} = \min\{C_h, C_c\},
\]

\[
C_h \equiv \dot{m}_h \cdot c_{p,h}, \quad C_c \equiv \dot{m}_c \cdot c_{p,c}
\]

\( \dot{m}_h, \dot{m}_c = \) mass flowrates on hot and cold sides,

\( c_{p,h}, c_{p,c} = \) average specific heats on hot and cold sides,

\( T_{h,i}, T_{c,i} = \) inlet temperatures on hot and cold sides.

The effectiveness of the crossflow region is calculated based on the Ntu parameter using the approximation from Kays and Crawford [6],

\[
\varepsilon = 1 - \exp\left\{\exp\left( -Ntu^{0.78}C^* \right) - 1 \right\} Ntu^{0.22}/C^*,
\]

where

\[
Ntu = \frac{UA}{C_{\text{min}}} = \text{number of transfer units},
\]

\( C^* = \frac{C_{\text{min}}}{C_{\text{max}}} \),

\( C_{\text{max}} = \max\{C_h, C_c\} \),

\( U = \) total heat transfer coefficient,

\( A_s = \) total surface area of the cross flow region.

It is assumed in the model that the average thermal resistance of the heat transfer area is equal to the thermal resistance per unit length calculated for the nearest counter-flow region (either first or last node) times the crossflow region length. It is also assumed that the flow geometry (channel diameter, zigzag angle, etc.) in the crossflow region is the same as in the counter-flow region.

\[
UA_s = H \cdot P \cdot L_{cf},
\]

where

\( H = \) total heat transfer coefficient based on the thermal resistance of the two fluids and the wall,

\( P = \) total perimeter of all channels on one side.
To account for the pressure drop and still conserve energy, the average specific heats are calculated as:

$$c_{p,h} = \frac{\Delta h_h}{\Delta T_h} = \frac{h_{h,i} - h_{h,o}}{T_{h,i} - T_{h,o}}.$$  \hspace{1cm} (3.15)

The inlet temperature for the crossflow region is either the heat exchanger inlet temperature or the outlet temperature from the two counter-flow regions (Figure 3-12). Since the temperature change in the crossflow region provides the inlet conditions for the counter-flow region, and vice versa, iterations are implemented to find the converged solution.

To calculate the pressure drop in the crossflow region, the value of the pressure drop per unit length calculated in the nearest counter-flow region is multiplied by the crossflow region length:

$$\Delta p_{cf} = \frac{\partial p}{\partial z_{1orN}} L_{cf},$$  \hspace{1cm} (3.16)

where

$$\frac{\partial p}{\partial z_{1orN}} = \text{pressure drop per unit length calculated for the first or last counter-flow node.}$$

Because the crossflow model relies on the e-Ntu method, it can only be used for finding a steady-state solution. For this reason, the Z/I PCHE is not supported by the PDC dynamic model. Instead, a user needs to create an equivalent platelet PCHE design for dynamic calculations. The simplest approach to finding equivalent platelet design is the following:

- Run steady-state calculations with the Z/I PCHE, record its performance in terms of heat transfer and pressure drop,
- Change the heat exchanger type to “Platelet PCHE,”
- Keep all the inputs, including HX dimensions the same,
- Adjust the header length (see Figure 3-10 – the input only used by platelet PCHE) to obtain the same performance as the original Z/I PCHE,
- If satisfactory agreement on both heat transfer and pressure drop could not be obtained with above steps, other HX inputs, such as HX length can be modified together with the header length to improve the agreement.

**Formed Plate PCHE**

All of the discussion in this section has so far assumed “classical” PCHE plates with semi-circular channels. However, the PDC also supports a formed plate PCHE design where the channels are formed by the addition of corrugated plates and un-etched flat plates. Figure 3-13 shows an example of the heat exchanger where such a formed plate is located between two “classical” PCHE plates.
Figure 3-13 also shows what inputs are required for the PDC model. For the formed plate design, both the channel width and the channel depth need to be provided independently. For a "classical" PCHE design, only the channel diameter is needed since the channel depth is assumed to be equal to the channel radius (i.e., ½ of the channel diameter). Since the channel depth is not needed for the PCHE design, that option is triggered in the PDC if the user specifies “0” for input (see, for example, Figure 2-12). For the platelet design (i.e., when channel depth ≠ 0), the input for the pitch-to-diameter ratio is used to calculate the thickness of the formed plate [= (PDR-1)*channel width], while the input for the “plate thickness” is used to calculate the thickness of the separating plate [= plate thickness – channel depth – formed plate thickness], as can be seen from Figure 3-13.

Special heat transfer and pressure drop correlations have been developed for the PDC PCHE models. Those correlations are provided in Section 3.4.1.2.

3.1.2.5 Cooler

The PDC cooler model is similar to the other heat exchanger models described above in many aspects, including the choice of the shell-and-tube and PCHE HX type options and general scheme for the steady-state solution. At the same time, there are specifics of the cooler model, which are described in this section.

As shown in Table 3-1, the hot side inlet and outlet conditions for the cooler are known from the cycle calculations. Therefore, the main goal of the cooler module is not to find the outlet conditions (at least, on the hot side), but is rather to find either the cooler design or the cold side conditions (flow rate) that would meet the target cooler performance on the hot side. That difference is solution target and is also described in Table 3-1. For this reason, the internal
iterations inside the cooler subroutine are organized to iterate on these parameters, - HX length, number of units, or cooling medium flow rate, which is the user’s choice in the input.

The target parameter for these iterations is also different for the cooler than for other heat exchangers. The PDC has been developed for analysis of supercritical cycles, where the cooler outlet is usually located close to the working fluid critical point. Because of significant properties variations at this location, the PDC is designed to avoid any iterations on the cooler-outlet conditions on the hot side. Instead, all the iterations for the cooler start at the hot-side outlet (cold end) and proceed to the hot end. This way, the solution scheme always moves away from the critical point. The calculations proceed to find the conditions on the hot end, which would be the hot-side inlet and the cold-side outlet. Then, the parameter on which the iterations are carried out is adjusted to match that calculated hot-side inlet conditions (temperature) to that obtained from the cycle calculations. Other than that difference, the solution approach is similar to that described in Section 3.1.2.2.

The PDC cooler model has been developed to include heat removal by air. It was found [7,8] that for this application, a counter-flow configuration may not be the best choice and crossflow designs may work better. For this reason, the PDC cooler model also includes the choice of the crossflow heat exchanger types and the solution scheme specifically developed for crossflow HX configurations. These cooler-specific model and the heat exchanger options are described below.

3.1.2.6 Crossflow Heat Exchangers for Cooler

The main difference between the crossflow and counter-flow heat exchangers is that the former has necessarily a two-dimensional temperature field, as demonstrated in Figure 3-14. As two fluids flow in perpendicular directions, fluids in parallel channels will “see” opposite side fluids of different temperature. For example, in Figure 3-14, the hot fluid in the top channel is in contact with the warmer cold side fluid near the exit of the heat exchanger, while the hot side fluid in the bottom channel will “see” much colder cold side fluid at the entrance of the heat exchanger. Therefore, the amount of heat transfer, which is proportional to the temperature difference between the two fluids, will not be the same for the parallel hot side channels. Therefore, the temperature change in the hot side fluid will be less in the top channel, compared to the bottom channel, which is schematically illustrated by arbitrary temperature changes in hot side channels in Figure 3-14.

In a similar fashion, the left-most cold side flow in Figure 3-14 will “see” colder hot side flow than the right-most channel, leading to smaller temperature rises and lower temperatures in that flow, compared to all other channels. Therefore, in a crossflow heat exchanger, a two-dimensional temperature field will always exist where the fluid temperatures are different both along the channel (or tube) length as well as between the channels (tubes).
Because of the two-dimensional temperature field, the solution approach for a crossflow heat exchanger must be different from that adopted previously for counter-flow heat exchanger. The first obvious difference is that two-dimensional temperature arrays need to be stored for heat transfer and properties calculations inside the heat exchanger. For the cooler application for supercritical cycles, this consideration is important since in order to track the hot side property changes, many axial nodes are required. If the same accuracy is retained for the crossflow heat exchanger, the total number of nodes would increase by a factor equal to the number of vertical nodes, leading to a proportional increase in properties calculations. In addition, in other HX calculations, a fast-running solution algorithm was developed (see Section 3.1.2.2) where once the fluid properties in each axial region are calculated, the heat transfer equations were solved simultaneously for the entire length of the heat exchangers using an analytical solution in each region. That approach could not be retained for the crossflow heat exchangers because it will require finding an analytical solution for the two-dimensional temperature field, which is much more complicated. Instead, the solution of temperature field needs to be found in each heat transfer region, shown in Figure 3-14, and then the iterations need to be done in calculating how heat transfer in each region affects the conditions and heat transfer in other locations downstream that particular region in both flow directions.

Other than those differences, the solution to the heat transfer equations is similar to that implemented previously for a counter-flow heat exchanger. The amount of heat transfer between the two fluids is defined by the temperature difference between the fluids and overall heat transfer coefficient for that region, while the same amount of heat transfer affects the temperature (or
enthalpy) change in each region for both fluids. For example, considering the heat transfer region in Figure 3-14, the heat transfer equations are formulated as:

\[ Q_{i,j} = H S_{i,j} (\bar{T}_{\text{hot}} - \bar{T}_{\text{cold}}); \]

\[ \dot{m}_{\text{hot}} (h_{\text{hot}}^{i,j} - h_{\text{hot}}^{i+1,j}) = Q_{i,j} = \dot{m}_{\text{cold}} (h_{\text{cold}}^{i,j} - h_{\text{cold}}^{i,j}); \]  

where

\[ Q_{i,j} = \text{heat transfer in region [i,j], W}, \]
\[ H S_{i,j} = \text{overall heat transfer coefficient times area for region [i,j], W/K}, \]
\[ \bar{T}_{\text{hot}} = \frac{T_{\text{hot}}^{i,j} + T_{\text{hot}}^{i+1,j}}{2} = \text{average hot side temperature in region [i,j], K}, \]
\[ \bar{T}_{\text{cold}} = \frac{T_{\text{cold}}^{i,j} + T_{\text{cold}}^{i+1,j}}{2} = \text{average cold side temperature in region [i,j], K}, \]
\[ T_{\text{hot}}^{i,j}, T_{\text{cold}}^{i,j} = \text{hot and cold side temperatures at node (i,j), respectively, K}, \]
\[ \dot{m}_{\text{hot}}, \dot{m}_{\text{cold}} = \text{hot and cold side flow rates in region [i,j], respectively, kg/s}, \]
\[ h_{\text{hot}}^{i,j}, h_{\text{cold}}^{i,j} = \text{hot and cold side enthalpies at node (i,j), respectively, J/kg-K}. \]

The overall heat transfer coefficient is defined through the total thermal resistance on the hot and cold side and the resistance of the wall:

\[ H S_{i,j} = \frac{1}{r e_{i,j}} = \frac{1}{r e_{h}^{i,j} + r e_{c}^{i,j} + r e_{w}^{i,j}}, \]  

while the resistance on each side is calculated through the heat transfer coefficient (HTC), surface area (S), and surface area efficiency (\( \eta \)) on that side:

\[ \frac{1}{r e_{h}^{i,j}} = H T C_{h}^{i,j} S_{h}^{i,j} \eta_{h}^{i,j}; \]

\[ \frac{1}{r e_{c}^{i,j}} = H T C_{c}^{i,j} S_{c}^{i,j} \eta_{c}^{i,j}. \]  

The wall thermal resistance depends on the surface geometry. For a round tube, it is equal to:

\[ r e_{w}^{i,j} = \ln \left( \frac{d_{o}}{d_{i}} \right) \frac{d_{i}}{2 \pi k_{w}^{i,j} \Delta l_{i,j}}, \]  

where

\( d_{o}, d_{i} = \text{outer and inner tube diameters, respectively, m}, \)
\( k_{w}^{i,j} = \text{average wall thermal conductivity in region [i,j], W/m-K}, \)
\[ \Delta l_{i,j} = \text{tube length in region } [i,j], \text{ m.} \]

In addition to the heat transfer equations above, the pressure drops are calculated in region \([i,j]\) for both fluids. Those pressure drops are used to calculate the pressure change in the node and, eventually, to relate the enthalpy change with the temperature change in the region to complete the heat transfer equations above.

The heat transfer equations above are solved in the code in an iterative fashion. First, based on the temperatures from previous iterations, the heat transfer coefficients and the amount of heat transfer are calculated for each region, along with the pressure drop. Then, the amount of heat transfer is used to re-calculate temperatures in each node, starting from inlet nodes.

The PDC crossflow cooler model makes an assumption of uniform flow distribution between the tubes (channels). In reality, though, common inlet and outlet pressures of the headers and different temperatures (densities) for each channel would mean that the flow rates should be different to provide the same pressure drop for all tubes. To avoid an additional layer of iterations to calculate flow re-distribution, an assumption of uniform flow distribution is made in the crossflow heat exchanger model. Under this assumption, the flow rates are assumed to be the same for all channels and the calculations proceed independently to obtain outlet pressures for each channel. Then, the channel-outlet pressures are averaged to obtain a common outlet pressure at the header pressure. This assumption is partially justified by the fact that differences in pressure drops are not that large. In one of the cooler calculations, it was found that the pressure drop on the hot side varied from 4.789 kPa to 4.892 kPa between the channels under a uniform-flow assumption, i.e., the difference in pressure drops was only about 2%.

Another assumption implemented in the code is no intermixing between the air flows. In the finned tube designs described below, there would always be a space between the tube fins, such that there would be some air flow along the tubes, rather than across the tubes. It is believed, though, that the air flow rate along the tubes and air intermixing would be small compared to the air flow across the tubes, such that these effects can be ignored.

A user should expect that calculations with a crossflow cooler would be noticeably slower than those of the other heat exchanger types. There are several reasons for that. The first obvious reason is that the two-dimensional temperature field needs more computational nodes and thus more calculations for fluid properties. Second, with crossflow, an analytical solution cannot be obtained (or is difficult to obtain) for the entire heat exchanger. Therefore, iterations need to be implemented to solve for heat transfer in one region before starting calculations in another region. These iterations have been shown to be prone to temperature cross-over, a condition where too much heat transfer in a node can result in the outlet temperature for a hot flow, for example, to drop below the cold-side temperatures in iterations. This issue is especially important for a cooler model due to properties variations close to the critical point. Also, because of the unavoidable temperature variation at the outlet on each side (see Figure 3-14), the cooler calculations could not start at the cooler hot-side outlet and move away from the critical point. Rather the calculations need to start at the inlet and approach the critical point, which requires more cautious iterations. For these reasons, limits on how much each parameter can change in one iteration are
implemented in the PDC cooler model, further slowing down calculations of crossflow cooler modules.

There is another aspect of the crossflow heat exchanger which has the potential to complicate the calculations even further. As mentioned in the previous paragraph, a non-uniform temperature distribution results in different pressure conditions between the parallel channels on both sides.

**Finned Tube Crossflow Heat Exchanger**

The schematic illustration of a finned tube heat exchanger is shown in Figure 3-15. For this air-cooler application, the hot-side fluid (CO₂ in Figure 3-15) flows inside of the horizontal tubes, while the air flow is vertical, from bottom to top, across the tubes, driven by air fans. The tubes have transverse fins on the outside (air) surface. The hot side flow arrangement can be either single-pass or multi-pass; the example in Figure 3-15 shows a three-pass arrangement, where the tubes are divided into three groups and the hot side flow goes three times across the heat exchanger. The advantage of a multi-pass arrangement is that it increases the hot side flow rate per tube, thus increasing the Reynolds number and the heat transfer coefficient. This is achieved, though, at the expense of higher pressure drop on the hot side; therefore, there would always be a trade-off between cycle efficiency (affected by the side pressure drop in the cooler) and cooler thermal performance and cost. The multi-pass arrangement can be implemented either in headers (as shown in Figure 3-15) or in tubes, where individual tubes will be connected by U-sections.

Figure 3-15 shows four rows of tubes in the air flow direction. This is again a design choice affecting the heat exchanger size (foot print) and the air side pressure drop. The tubes can be either in a triangular lattice (as shown in Figure 3-15) or in a square lattice, where the tubes will be located directly above the previous row.

![Figure 3-15. Finned Tube Crossflow Heat Exchanger.](image)
The solution approach for the finned tube heat exchanger is based on the concept described above. The hot side channels in Figure 3-14 are the tubes in one vertical section; the number of tubes is equal to the number of tube rows \((N_{\text{row}})\) – four for the design in Figure 3-15. There are \(N_{\text{row}} + 1\) vertical nodes on the air side. This means that hot side conditions inside a tube and air conditions outside a tube are resolved for each tube. It is assumed that all parallel tubes in one pass are identical from a heat transfer point of view, so the solution is obtained for one vertical stack of tubes. The number of nodes in the direction of the hot side flow should be determined by the user based on a trade-off between the required accuracy for properties and computational time.

As mentioned above, the tubes can be arranged either in a triangular or square lattice, as shown in Figure 3-16. In Figure 3-16,

\[
\begin{align*}
d_f & = \text{fin outer diameter}, \\
d_t & = \text{tube outer diameter}, \\
p_v & = \text{tube lattice vertical pitch}, \\
p_h & = \text{tube lattice horizontal pitch}.
\end{align*}
\]

![Figure 3-16. Tube Lattices: Triangular (Left) and Square (Right).](image)

In the calculations, the off-centered arrangement of a triangular lattice is ignored; instead, it is assumed that tubes are located directly above each other, as in the square lattice. However, both the horizontal and vertical tube pitches in Figure 3-16 are input to the code (as pitch-to-diameter ratios), so the flow path length (height) on the air side is correctly accounted for in both the triangular and square lattices.

To calculate the multi-pass arrangement on the hot side, the following approach is taken in the code (see Figure 3-17). In the modeled heat exchanger (top of Figure 3-17, a three-pass example is shown), the hot side flow goes multiple times through the HX tubes. On the air side, though, the flows and temperatures for each tube are independent of each other. Also, each pass “sees” the same air inlet temperature. These facts mean that there are basically multiple heat exchangers,
located in series, as demonstrated at the bottom of Figure 3-17. Except for the hot side inlet conditions to each section, there is no other connection between these heat exchangers.

![Diagram of multi-pass heat exchanger with separate headers and U-tube sections.]

**Figure 3-17. Treatment of Multi-Pass HX with Separate HXs.**

Therefore, in the code, a multiple-pass heat exchanger is treated as a series of multiple heat exchangers. The number of tubes in each heat exchanger is equal to the number of tubes in each pass (1/3 of total number of tubes for the three-pass example in Figure 3-17). The inlet conditions on the air side are the same for all heat exchangers. The hot side conditions at the first HX (first pass) inlet are the same as the given hot side inlet conditions. When the calculations for the first HX are completed, the hot side outlet conditions for that HX are calculated. If the input specifies that pass connections are done in U-tube sections, those outlet conditions are transferred directly, tube-by-tube, to the inlet of the next heat exchanger (possible temperature and pressure changes in the U-sections of the tubes are ignored). In the case where the connection is implemented in headers, the outlet conditions from all tubes are combined to find the average conditions for this header. This averaging is done for the pressure (as discussed in the assumptions on page 108) and for the enthalpy to preserve energy. The enthalpy-pressure pair is then used to define the rest of the hot side properties in that header, which are used as the inlet conditions for the next HX section. These calculations are repeated for all passes. The outlet conditions at the last heat exchanger are always averaged to calculate the hot side conditions at the heat exchanger outlet header. The air outlet conditions from all nodes in all heat exchanger sections are averaged (again, based on enthalpy-pressure averaging) to calculate the overall air outlet pressure and temperature.

To determine the heat transfer and pressure drop in the finned tube cross-flow heat exchanger, some geometric parameters must be defined, including the flow area, surface area, heat transfer
perimeter (surface area per unit length), hydraulic diameter, etc. The definitions of these parameters for the air side are discussed first.

When the air flows across the finned tubes, the free flow area varies. Depending on how the heat transfer and pressure drop correlations are developed, the air-side flow area can be defined differently. For the correlations currently adopted in the PDC, the air-side flow area is defined as the minimum free flow area when the air goes across the finned tube bank (and correspondingly the local air velocity will be the maximum). Specifically, it is defined as:

\[
A_{c,a} = \left[ (p_h - d_{t,o})L_t - (d_f - d_{t,o})t_f N_f \right] N_c ,
\]

where

- \( A_{c,a} \) = air-side flow area, m\(^2\),
- \( p_h \) = horizontal tube pitch, m,
- \( d_{t,o} \) = tube outer diameter, m,
- \( L_t \) = tube length, m,
- \( d_f \) = fin diameter, m,
- \( t_f \) = fin thickness, m
- \( N_f \) = number of fins per tube,
- \( L_t \) = tube length, m,
- \( N_c \) = number of tube columns (number of tubes per row).

The air-side surface area (heat transfer area) includes that for both the fins and the bare tubes, and is defined as:

\[
A_a = \left[ \pi d_{t,o} \left( L_t - t_f N_f \right) + \frac{\pi}{2} \left( d_f^2 - d_{t,o}^2 \right) \right] N_c N_r ,
\]

where

- \( A_a \) = air-side surface area, m\(^2\),
- \( N_r \) = number of tube rows.

It should be noted that the circumferential surface of the fins have been ignored in the above definition. The main reason is that the fins are touching with each other in some designs, such that part of that surface will not participate in heat transfer. In additional, the fin circumferential area is negligible compared to its side surface area, which is the second term in the above definition.

With the air-side surface area defined, the air-side heat transfer perimeter can be defined as:

\[
HTP_a = \frac{A_a}{L_t} ,
\]

where

\( HTP_a \) = air-side heat transfer perimeter, m.
The use of fins in the finned tube cross-flow heat exchanger helps to enhance the air-side heat transfer through the creation of an extended heat transfer surface. However, considering the heat flow path from the tube-side fluid through the tube wall and fins, and eventually into the air, there is clearly an additional thermal resistance due to the fins, compared to plain tubes. To account for this resistance in heat transfer calculations, a fin efficiency is defined in the following manner: fin efficiency is the ratio of the total heat transferred from the actual fins to the total heat that would be transferred if the fins were isothermal at the tube temperature. Correlations to determine the fin efficiency are presented below. With the fin efficiency determined, the air-side surface area efficiency can be calculated as:

\[
\eta_a = 1 - \frac{A_f}{A_a} (1 - \eta_f),
\]

(3.26)

where

- \( \eta_a \) = air-side surface area efficiency,
- \( \eta_f \) = fin efficiency,
- \( A_f \) = fin surface area, \( m^2 \), and is defined as:

\[
A_f = \frac{\pi}{2} \left( d_f^2 - d_t^2 \right) N_c N_r.
\]

For fined tubes with circular fins, the fin efficiency can be calculated based on a complex analytical derivation by Kern and Kraus [9]:

It should be noted that the circumferential surface area of the fins has been neglected in the above definition, to be consistent with the definition of the total air-side surface area.

For the tube side, no interior fins are adopted in the present design. Therefore, the definitions of the geometric parameters for the tube side are quite straightforward, summarized as follows:

\[
A_{c,t} = \frac{\pi}{4} d_{t,i}^2 N_c N_r; \quad (3.27)
\]

\[
A_t = \pi d_{t,i} L_t N_c N_r; \quad (3.28)
\]

\[
HTP_t = \frac{A_t}{L_t} = \pi d_{t,i} N_c N_r; \quad (3.29)
\]

\[
D_{h,t} = d_{t,i}; \quad (3.30)
\]

where

- \( A_{c,t} \) = tube-side flow area, \( m^2 \),
- \( d_{t,i} \) = tube inner diameter, \( m \),
- \( A_t \) = tube-side total surface area, \( m^2 \),
- \( HTP_t \) = tube-side heat transfer perimeter, \( m \),
- \( D_{h,t} \) = tube-side hydraulic diameter, \( m \).
\[
\eta_f = \frac{4d_{t,o}}{m(d_f^2 - d_{t,o}^2)} \left[ \frac{I_1(md_f/2)K_1(md_{t,o}/2) - K_1(md_f/2)I_1(md_{t,o}/2)}{I_0(md_{t,o}/2)K_1(md_f/2) + I_1(md_f/2)K_0(md_{t,o}/2)} \right] 
\]

(3.31)

where

\[ I_1 = \text{first order modified Bessel function of the first kind}, \]

\[ I_0 = \text{zero}^{\text{th}} \text{order modified Bessel function of the first kind}, \]

\[ K_1 = \text{first order modified Bessel function of the second kind}, \]

\[ K_0 = \text{zero}^{\text{th}} \text{order modified Bessel function of the second kind}, \]

\[ m = \text{a geometric parameter (m}^{-1}) \text{defined as:} \]

\[
m = \sqrt{ \frac{2}{\left( \frac{1}{R_a} + R_{f,a} \right) k_f t_f}} ,
\]

(3.32)

where,

\[ R_{f,a} = \text{air-side fouling resistance, m}^2\text{-K/W, if present}, \]

\[ k_f = \text{thermal conductivity of the fin, W/m-K}. \]

The above analytical formulation for the fin efficiency, although accurate, is relatively difficult to implement in Fortran, due to the Bessel functions. An empirical correlation that approximates the above analytical solution well, but much simpler to implement in Fortran, has been identified:

\[
\eta_f = \frac{1}{1 + \left( \frac{(mH_f)^2}{d_f} \right) \frac{d_f}{d_{t,o}}} .1
\]

(3.33)

In the air cooler application (as well as most other applications), the air-side heat transfer coefficient is expected to lie in the range of ~ 0 – 200 W/m\(^2\)-K. Over this range, the empirical correlation approximates the analytical solution with a maximum relative error less than 2.5%.

**Crossflow PCHE**

Another option in the PDC for the cooler is the crossflow compact Printed Circuit Heat Exchanger (PCHE). It needs to be pointed out, though, that unlike the designs described in the previous sections, the heat exchanger design and corresponding analysis described here is just a concept investigated by the authors. It has not been proposed or quoted by a heat exchanger manufacturer. For these reasons, the proposed design may not be optimal (or even practical) for this particular application. Therefore, the use of this heat exchanger type in the PDC calculations should only be considered by the user as a preliminary investigation of this type of heat exchanger.

The crossflow PCHE air cooler concept is schematically illustrated in Figure 3-18. The hot side (CO\(_2\) in Figure 3-18) consists of conventional semi-circular zigzagged etched channels in a metal
plate. In a simplest configuration, there would be a simple pass of the hot side channels across the plate. However, as Figure 3-18 demonstrates, the PCHE technology allows for a multi-pass channel configuration on the plate, without a need of external headers. Figure 3-18 shows just one example of a three-pass arrangement on the hot side; other options are possible. The channel dimensions in Figure 3-18 are only shown for demonstration purposes as those that are considered practical at the current phase of the PCHE development. All these dimensions can be changed by the PDC user.

![Figure 3-18. Concept of Crossflow PCHE.](image)

On the air side, the formed plate concept with large channel sizes (described in Section 3.1.2.4) is adopted to increase the flow area and reduce the pressure drop on the air side. The channels are formed by a deformed plate. The air channels could be straight or have a small zigzag angle to promote turbulence. The air flow is perpendicular to the general direction of the hot side flow, i.e. the air flow is in the direction of the heat exchanger width.

As shown in Figure 3-18, there would be hot side inlet and outlet headers on each side of the heat exchanger. The air side does not need headers and could be open to the environment as long as it is connected by a duct to air fans, much like the finned tube design in the previous section.

In this heat exchanger configuration, there would still be a crossflow pattern between the hot and air sides. The difference from the finned tube arrangement in the previous section is that the hot side channels in one plate will include channels from all passes. Therefore, logic, specific to this design, was included in the code to calculate inlet conditions for each additional pass based on what channel in the previous pass this channel is connected to. To simplify the calculations, an
assumption is made to ignore any heat transfer and condition changes in the sections connecting the channels, such that a pure crossflow configuration is analyzed.

Because of this flow arrangement, the number of regions in the direction of the air flow is set equal to the total number of the hot side channels in each plate, such that the hot side conditions in each individual channel are resolved. In the direction of HX length, the number of points selection is defined by the user and, similar to other options, should be based on a trade-off between accuracy and computational speed. Under an assumption of a uniform flow distribution, all the plate pairs are identical, so the calculations are performed to calculate heat transfer between one hot side plate and one air plate; the results for all other plates would be identical.

Similar to the finned tube concept, the hot side conditions are the outlet of the last pass’s channels averaged to calculate average cooler-outlet conditions. Similarly, the conditions on the outlet of all air channels are averaged to calculate air outlet conditions.

Since the channel configurations on both the hot and air sides are exactly the same as in the other PCHE concepts described in Section 3.1.2.4, the calculation of parameters, such as hydraulic diameter, flow areas, surface areas, etc., is the same as for other PCHE designs. The only change needed for the crossflow arrangement is that the heat transfer equations described above in this section are now solved on a per-region basis, rather than a per-unit length basis.

### 3.1.3 Electrical Heater

An Electrical Heater is included in the PDC as an option for heat addition to the cycle as an alternative to a Heat Addition Heat Exchanger (HAHX). In the electrical heater, heat is added directly from the heater rods to the working fluid (i.e., no hot-side fluid exists, as in the HAHX). The electrical heater option is intended for modeling of experiment loops. It is triggered by selecting “Electrical Heater” for the “Heat Addition Mode” field in the cycle input form (see Figure 2-9).

The electrical heater in the PDC is assumed to consist of straight cylindrical heater rods and the working fluid flowing along the rods in a shell. Since this configuration is similar to a shell-and-tube heat exchanger, in the electrical heater mode all the input is provided as it would be for a shell-and-tube heat exchanger. However, no calculations are done on the primary side of this heat exchanger either in steady-state or in transient calculations. Instead, the heat is assumed to be added directly to the heat exchanger wall (tubes). This heat input is assumed to be uniform along the heater length based on either user input for the total heater power in steady-state or either automatic or manual control in transients. In steady-state mode, the heat input in each node is equal to the total working fluid enthalpy rise in that node. In transients, the heat input in each node is used to calculate the heat balance for the changing wall temperature. The fluid side calculations, including heat transfer and pressure drop, are still the same as for the shell-and-tube heat exchanger.

There are two options for the steady-state solution for an electrical heater in the PDC: given power and given outlet temperature (see the heater input form in Figure 2-18). In the “Given
power” mode, the working fluid outlet temperature is calculated based on the heat balance and the inlet conditions and flow rate. In the “Given outlet temperature” mode, the temperature is given and the heater power is calculated from the heat balance on the working fluid side, again, given the inlet conditions and the flow rate.

In the dynamic calculations, several options for the electrical heater control exist in the PDC, as described in Section 3.3.3.2.

3.1.4 Turbomachinery

The approach to turbomachinery (turbines and compressors) calculations in the PDC is based on a one-dimensional mean streamline analysis. Under this approach, the fluid conditions are calculated before and after a stage row (either rotor or stator blades) along an “average” streamline which, for simplicity, can be envisioned as located in the mid-height of the blades (the actual streamline location will be discussed later). Therefore, any variation in either fluid properties or the blade performance along the blade height is not considered in this analysis. Also, the variation of the fluid properties and passage width inside the blade row is not included; only inlet and outlet conditions are calculated (with the possible exception of the throttle location, where knowing the fluid velocity at the narrowest passage between the blades is needed for some loss models).

Under the mean streamline approach in the PDC, the fluid properties, including velocities, and the turbomachinery performance, such as work and efficiency, are related based the velocity triangles. An example of a velocity triangle is shown in Figure 3-19. It relates the absolute flow velocity ($C$) with the blade speed ($u$) and the relative velocity of the fluid in relation to the blade ($W$).

![Figure 3-19. Turbomachinery Stage Velocity Triangles for Rotor Inlet and Outlet.](image)

From Figure 3-19, the relative velocity of the flow with respect to the blades is defined as:

$$\bar{W} = \bar{C} - \bar{u}, \quad (3.34)$$
and its component in the axial (along the axis of blade rotation) and tangential (perpendicular to the axis of blade rotation) are defined as:

\[ W_z = C_z \], \hspace{1cm} (3.35) \\
\[ W_\theta = C_\theta - u \]. \hspace{1cm} (3.36)

The blade speed is always calculated from its rotational speed and the mean radius of the blade:

\[ u = \omega r \], \hspace{1cm} (3.37)

where \(\omega = 2\pi n_r\) = angular rotational speed, \\
\(n_r = \) shaft rotational speed in rev/s.

Figure 3-19 also defines the velocity angles with respect to the axial direction, both for the absolute velocity (\(\alpha\)) and relative velocity (\(\beta\)). Note that for the stator components, the blade velocity is zero such that the absolute and relative velocities and angles are identical. The flow angles will be compared to the blade angles (\(\kappa\)) at the inlet and outlet. The incidence angle is defined as the difference between the relative flow angle and the blade angle at the inlet, while the deviation angle is defined as that difference at the outlet.

The turbomachinery analysis in the PDC uses the concepts of static and total fluid conditions. The static conditions are those that define the fluid properties. The total conditions include the effect of the fluid speed and are calculated from the static conditions using the fluid speed along the constant entropy line, as shown in Figure 3-20.

![Figure 3-20. Total and Static Conditions in Turbomachinery.](image)

According to definition of total conditions in Figure 3-20:
\[ H_{total} = h_{static} + \frac{C^2}{2} , \]  
(3.38) 

\[ s_{total} = s_{static} . \]  
(3.39) 

Total pressure, as well as other properties, if needed, at total conditions are defined through the total enthalpy and entropy:

\[ P_{total} = \text{Pressure} \ (H_{total}, s_{total}) . \]  
(3.40)

For an ideal gas, there is an analytical expression for an isentropic process, such that total properties can be easily calculated based on static properties. However, for real gases, there is no such formulation and the total conditions need to be either defined in the tables of properties versus entropy and enthalpy or to be iterated on. The PDC turbomachinery models are specifically formulated to avoid ideal gas approximations and use a hybrid approach, where the pre-calculated h-s tables define only the first guess for iterations on properties.

In this report and in the code equations, the total conditions are denoted by either using capital letters, as in Figure 3-20, or using a subscript “0.” The subscript “static” will be dropped from the equations such that the properties in lower case letters without subscript “0” will always refer to static conditions. The total relative conditions are defined similarly to those in Figure 3-20, but with relative speed instead of absolute speed. The total relative conditions are denoted with an apostrophe mark (']):

\[ H'_{total} = h + \frac{W^2}{2} . \]  
(3.41)

The change in the tangential component of the fluid velocity is caused in turbomachinery by the torque acting on the fluid by the blades. The energy transfer between the blades and the fluid is described by the well-known Euler turbine equation [10]:

\[ H_2 - H_1 = u_2 C_{\theta 2} - u_1 C_{\theta 1} . \]  
(3.42)

The Euler equation holds for both a turbine and compressor, although the direction of the heat transfer is reversed: in a turbine the fluid drives the blades, while in a compressor the energy is transferred from the rotating blades to the fluid. Also note that for stationary components, such as diffusers and nozzles, the rotational speed is zero such that the total enthalpy is conserved in these components.

In the PDC, the Euler equation is used to calculate the energy transfer between the blades and the fluid. It is combined with the continuity equation and the definitions of the velocity triangles (Figure 3-19) to complete the principal set of the equations. The continuity equation relates the fluid density and the flow rate with the flow area and the flow rate:

\[ \rho_1 C_1 A_1 = \dot{m} = \rho_2 C_2 A_2 , \]  
(3.43)
where the flow area, $A$, is measured in the direction perpendicular to the flow velocity.

Note that the above equation assumes that the flow rate is preserved in the stage (or between the stages). This means that in the PDC, the internal leakage flow from the turbomachinery is neglected. The leakage across the blade tip or blade shroud is included in the leakage loss formulation (discussed below) and does not affect the inlet/outlet blade flows since those leakages are internal to the blades.

The turbomachinery blade row performance is characterized in the PDC models by the decrease in the total pressure relative to an ideal process and is formulated in terms of a pressure loss coefficient [10]:

$$ P_2' = P_{2id}' - Y(P_2' - p_2). $$  \hspace{1cm} (3.44)

In the above equation, $P_{2id}'$, is the total relative pressure in an ideal (isentropic) process. For both stationary and rotating components, it is calculated from the outlet total relative enthalpy (from the Euler equation) at the stage outlet and the entropy at the stage inlet. If the loss coefficient is zero, the process would be isentropic, meaning that the inlet and outlet entropies are the same. However, in a real stage, there would always be losses, such that $Y>0$ and the total pressure at the outlet will always be less than that in the ideal (isentropic) process. As shown in Figure 3-21, the decrease in pressure always leads to an increase in entropy. As a result, the stage efficiency and the overall component efficiency would be less than 100%, as defined below.

![Figure 3-21. Concept of Pressure Loss and Increase in Entropy.](image)

For the stationary blades, the total enthalpy is conserved and the relative and absolute velocities are identical. Therefore, $P_{2id}'$ in the above equation will be equal to the total pressure at the inlet. In other words, for this component, both the total enthalpy and the total pressure are conserved in
a stage as if there were no losses. For rotating blades, the total enthalpy is changed by the amount defined by the Euler equation, so the total pressure would not be preserved from inlet to outlet. This pressure change is what makes the pressure increase in a compressor and decrease in a turbine. But the overall solution approach would still be the same, with the pressure loss coefficient defining the entropy increase in the stage and thus the stage and overall component efficiency.

Note also that the definition of the pressure loss coefficient uses the static outlet pressure, $p_2$. This pressure needs to be calculated based on the outlet entropy, $s_{out}$, and outlet static enthalpy. It also needs to be in agreement with the outlet static density from the continuity equation. Therefore, iterations on the outlet conditions are always required in the turbomachinery analysis in the PDC.

Figure 3-22 shows the overall processes on the enthalpy-entropy diagram for a turbine and a compressor, from inlet to outlet. It is common for the turbomachinery analyses to use several definitions of component efficiency depending on what conditions, total or static, are used. The efficiency definitions used in the PDC are provided in Table 3-2 with the values defined in Figure 3-22. For a conservative analysis, the PDC always ignores any kinetic energy at the component inlet, $C_{in}=0$. 

Figure 3-22. Enthalpy-Entropy Diagram of Expansion in Turbine (Left) and Compression in Compressor (Right).
Table 3-2. Turbomachinery Efficiency Definitions in the PDC

<table>
<thead>
<tr>
<th>Efficiency</th>
<th>Turbine</th>
<th>Compressor</th>
</tr>
</thead>
<tbody>
<tr>
<td>Static-to-Static</td>
<td>$\varepsilon_{S-S} = \frac{h_{in} - h_{out}}{h_{in} - h_{s, out}}$</td>
<td>$\varepsilon_{S-S} = \frac{h_{s, out} - h_{in}}{h_{out} - h_{in}}$</td>
</tr>
<tr>
<td>Total-to-Static</td>
<td>$\varepsilon_{T-S} = \frac{h_{in} - h_{out} - \frac{c_{out}^2}{2}}{h_{in} - h_{s, out}}$</td>
<td>$\varepsilon_{T-S} = \frac{h_{s, out} - h_{in}}{h_{out} + \frac{c_{out}^2}{2} - h_{in}}$</td>
</tr>
<tr>
<td>Total-to-Total</td>
<td>$\varepsilon_{T-T} = \frac{h_{in} - h_{out} - \frac{c_{out}^2}{2}}{h_{in} - h_{s, out} - \frac{c_{out}^2}{2}}$</td>
<td>$\varepsilon_{T-T} = \frac{h_{s, out} + \frac{c_{out}^2}{2} - h_{in}}{h_{out} + \frac{c_{out}^2}{2} - h_{in}}$</td>
</tr>
</tbody>
</table>

Since the properties are always calculated based on static conditions, the PDC uses the static-to-static definitions for a turbine and a compressor in Table 3-2 for the cycle calculations and iterations.

Note from Table 3-2 that the total-to-static efficiency is always the smallest value among all of the definitions. Therefore, for a conservative analysis, the total-to-static efficiency definition is used in the PDC to report turbine and compressor efficiencies. To be consistent with that definition, the turbine work is calculated in the PDC to subtract the kinetic energy at the outlet, while the compressor work always adds that kinetic energy. These definitions are equivalent to an assumption that the exit kinetic energy from a turbomachinery component will be dissipated in the cycle heat exchangers (as usually is the case) and will not be available as inlet energy to other turbomachinery components,

\[
W_{turb} = \dot{m}_{turb} \left( h_{in} - h_{out} - \frac{c_{out,turb}^2}{2} \right), \tag{3.45}
\]

\[
W_{comp} = \dot{m}_{comp} \left( h_{out} + \frac{c_{out,comp}^2}{2} - h_{in} \right). \tag{3.46}
\]

The turbine and compressor work in the PDC are also corrected by the mechanical loss, $l_{mech}$, (a loss occurring outside the stages, such as in bearings) and the generator efficiency, $\varepsilon_{gen}$, to obtain the gross generator output. The mechanical loss fraction and the generator efficiency are user inputs for each shaft.

\[
W_{gen} = \left[ (1 - l_{mech}) \sum_{N_t} W_{turb} - \frac{1}{1 - l_{mech}} \sum_{N_c} W_{comp} \right] \varepsilon_{gen}, \tag{3.47}
\]

where $N_t$ and $N_c =$ number of turbines and compressors in the cycle, respectively.
The gross generator output from Equation (3.47) is corrected by the power requirement for the cooling fluid pump to obtain the net generator output for the cycle efficiency definition.

Each turbomachinery component in the PDC has an inlet nozzle. The goal of this nozzle is to accelerate the flow from the inlet pipe to the flow area existing at the first stage inlet. It is assumed that the flow velocity at the component inlet is zero, while the flow velocity at the first stage inlet is calculated from the continuity equation and the first stage frontal area. No detailed analysis of the inlet nozzle is carried out, instead the user specifies the nozzle efficiency, which is similar in meaning to the turbine static-to-static efficiency in Figure 3-22 and Table 3-2. Since the nozzle is a stationary component, the total enthalpy is conserved and it is equal to the static enthalpy (for $C_{in}=0$) at the component inlet. That total enthalpy and the efficiency definition in Figure 3-22 and Table 3-2 are used to calculate the outlet static enthalpy, with iterations on the flow speed and density from the continuity equations. The user-specified inlet nozzle efficiency is assumed to be fixed in the PDC and doesn’t change in both steady-state and dynamic calculations. The inlet nozzle outlet conditions, including flow speed, are used as the inlet conditions for the turbomachinery stages. For the compressors where the minimum conditions are defined, the inlet nozzle calculations start from the given conditions at the first stage inlet, i.e., at the nozzle outlet. Then, the same equations and efficiency definition are used to calculate the compressor-inlet conditions, which are provided to the cycle calculations to define the required cooler-outlet conditions. This exception only applies to the compressor calculations in the design mode, in performance mode and in all transient calculations, the inlet nozzle analysis still starts from the nozzle inlet and the first-stage inlet conditions are calculated for all compressors.

In the PDC, there are two modes of turbomachinery calculations: design and performance. In the design mode, the required inlet and outlet conditions (except for outlet temperature) are calculated by the cycle subroutine. Then, the geometric parameters (flow areas, blade angles, etc.) are calculated by the turbine or compressor design subroutine to match the outlet pressure. As part of this calculation, the losses are also calculated which provide the component efficiency and thus the outlet temperature. In the performance mode, the turbomachinery design is given and is used to calculate the performance of the turbine or compressor, including outlet pressure and temperature, which is used to calculate the efficiency. The selection between the design and performance mode is the user’s choice for the steady-state cycle calculations (see Figure 2-9). For dynamic calculations, the performance subroutines are always used since the design will be known, either from direct user input or from design calculations at steady-state.

3.1.4.1 Axial Compressor

As for all other types of turbomachinery components\(^1\), the PDC model for an axial compressor includes the compressor design and performance subroutines.

Axial Compressor Design

\(^1\) Except for the radial turbine, which only includes the performance subroutine as described in Section 3.1.4.4.
The compressor design model calculates steady-state design parameters for compressors for given cycle conditions. The input parameters are:

- Working fluid
- Inlet pressure and temperature
- Outlet pressure
- Flow rate
- Rotational speed
- Blade material density
- Maximum allowable blade stress
- Number of stages.

The design parameters which need to be calculated include:

- Fluid property (pressure and temperature) distributions throughout the compressor
- Flow angles and speeds
- Blade parameters for each stage:
  - Hub and tip radii
  - Blade height
  - Blade chord
  - Spacing
  - Number of blades
  - Blade angles
- Stresses in the blades
- Compressor efficiency.

An attempt is always made to simplify the design procedure. In that regard, assumptions are made for the values for several parameters which in general need to be optimized based upon specific recommendations and engineering judgment. The parameters have to be changed only if the design or off-design characteristics turn out to be unsatisfying. It is understood that this approach will not produce the best optimal design, but it does produce a reasonable design that is good enough to perform the cycle analysis which is the real goal of the PDC. Since this approach does not produce a fully-optimized design, the results of the PDC compressor design model are conservative meaning that the compressor performance predicted by the PDC would be lower than that of the fully-optimized design. This approach is used for the following parameters.

The axial component of the flow speed is assumed to be constant in the compressor. A repeating stage design is selected meaning that the flow angles are the same at each stage inlet.

The stage reaction is selected to be 50% which allows simplification of the design procedure. For example, for 50% reaction, it is possible to derive an analytical correlation between the inlet guiding vane (IGV) angle and blade deflection angle independent of other parameters to satisfy the de Haller criteria:

\[ \frac{W_2}{W_1} \leq 0.72 \]  

(3.48)
The components of the flow speed are shown in Figure 3-23.

![Figure 3-23. Compressor Stage Velocity Triangles.](image)

Under the assumption of constant axial speed,

\[
\frac{W_2}{W_1} = \frac{C_z/\cos \beta_2}{C_z/\cos \beta_1} = \frac{\cos \beta_1}{\cos \beta_2}.
\]  

(3.49)

For the 50%-reaction stage, the velocity triangles are symmetric meaning that \(\beta_2 = \alpha_1\) which for the first stage is equal to the IGV angle, \(\alpha_{IGV}\), and remains the same for all stages under the repeating stage assumption. The deflection angle is defined as \(\beta_1 - \beta_2\) and its limiting value can be found from Equations (3.48) and (3.49) as a function of the IGV angle:

\[
defl_{\text{max}} = \beta_1^{\text{max}} - \beta_2 = \arccos (0.72 \cos \alpha_{IGV}) - \alpha_{IGV}
\]  

(3.50)

Table 3-3 shows the relationship between IGV angle and maximum deflection angle.

<table>
<thead>
<tr>
<th>IGV angle, deg</th>
<th>Max. deflection, deg</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>43.9</td>
</tr>
<tr>
<td>5</td>
<td>39.2</td>
</tr>
<tr>
<td>10</td>
<td>34.8</td>
</tr>
<tr>
<td>15</td>
<td>30.9</td>
</tr>
<tr>
<td>20</td>
<td>27.4</td>
</tr>
<tr>
<td>30</td>
<td>21.4</td>
</tr>
<tr>
<td>40</td>
<td>16.5</td>
</tr>
<tr>
<td>50</td>
<td>12.4</td>
</tr>
<tr>
<td>60</td>
<td>8.9</td>
</tr>
</tbody>
</table>

It is always desirable for higher efficiency to select the deflection angle as high as possible. At the same time, Table 3-3 shows that a large deflection angle requires a small IGV angle increasing the Mach number at the first stage inlet. The maximum Mach number and compressor efficiency should be checked after the design is complete to see if this selection is satisfactory.
The blade row solidity (spacing-to-chord ratio) is selected following the recommendations for optimal turbine blade row spacing described in [11]. The NACA 65-series blade profiles are used for profile coefficients.

The design procedure starts by determining the pressure distribution between the stages. It is recommended for compressor design [11] that the enthalpy change for each stage should be approximately the same. Assuming that the stages are of equal efficiencies, the condition of equal enthalpy change in an isentropic process is used to determine the pressure and enthalpy at each stage inlet and outlet.

The known change in enthalpy in an isentropic process defines the axial component of the flow speed as follows. As mentioned above, under the repeating stage assumption, the flow inlet angle for every stage is equal to the IGV angle, and the flow velocity at each stage outlet is equal to that at the inlet. If the average deflection angle is specified, then one can calculate the average flow angle at the rotor outlet. For 50% reaction, this relation is explicit:

\[ \text{defl} \equiv \beta_1 - \beta_2 = \alpha_2 - \alpha_1. \]  

(3.51)

For reactions other than 50%, Equation (3.51) becomes implicit and more complicated but it has been shown that this relationship still exists.

Since the flow velocities at each stage outlet and inlet are equal, the change in enthalpy in the stage is equal to the change in total enthalpy which is defined by Euler equation:

\[ \Delta h = \Delta h_0 = u(C_{2\theta} - C_{1\theta}). \]  

(3.52)

Blade speed, \( u \), can be derived from the reaction definition:

\[ R \equiv 1 - \frac{C_{2\theta} + C_{1\theta}}{2u}; \]  

(3.53)

\[ u = \frac{C_{2\theta} + C_{1\theta}}{2(1 - R)}. \]  

(3.54)

Assuming that the compressor efficiency is known (iterations are required), the average change in enthalpy can be related to the change in enthalpy in an isentropic process. Using the definition of efficiency and combining Equations (3.52)-(3.54), the following relationship is obtained:

\[ \frac{\Delta h}{\epsilon} = \Delta h = \frac{C_{2\theta} + C_{1\theta}}{2(1 - R)}(C_{2\theta} - C_{1\theta}) = \frac{C_{2\theta}^2 - C_{1\theta}^2}{2(1 - R)}(\tan^2 \alpha_2 - \tan^2 \alpha_1) \]  

(3.55)

from which the axial component of flow speed is calculated:
\[ C_z = \sqrt{\frac{\Delta h}{\varepsilon} 2(1-R) \frac{1}{\tan^2 \alpha_z - \tan^2 \alpha_i}}. \quad (3.56) \]

The axial speed component is known, and the calculations can proceed for every stage. As mentioned above, the flow angle at a stage inlet is equal to the IGV angle, such that the remaining flow speed components can be found (Figure 3-23). The known inlet conditions specify the density at the inlet, \( \rho_1 \). The continuity equation is used to calculate the required flow area measured perpendicular to the compressor axis:

\[ A_\perp = \frac{A}{\cos \alpha_1} = \frac{\dot{m}}{\rho_1 C \cos \alpha_1} = \frac{\dot{m}}{\rho_1 C_z}. \quad (3.57) \]

At the same time, the flow area is defined by the tip and hub radii of the blades

\[ A_\perp = \pi \left( r_t^2 - r_h^2 \right). \quad (3.58) \]

The PDC compressor design code is organized in such a manner that the hub radius is selected such that the calculated pressure at the stage outlet matches the required pressure from the distribution obtained earlier. Equation (3.58) is used to calculate the tip radius and then the medium radius, blade height, and blade speed:

\[ r_t = \sqrt{\frac{A_\perp}{\pi} - r_h^2}; \quad (3.59) \]

\[ r_m = \frac{r_t + r_h}{2}; \quad (3.60) \]

\[ H_b = r_t - r_h; \quad (3.61) \]

\[ u = 2\pi n_r r_m. \quad (3.62) \]

The relative-to-the-blade speeds and angles are calculated based on Figure 3-23

\[ W_{1z} = C_z, \quad (3.63) \]

\[ W_{1\theta} = C_{1\theta} - u, \quad (3.64) \]

\[ W_1 = \sqrt{W_{1\theta}^2 + W_{1z}^2}, \quad (3.65) \]

\[ \sin \beta_1 = \frac{W_{1\theta}}{W_1}. \quad (3.66) \]
The flow speed components at the rotor outlet are calculated using the definition (3.53) of the stage reaction and velocity triangles on Figure 3-23,

\[ C_{2\theta} = 2u(1 - R) - C_{1\theta}, \]  
(3.67)

\[ C_{2z} = C_z, \]  
(3.68)

\[ C_2 = \sqrt{C_{2\theta}^2 + C_{2z}^2}, \]  
(3.69)

\[ \sin \alpha_2 = \frac{C_{2\theta}}{C_2}, \]  
(3.70)

\[ W_{2z} = C_z, \]  
(3.71)

\[ W_{2\theta} = C_{2\theta} - u, \]  
(3.72)

\[ W_2 = \sqrt{W_{2\theta}^2 + W_{2z}^2}, \]  
(3.73)

\[ \sin \beta_2 = \frac{W_{2\theta}}{W_2}. \]  
(3.74)

The optimum solidity [11] for the rotor blades is:

\[ \sigma = 2.5(\tan|\beta_2| + \tan|\beta_1|)\cos^2 \beta_1. \]  
(3.75)

Blade profile angles can now be calculated using the methodology described in [12] (Figure 3-24).
Design incidence angle (i.e., incidence angle at design conditions):

\[ t^* = K_{t,i} (t^*_0)_{0,0} + n\theta , \]  

where

\[ K_{t,i} = (10t_b/c)^q, \]
\[ q = 0.28/\left[ 0.1 + (t_b/c)^{0.3} \right], \]
\[ \left( t^*_0 \right)_{0,0} = \frac{\beta_i}{5 + 46\exp(-2.3\sigma)} - 0.1\sigma^3 \exp\left[ \frac{\beta_i - 70}{4} \right], \]
\[ x = 0.914 + \sigma^3/160, \]
\[ n = 0.025\sigma - 0.06 - \left( \frac{\beta_i/90}{1.5 + 0.43\sigma} \right), \]
\[ t_b/c = \text{blade maximum thickness-to-chord ratio (0.1 for NACA-65 series blades)}. \]

Design deviation angle:

\[ \delta^* = K_{t,\delta} (\delta^*_0)_{0,0} + m\theta , \]  

where

\[ K_{t,\delta} = 6.25(t_b/c) + 37.5(t_b/c)^2, \]
\[ \left( \delta^*_0 \right)_{0,0} = 0.01\sigma\beta_i + \left[ 0.7\sigma^{1.9} + 3\sigma \right] \beta_i/90)^{(1.67+1.098\sigma)}, \]
\[ m = m_{1,0}/\sigma^b, \]
\[ m_{1,0} = 0.17 - 0.0333x + 0.333x^2, \]
\[ x = \beta_i/100, \]
\[ b = 0.9625 - 0.17x - 0.85x^3. \]

The rest of the blade profile angles are defined in Figure 3-24. Note that the camber angle, \( \theta \), needed for Equations (3.76) and (3.77) is defined through blade angles which are functions of the incident and deviation angles. Therefore, iterations are required on the camber angle.

When the blade profile parameters are calculated, it is possible to calculate flow conditions in the blade row. The total relative enthalpy at the rotor outlet is equal the total relative enthalpy at the rotor inlet:

\[ h'_{02} = h'_{01} = h_1 + \frac{W_i^2}{2}. \]  

The total relative pressure at the rotor inlet is the pressure corresponding to the total relative enthalpy and inlet entropy:

\[ p'_{01} = p(h = h'_{01}, s = s_1). \]
The total pressure at the rotor outlet is equal to the total relative pressure at the inlet minus losses

\[ p'_{02} = p'_{01} - \bar{\omega}(p'_{01} - p_1) - \Delta p_{0c}, \]  

where

- \( \bar{\omega} \) = loss coefficient,
- \( \Delta p_{0c} \) = tip clearance gap total pressure loss.

(The equations for the loss coefficient and clearance loss are provided below.)

Total relative pressure and enthalpy at the rotor outlet define the entropy at this point

\[ s_2 = s'_{02} = s(p = p'_{02}, h = h'_{02}) \]  

Enthalpy and other conditions at the rotor outlet can now be found:

\[ h_2 = h'_{02} - \frac{W_2}{2}, \]

\[ p_2 = p(h = h_2, s = s_2), \quad T_2 = T(h = h_2, s = s_2). \]

When the inlet and outlet conditions are known, the centrifugal, bending, vibrational, and total stresses can be calculated using Equation (3.84)-(3.87), respectively [13].

\[ \sigma_c = 2\pi \rho_B n_r^2 A_\perp, \]  

\[ \sigma_B = \frac{x}{I_{yy}}[M_\phi \cos\phi - M_a \sin\phi] - \frac{y}{I_{xx}}[M_a \cos\phi + M_\phi \sin\phi], \]

\[ \sigma_v = \alpha \sigma_B, \]

\[ \sigma_r = \sigma_c + \sigma_B + \sigma_v, \]

where

- \( \rho_B \) = blade material density,
- \( n_r \) = rotational speed,
- \( x,y \) = coordinate system based on the principal axes of inertia,
- \( I \) = polar moment of inertia,
- \( \phi \) = moments of inertia angle,
- \( \alpha \) = vibrational stress constant (\( \alpha = 0.75 \)).

In the equation for the bending stress, \( \sigma_B \), the coordinates \( x \) and \( y \) are proportional to the blade chord. The blade chord is calculated by the code such that the total stress is below the allowable limit, which is a user input.
The loss coefficient and tip leakage loss calculations follow the recommendations of [12].

The design loss coefficient,

$$\bar{\omega}^* = \frac{2\sigma}{\cos \beta_2} \left( \frac{W_2^*}{W_1} \right)^2 K_1 \left[ K_2 + 3.1(D_{eq}^*-1)^2 + 0.4(D_{eq}^*-1)^4 \right], \quad (3.88)$$

where

$$D_{eq} = \frac{W_{\max}}{W_2},$$

$$W_{\max} = W_1 \left[ 1.12 + 0.61 \frac{\cos^2 \beta_1}{\sigma} (\tan \beta_1 - \tan \beta_2) + \alpha (i-i^*)^{1.43} \right],$$

$$\alpha = 0.0117, \ K_1 = 0.0073, \ K_2 = 1 + (s/H_b) \cos \beta_2 + 0.004 K_{Re} / K_1, \ K_{Re} = \begin{cases} \sqrt{2.5 \times 10^5/Re_c} - 1, & Re_c < 2.5 \times 10^5 \\ \left[\log(2.5 \times 10^5) / \log(Re_c) \right]^{0.58} - 1, & Re_c > 2.5 \times 10^5 \end{cases}.$$  

Correlation (3.88) includes the secondary flow effect ($K_1$), Re number correction ($K_{Re}$), and end-wall losses ($s/H_b$). The Mach number effect is taken into account as follows:

$$\bar{\omega} = \bar{\omega}_m \left(1 + \xi^2 \right), \quad (3.89)$$

where

$$\bar{\omega}_m = \bar{\omega} \left[1 + (i_m - i^*)^2 / R_s^2 \right],$$

$$\xi = \begin{cases} (i - i_m) / (i_m - i^*), & i < i_m \\ (i - i_m) / (i_m - i^*), & i \geq i_m \end{cases},$$

$$i_m = i_c + (i_s - i_c) \frac{R_c}{R_c + R_s},$$

$$i_s = i^* + \frac{R_s}{1 + 0.5(K_{sh M_1}^3)},$$

$$i_c = i^* - \frac{R_c}{1 + 0.5 M_1^3},$$

$$R_s = \alpha_s - \alpha^*,$$

$$\alpha_s = \alpha^* + 10.3 + \left[ 2.92 - \frac{\beta_{1s}}{15.6} \right] \theta / 8.2,$$

$$\beta_{1s} = \alpha_s + \gamma,$$

$$R_c = \alpha_c - \alpha^*,$$

$$\alpha_c = \alpha^* - 9 + \left[ 1 - \left( \frac{30}{\beta_{1c}} \right)^{0.48} \right] \theta / 4.176,$$
\[ \beta_{ic} = \alpha_c + \gamma. \]

The total pressure loss due to tip clearance leakage is:

\[ \Delta p_0 = \Delta p \frac{\dot{m}_c}{m}, \]

where

\[ \dot{m}_c = \bar{\rho} U_c \delta_c c \cos \gamma, \]
\[ U_c = \frac{0.816}{N_{row}^{0.2}} \sqrt{\frac{2\Delta p}{\bar{\rho}}}. \]

The technique described above is also applied for the stator row to calculate the flow conditions and geometry of one stage. For the stator, the absolute (not relative) parameters (speed, angles, total pressure, enthalpy, and so on) are used. As described above, the hub radius is adjusted if needed to match the specified stage-outlet pressure. The process is then repeated for every stage.

To calculate the compressor length, the blade row axial dimension is calculated as the chord, \( c \), multiplied by the cosine of the stagger angle, \( \gamma \) (Figure 3-24). The compressor length is equal to the sum of all rotor and nozzle blade axial dimensions.

The selection of the number of stages for each compressor is a user input and should be based on engineering judgment using comparison of the main performance characteristics and desired compressor efficiency on one hand and the size and cost of the compressor on another hand.

**Axial Compressor Off-Design Performance Model**

An off-design performance prediction model is used in the PDC steady-state calculations, if the performance mode is selected for the turbomachinery. The performance model is also always used to generate the compressor performance maps for the dynamics calculations.

For the off-design model the following parameters are given:
- Inlet conditions
- Flow rate
- Stage geometry
- Rotational speed
- Blade profile and angles.

The goal of the performance model is to calculate the flow conditions inside the compressor and at the compressor outlet. The flow velocities and angles at each row are also calculated by the model.

The calculations start from the inlet. Given the flow conditions and flow rate, together with the design parameters of the IGV (flow area and IGV angle), that information specifies the flow velocity and direction at the IGV outlet or first stage inlet. Using Equations (3.63)-(3.66) described in the design section above, the relative to the blade flow velocity and angles are
calculated at the stage inlet. The blade angle and flow angle define the incidence angle, \( i \), according to Figure 3-24. To determine the flow conditions at the outlet, iterations are required. It is assumed that the row-outlet density is known. The axial speed component at this point can then be found from the continuity Equation (3.57) with specified flow area by the design calculations.

The flow angle and the loss coefficient are to be found using the recommendations in [12]. The deviation angle is:

\[
\delta = \delta^* + \left[ \frac{\partial \delta}{\partial i} \right]^* (i - i^*) + 10 \left( 1 - \frac{W_2}{W_{cl}} \right),
\]

(3.91)

where

\[
\left[ \frac{\partial \delta}{\partial i} \right]^* = \frac{1 + (\sigma + 0.25\sigma^4)(\beta_i/53)^{2.5}}{\exp(3.1\sigma)}
\]

is defined at design point.

The outlet flow angle is defined by Figure 3-24. The flow angle and axial speed component provide the relative flow speed. The absolute speed, its components, and angles can be found using a relationship similar to Equations (3.71)-(3.74).

The loss coefficient is expressed as a function of the design loss coefficient and incidence angle:

\[
\bar{\omega} = \bar{\omega}_m \begin{cases} 
1 + \frac{\xi^2}{2}, & -2 \leq \xi \leq 1 \\
5 - 4(\xi + 2), & \xi < -2 \\
2 + 2(\xi - 1), & \xi > 1
\end{cases},
\]

(3.92)

where

\[
\xi = \frac{(i - i_m)/(i_m - i_i), \quad i < i_m}{(i - i_m)/(i_s - i_m), \quad i \geq i_m}
\]

The flow conditions at the rotor outlet are defined by Equations (3.78)-(3.83) with current values for the loss coefficient and flow speeds. The iterations on the rotor-outlet density are repeated, if necessary.

The same procedure is repeated for the stator and then for every stage until the outlet conditions are found.

Based on the inlet conditions and the outlet pressure, the outlet enthalpy in an isentropic process is calculated:

\[
h_{s,out} = h(p = p_{out}, s = s_{in})
\]

(3.93)

The total-to-total compressor efficiency is:
To calculate the stall conditions, the stall criterion recommended by [12] is used:

\[ W_{RE} < W_{RE}^{\text{min}}, \quad (3.95) \]

where

\[ W_{RE} = \sqrt{\frac{p_0^2 - p_1^2}{p_0^2 - p_1}} = \text{equivalent relative velocity ratio across the blade}, \]
\[ W_{RE}^{\text{min}} = k \left[ \frac{0.15+11t_b/c}{0.25+10t_b/c} \right] \frac{1+0.4[\theta/c(2\sin(\theta/2)\cos \gamma)]^{0.65}}{\theta} = \text{stall velocity ratio}, \]

with condition \( \theta/c(2\sin(\theta/2)\cos \gamma) \geq 1.1 \) applied,

\[ k = \begin{cases} 1, & D_{eq} \leq 2.2 \\ (2.2/D_{eq})^{0.6}, & D_{eq} > 2.2 \end{cases} \]

In order to have a quantitative equivalent of Criterion (3.95), the stall coefficient is introduced:

\[ f_{\text{stall}} = \frac{W_{RE}}{W_{RE}^{\text{min}}}. \quad (3.96) \]

The stall criterion would then be \( f_{\text{stall}} < 1 \), and \( f_{\text{stall}} \) will show how far the compressor is from the stall conditions.

Choke conditions occur when the calculated Mach number (i.e., ratio of the local speed to the speed of sound) at any row inlet or outlet reaches unity. Therefore, the maximum Mach number in the compressor is used to measure how far the compressor is from the choking condition.

3.1.4.2 Centrifugal Compressor

The centrifugal compressor design and performance models are based on Reference [14]. A centrifugal compressor stage (Figure 3-25) consists of an inlet duct, inlet guiding vane (IGV), impeller, diffuser, and volute or collector. In case of a multi-stage compressor, the collector/volute is replaced with a crossover and a return channel for each stage, except for the last one.
The performance analysis of a centrifugal compressor is similar to that of an axial compressor. The main differences include:

- Different geometry, which is reflected by different loss correlations and different flow area calculations for the continuity equations, and a
- Change in blade speed due to the change in radius from the impeller inlet to the impeller discharge, which affects the energy conservation equation as shown below.

The centrifugal compressor impeller geometry is shown in Figure 3-26 along with the notation used in this report and in the PDC equations. For the purely axial inlet ($\phi_1=0$) and pure radial discharge ($\phi_2=90^\circ$), the impeller frontal areas are calculated as shown below. The flow areas are equal to the frontal areas, minus the area blocked by the blades.

$$A_1 = \pi (r_{tip}^2 - r_{hub}^2) ,$$  \hspace{1cm} (3.97)

$$A_2 = 2\pi r_2 b_2 .$$  \hspace{1cm} (3.98)

![Figure 3-26. Centrifugal Compressor Impeller Passage (Left) and Blade Geometry (Right).](image)

The centrifugal compressor diffuser geometry is shown in Figure 3-27. Equations similar to Equation (3.98) are used in the code to calculate the diffuser area at inlet and outlet.
Aside from the differences described above, the approach for a centrifugal compressor design and performance analysis is similar to that of an axial compressor. In particular, the same one-dimensional analysis is implemented under which flow conditions are calculated only at the impeller inlet and outlet (i.e., exact flow parameters inside an impeller are not calculated). Also, a realistic equation of state is used for the fluid properties and no ideal-gas simplifications are made for the fluid properties or the compression/expansion processes in the compressor.

The impeller performance is based on the energy conservation equation, equation of state, and loss correlation (Equations (3.99)-(3.102)).

Energy conservation equation:

$$ h'_{2} = h'_{1} + \left( U_{2}^{2} - U_{1}^{2} \right)/2, \quad (3.99) $$

where

$$ h' = h + \frac{W^{2}}{2} = \text{total relative enthalpy}. $$

Total outlet pressure for ideal process (without losses):

$$ p'_{t2id} = p(h'_{2}, s_{2}). \quad (3.100) $$

Total outlet pressure with losses:

$$ p'_{t2} = p'_{t2id} - f_{c} \left( p'_{t1} - p_{t} \right) \bar{\omega}, \quad (3.101) $$

where

$$ f_{c} = \frac{p'_{t2} T_{t2}}{p'_{t1} T_{t1}} = \text{correction factor to account for total pressure loss variation from impeller inlet to impeller discharge}, $$
\( \bar{\omega} = \) loss coefficient.

The loss coefficient is calculated as a sum of loss components (such as, incident, diffusion, choke, and so on), as described in Reference [14],

\[ \bar{\omega} = \bar{\omega}_{inc} + \bar{\omega}_{dif} + \bar{\omega}_{ch} + \bar{\omega}_{sl} + \bar{\omega}_{st} + \bar{\omega}_{mix} + \bar{\omega}_{cl} + \bar{\omega}_{tr} \]  \hspace{1cm} (3.102)

The impeller design is based on so-called “good design practice” [14]. Under this approach, the design parameters (for example, impeller blade angle at discharge) are expressed as empirical functions of flow coefficient. The flow coefficient is based on the volumetric inlet flow rate, impeller discharge radius, and rotational speed:

\[ \phi = \frac{\dot{m}}{\rho_0 \pi r_2^2 U_2} . \]  \hspace{1cm} (3.103)

The parameters selected based on “good design practice” include:

- Blade load coefficient, which defines the change in the tangential component of flow speed,
  \[ I_B = C_{U_2}/U_2 - U_i C_{U_1}/U_2 , \]
  \[ I_B = 0.68 - (\phi/0.37)^2 . \]

- The slip factor, which defines the blade angle at discharge
  \[ \sigma = 1 - \sqrt{\cos \kappa_2 \sin \alpha_{C_2}/z^{0.7}} , \]
  \[ I_B = \sigma(1 - \lambda \phi_2 \tan \kappa_2) - U_i C_{U_1}/U_2^2 . \]

- Blade, flow, and incidence angles at impeller inlet,
  \[ \beta_i = -60^\circ , \]
  \[ \alpha_i = 0^\circ , \]
  \[ i_i = 0^\circ , \]
  \[ i_i = k_i - \beta_i . \]

- Flow angle at discharge, and
  \[ \cot \alpha_2 = 0.26 + 3\phi . \]

- Impeller axial length,
  \[ \Delta z_i = (0.014 + 0.023 d_i/d_0 + 1.58\phi)d_2 . \]

All other design parameters are calculated from the continuity (3.43) and Euler (3.42) equations and from velocity triangles. The impeller discharge radius, \( r_2 \), which goes into the definition of the flow coefficient, is selected such that the stage-discharge pressure matches the design value.
The limiting design criterion is a blade loading which is designed as a ratio of an average blade velocity difference to the average velocity in the impeller. The design value for the blade loading should not exceed 0.9:

$$\frac{2 \Delta W}{W_1 + W_2} \leq 0.9,$$

(3.104)

where

$$\Delta W = 2\pi d_z U_z I_f / (z L_g) = \text{average blade velocity difference}.$$

The blade loading limitation is used to calculate the required number of impeller blades, \( z \), according to Equation (3.104).

The design and performance of a diffuser is similar to that of the impeller, except that there is no rotation and there is no external energy input in the diffuser. Again, some parameters are calculated based on conservation equations; the rest is assumed based on “good design practice” to match the impeller design. Both design parameters and the loss coefficient depend on whether a vaned or vaneless diffuser is utilized (both are supported by the code). The loss coefficient for a vaned diffuser has several components, defined in Reference [14].

The fluid conditions at the diffuser outlet are defined by the conservation of total energy and the change in total pressure due to losses (Equations (3.105) and (3.106)). The continuity equation relates the outlet density to the flow speed used in the energy equation.

$$h_{t3} = h_{t4},$$

(3.105)

where

$$h_t = h + \frac{C^2}{2} = \text{total enthalpy},$$

$$p_{t4} = p_{t3} - (p_{t3} - p_3)\omega.$$  

(3.106)

The volute or collector is not modeled in the centrifugal compressor design and analysis models in the PDC. It is assumed that the flow conditions at the compressor outlet are the same as the conditions at the diffuser discharge. The return channel is modeled with an assumed value of the pressure loss coefficient, which is a user input.

3.1.4.3 Axial Turbine

An axial flow turbine usually consists of several stages. Each stage has a nozzle, a set of stationary blades, and a rotor with rotating blades. In a rotor, the expanding gas forces the blades to rotate producing a mechanical energy of rotation which is converted into electricity in the generator. In the nozzle, the gas is accelerated so it can produce more energy in the rotor. Both
the nozzle and the rotor have blades which are designed to achieve the required change in gas pressure. The blades are mounted on the hub, which is connected to the shaft (Figure 3-28).

![Figure 3-28. Axial Turbine Stages.](image)

The axial turbine stage dimensions used in the PDC are shown in Figure 3-29. Figure 3-30 shows the change in gas velocity as it goes through the nozzle and rotor blades in an axial turbine.

![Figure 3-29. Axial Turbine Stage Dimensions.](image)
The approach to the axial turbine analysis is based on the general turbomachinery equations described in Section 3.1.4 above. The Euler and continuity equations are used with the velocity triangles to define the fluid condition changes in a turbine stage.

**Axial Turbine Loss Model**

The loss model for the axial turbine blades implemented in the PDC uses the loss correlations presented in Reference [15]. The loss model includes the following components:

- Blade profile losses,
- Mach number correction,
- Shock losses,
- Tip clearance leakage,
- Reynolds number correction,
- Secondary flow losses, and
- Trailing edge losses.

The total loss coefficient is calculated as a sum of loss coefficients from profile, secondary, and tip leakage losses:

\[
Y = Y_p + Y_s + Y_{tip}.
\]  \hspace{1cm} (3.107)

The profile loss coefficient is calculated as the combination of the profile loss coefficient derived in Reference [16] and the effects of Mach number and Reynolds number. The incident loss coefficient is added to the profile loss coefficient following the recommendations of [16] as described below.

\[
Y_p = 0.914 \left( \frac{2}{3} Y_{p(i=0)} K_{tip} K_p + Y_{shock} \right) f_{Re},
\]  \hspace{1cm} (3.108)

where

\[
Y_{p(i=0)} = \text{profile loss coefficient at zero incidence},
\]
The profile loss coefficient at zero incidence is defined as

\[
Y_{p[0]} = Y_{p,n} + \frac{\kappa_1}{\alpha_2} \left( Y_{p,i} - Y_{p,n} \right) \left( \frac{t_b}{c} \right)^{\kappa_1},
\]

where

- \( Y_{p,n} \) = profile loss coefficient for nozzle \((\kappa_1=0)\) blades,
- \( Y_{p,i} \) = profile loss coefficient for impulse \((\kappa_1=\alpha_2)\) blades,
- \( \kappa_1 \) = blade angle at the inlet,
- \( \alpha_2 \) = flow angle at the outlet,
- \( t_b \) = maximum blade thickness,
- \( c \) = blade chord.

The indices, 1 and 2, denote blade inlet and outlet, respectively.

The profile loss coefficients for nozzle and impulse blades are given in Reference [16] as plots versus blade spacing-to-chord ratio, \( s/c \), for different flow outlet angles, \( \alpha_2 \). Those plots were fitted with the TableCurve 3D software (demo version) [17] to find the fitting function which provides the best approximation,

\[
Y_{p,n} = f_1(\frac{s}{c}, \alpha_2),
\]

\[
Y_{p,i} = f_2(\frac{s}{c}, \alpha_2),
\]

The incidence loss coefficient is reported in Reference [16] as a plot versus the ratio of incidence angle, \( i \), to stalling incidence angle, \( i_s \). The stalling incidence, \( i_s \), is derived through a series of plots versus spacing-to-chord ratio and flow outlet angle. Again, those plots, as well as the plot for incidence loss coefficient, were fitted with functions using the TableCurve software.

\[
K_{yp} = f_3\left(\frac{i}{i_s}\right),
\]

\[
i_s = i_s(\frac{s}{c} = 0.75) + \Delta i_s,
\]

\[
i_s(\frac{s}{c} = 0.75) = f_4\left(\frac{\kappa_1}{\alpha_2(s/c = 0.75)}, \alpha_2(s/c = 0.75)\right),
\]
\[
\frac{\alpha_2}{\alpha_5(s/c = 0.75)} = f_5(s/c), \quad (3.115)
\]

\[
\Delta \iota = f_6(s/c, \alpha_2). \quad (3.116)
\]

As examples of plot fitting, Figure 3-31 shows the 3D fitting function (for the stalling incidence angle for a blade spacing-to-chord ratio = 0.75) and Figure 3-32 shows the 2D fitting of the incidence loss coefficient.
The correction coefficient from exit Mach number, channel acceleration, and their combined effects are defined in Reference [15], respectively:

\[
K_1 = \begin{cases} 
1, & \text{if } M_2 \leq 0.2 \\
1 - 1.25(M_2 - 0.2), & \text{if } M_2 > 0.2 
\end{cases}, \quad (3.117)
\]

\[
K_2 = \left( \frac{M_1}{M_2} \right)^2, \quad (3.118)
\]

\[
K_p = 1 - K_2(1 - K_1), \quad (3.119)
\]

where

\[ M = \text{Mach number}. \]

The subsonic shock loss coefficient is defined as:

\[
Y_{\text{shock}} = 0.75(M_1 - 0.4)^{0.75} \frac{r_h}{r_i} \frac{P_1}{P_2} \frac{1 - \left( 1 + \frac{\gamma - 1}{2} M_i^2 \right)^{\frac{\gamma - 1}{\gamma}}}{1 - \left( 1 + \frac{\gamma - 1}{2} M_z^2 \right)^{\frac{\gamma - 1}{\gamma}}}, \quad (3.120)
\]
where

\( r_h \) and \( r_t \) = hub and tip radii, respectively,
\( p \) = pressure,
\( \gamma = \frac{c_p}{c_v} \) = ratio of specific heats.

The correction for the Reynolds number is defined as:

\[
f_{Re} = \begin{cases} 
\left( \frac{\text{Re}}{2 \cdot 10^5} \right)^{-0.4}, & \text{if} \; \text{Re} \leq 2 \cdot 10^5 \\
1, & \text{if} \; 2 \cdot 10^5 < \text{Re} \leq 10^6 \\
\left( \frac{\text{Re}}{10^6} \right)^{-0.2}, & \text{if} \; \text{Re} > 10^6 
\end{cases}
\]  

(3.121)

where

\( \text{Re} = \frac{\rho_2 V^2}{\mu_2} \) = Reynolds number based on blade chord and outlet conditions.

The secondary loss coefficient is defined in Reference [15] as the original secondary loss coefficient from Reference [16] corrected for the subsonic Mach number:

\[
Y_s = 1.2 Y_{s,i} K_s ,
\]

(3.122)

\[
Y_{s,i} = 0.0334 f_{AR} \left( \frac{\cos \alpha_2}{\cos \alpha_1} \right) \left( \frac{C_L}{s/c} \right)^2 \frac{\cos^2 \alpha_2}{\cos^3 \alpha_m} ,
\]

(3.123)

where

\[
C_L = \frac{2(\tan \alpha_1 + \tan \alpha_2) \cos \alpha_m}{} ,
\]

\[
\alpha_m = \tan^{-1} \left[ \frac{\tan \alpha_1 + \tan \alpha_2}{2} \right] ,
\]

\[
f_{AR} = \begin{cases} 
\frac{1 - 0.25 \sqrt{2 - h/c}}{h/c}, & \text{if} \; h/c \leq 2 \\
\frac{1}{h/c}, & \text{if} \; h/c > 2 
\end{cases}
\]

\( h/c \) = blade height-to-chord ratio.

\[
K_s = 1 - K_3 \left( 1 - K_p \right)
\]

(3.124)

where

\[
K_3 = \left( \frac{c_x}{h} \right)^2
\]
$c_x = \text{axial projection of the blade chord.}$

The tip leakage loss coefficient is defined for shrouded blades only:

$$Y_{tip} = 0.37 \left( \frac{L}{h} \right)^{0.78} \left( \frac{s}{c} \right)^2 \frac{\cos^2 \alpha}{\cos^3 \alpha_m},$$

(3.125)

where

$$t' = \frac{t}{N_{seal}^{0.42}},$$

$t = \text{tip clearance},$

$N_{seal} = \text{number of seals}.$

For unshrouded blades, the tip leakage coefficient is set to be zero, but the overall blade row efficiency is corrected for the tip leakage losses:

$$\Delta \eta = 0.93 \frac{t}{h \cos \alpha_2} \frac{r_i}{r_m},$$

(3.126)

where

$\Delta \eta = \text{correction to the blade efficiency},$

$\eta_0 = \text{blade efficiency without tip leakage losses},$

$r_m = \text{blade mean radius}.$

**Design Analysis of Axial Turbine**

The axial turbine design procedure in the PDC uses several simplifying assumptions. The goal of these assumptions is to reduce the number of independent design variables such that the turbine design can be automated. It is understood that as a result of these assumptions, the turbine design calculated by the PDC may not be optimal, i.e., yielding the highest possible efficiency. For this reason, the design analysis in the PDC is conservative meaning that the calculated performance will be somewhat less when compared with detailed design calculations carried out using the best design practices.

First, it is assumed that the axial component of gas speed is constant everywhere in the turbine. This is a common assumption for turbine design [13]. Second, the rotor geometry is selected in such a way that the flow at every stage inlet and outlet is purely axial, i.e., the tangential component of gas velocity is equal to zero. This makes every stage calculation similar and independent from other stages. Also, the stage reaction, which is defined as the ratio of change in enthalpy to the change in total enthalpy [13], is set to be 50% for the calculation of the axial speed component as described below. This means that half of the pressure decrease in the stage occurs in the nozzle and half in the rotor. This is also a common choice for turbine design.

It can be analytically shown [2] that with the above assumptions, the gas velocity components and the blade rotational speed can be calculated as follows:
\[ C_{2\theta} = u = \sqrt{\frac{h_1 - h_{5,\text{out}}}{N_{st}}} , \]  
(3.127)

\[ C_z = \frac{C_{2\theta}}{\tan(\alpha)} , \]  
(3.128)

where \( N_{st} \) = number of stages (user input), 
\( \alpha \) = blade angle (user input).

The blade speed is used to calculate the average blade radius. When the calculations for each stage are completed, the continuity equation provides the required flow area, which, together with the average blade radius, defines all other dimensions in Figure 3-29, including blade height and hub and tip radii.

The velocity triangles define the blade angles. From those and the user input of the blade incidence and deviation angles (it’s a common practice to have zero incidence and deviation at the design point), the blade angles are calculated.

The blade chord (the distance between the leading and trailing edges of the blade) is calculated based on the stress criteria on the blade [13,18] using the user input for the desired blade profiles. The centrifugal, bending, vibrational, and total stresses, respectively, are defined as [13]:

\[ \sigma_c = 2 \pi \rho_B n_r^2 A_{\perp} , \]  
(3.129)

\[ \sigma_B = \frac{x}{I_{yy}} [M_\phi \cos \phi - M_a \sin \phi] - \frac{y}{I_{xx}} [M_a \cos \phi + M_\phi \sin \phi] , \]  
(3.130)

\[ \sigma_v = \alpha \sigma_B , \]  
(3.131)

\[ \sigma_r = \sigma_c + \sigma_B + \sigma_v , \]  
(3.132)

where
\( \rho_B \) = blade material density,
\( n_r \) = rotational speed,
\( x,y \) = coordinate system based on the principal axes of inertia,
\( I \) = polar moment of inertia,
\( \phi \) = moment of inertia angle,
\( \alpha \) = vibrational stress constant (\( \alpha=0.75 \)).

In the equation for the bending stress, \( \sigma_B \), the coordinates, \( x \) and \( y \), are proportional to the blade chord. The blade chord is calculated by the code such that the total stress is below the allowable limit, which is a user input.
For the turbine axial length estimate, it is assumed in the PDC that the blade row axial length is equal to the blade chord.

**Exit Diffuser**

The axial turbine is assumed to have an outlet diffuser after the last stage. The goal of this component is to decelerate the flow in order to recover at least a portion of the flow kinetic energy and transform it into the fluid pressure. An exit diffuser is usually a diverging nozzle with increasing flow area. As flow area increases, the fluid speed decreases according to the continuity equation. Since the total enthalpy in non-rotating diffuser is conserved, the decrease in speed means an increase in static enthalpy and, therefore, pressure.

The PDC uses an approach similar to that for the inlet nozzle (see Section 3.1.4) to perform the calculations for the exit diffuser. The user provides the diffuser efficiency, which characterizes loses in the diffuser and is used to calculate static pressure at the diffuser outlet. The user also provides the input for the pressure recovery coefficient which determines what fraction of the kinetic energy of the fluid at the last stage outlet is converted into an increase in static pressure. The higher the pressure recovery coefficient, the longer the diffuser that will be required to achieve that goal. The diffuser length is estimated in the PDC assuming an 8° diffuser divergence angle.

### 3.1.4.4 Radial Turbine

The PDC has been developed for the design and analysis of energy conversion systems. These systems are usually designed for large power plants, with typical power in 10-1000 MWe range. For systems in this power range, axial flow turbines are usually a preferred choice since they have better potential to achieve higher efficiencies and thus increase the cycle efficiency. For this reason, only axial turbine models were originally included in the PDC. Later, the code was extended to include a radial turbine model for analysis of small-scale experiment loops, where axial turbines may not be practical. However, since the analysis of the experiment loops does not usually require a turbomachinery design (for this system, the design is already known), the PDC now only includes a performance model for a radial turbine, and not a radial turbine design subroutine.

The PDC radial turbine performance model follows the general turbomachinery analysis approach in Section 3.1.4 with the loss models from Reference [10]. The radial turbine model is similar to the centrifugal (radial) compressor model (described in Section 3.1.4.2), except that the flow is in the reverse direction – from the volute to the diffuser to the impeller. The most important difference between the compressor and turbine models is the loss model and correlations.

**Boundary Layer Loss Coefficient**

The profile loss coefficient, $Y_p$, is expressed in terms of the ideal (no loss) component discharge dynamic head rather than the inlet dynamic head due to surface boundary layers in compressor.
The derivation of this approximation for the total pressure losses assumes the instant mixing of the boundary layers and mainstream fluid while conserving mass and momentum. This profile loss coefficient works for nozzles and rotors as they both have end-wall and blade surface boundaries, which overlap in the passage corners.

\[
Y_p = \frac{\Delta P_i}{P_{i,3} - P_3} = \frac{2\Theta + \Delta^2}{(1 - \Delta)^2}
\]  

(3.133)

where,

\[\Theta = \sum \frac{\theta}{b}, \text{ summed over all end walls,}\]
\[\Delta = \sum \frac{\delta^*}{b}, \text{ summed over all blade surfaces.}\]

The normalized defect thicknesses used in the loss coefficient equation are defined by,

\[
\Theta = 1 - \left[1 - \sum \frac{\theta_w}{b_w}\right]\left[1 - \sum \frac{\theta_b}{b_b}\right]
\]  

(3.134)

\[
\Delta = 1 - \left[1 - \sum \frac{\delta^*_w}{b_w}\right]\left[1 - \sum \frac{\delta^*_b}{b_b}\right]
\]  

(3.135)

where the effective blade-to-blade pitch passage is calculated from the blade pitch and the camber line angle at the blade discharge,

\[b_b = s_3 \sin \beta_3.\]  

(3.136)

The boundary layer momentum thickness at the component discharge is,

\[
\theta = c_f \rho_{ave} \left[\left(u_1/u_3\right)^5 + 2\left(u_2/u_3\right)^2 + 1\right]L/(8\rho_3),
\]  

(3.137)

where,

\[u_1 = \text{inlet velocity},\]
\[u_2 = \text{throat velocity},\]
\[u_3 = \text{discharge velocity},\]
\[L = \text{flow path length},\]
\[c_f = \text{friction coefficient}.\]

Here the average density takes into account the inlet, throat, and exit density as,

\[\rho_{ave} = \left[\rho_1 + 2\rho_2 + \rho_3\right]/4.
\]  

(3.138)

Also the coefficient of friction, \(c_f\), is defined here as it is used in the compressor. The displacement thickness by definition of the shape factor is given by,

\[\delta^* = H\theta.
\]  

(3.139)

The boundary layer thickness, \(\delta\), is defined by the power-law velocity profiles. It is assumed that the boundary layer shape factor for the 1/7th power-power law velocity profile is \(H\).
\[ \delta = \theta H (H + 1) / (H - 1) \]  \hspace{1cm} (3.140)

where 
\[ H = 1.2857 \].

**Volute Analysis**

The first component for analysis is the volute. The thermodynamic conditions are determined from the inlet temperature, pressure, and inlet flow rate. For this stationary component, neglecting frictional losses, the total enthalpy is conserved, thus it is found that \( H_1 = H_3 \). Station 1 is defined as the inlet and Station 3 as the outlet of the component in consideration throughout this report. Hence, Station 2 is a point between the inlet and the outlet of the component. The total static enthalpy of the volute is defined by,

\[ h_3 = H_3 - \frac{1}{2} C_3^2 . \]  \hspace{1cm} (3.141)

**Nozzle Analysis**

The nozzle row in the radial inflow turbine consists of a simple radial passage of constant width. The flow passage area is defined as:

\[ A = b [2 \pi r \sin \beta - t_b N] \], \hspace{1cm} (3.142)

where
\[ b = \text{passage height}, \]
\[ r = \text{radius}, \]
\[ \beta = \text{blade angle with respect to tangent}, \]
\[ t_b = \text{blade thickness}, \]
\[ N = \text{number of blades}. \]

The values for the blade pitch are defined as shown in the equations below, which is then used to find the subsonic discharge angle:

\[ s = 2 \pi r / N , \]  \hspace{1cm} (3.143)

\[ \tan \alpha_3 = \left( r_3 / r_{th} \right) \tan \alpha_{os} , \]  \hspace{1cm} (3.144)

\[ \sin \alpha_{os} = b_{th} o / (s_3 b_3) , \]  \hspace{1cm} (3.145)

where
\[ o = \text{blade to blade width}. \]

The optimum incidence angle, \( i^* \), and the optimum inlet flow angle, \( \alpha^* \), are defined by,

\[ i^* = \left[3.6 \sqrt{10 t_b / L} + |\beta_3 - \beta_i| / 3.4 \sqrt{L / s_3} - |\beta_3 - \beta_i| / 2 \right] , \]  \hspace{1cm} (3.146)
\[ \alpha^* = \beta_1 - i^* \text{sign} (\beta_3 - \beta_1) \] \hspace{1cm} (3.147)

The incidence loss coefficient, \( Y_{inc} \), is proportional to the inlet velocity pressure. Thus, one uses the fraction of the discharge pressure. Here, \( \alpha_1 \), is the inlet flow angle.

\[ Y_{inc} = \sin^2 (\alpha_1 - \alpha^*) \frac{P_{i1} - P_1}{P_3 - P} . \] \hspace{1cm} (3.148)

The nozzle exit total pressure is defined by \( P_{i3} \), where the total loss coefficient for the nozzle is given by \( Y \),

\[ P_{i3} = \left( P_{i1} + YP_3 \right) / (1 + Y) , \] \hspace{1cm} (3.149)

\[ Y = Y_p + Y_{inc} = \left( P_{i1} - P_{i3} \right) / \left( P_3 - P_3 \right) . \] \hspace{1cm} (3.150)

**Rotor Analysis**

For a radial inflow turbine, the flow is turned by 90 degrees from the radial inlet to the axial outlet. There are several losses which need to be accounted for and one begins by first defining a few parameters. The first is the average mean surface curvature which is given by,

\[ \kappa_m = |\phi_3 - \phi_1| / m_3 , \] \hspace{1cm} (3.151)

where

- \( \phi \) = passage curve angle with respect to tangent,
- \( m_3 \) = total meridional path length.

As was done for the nozzle row, it is important to define the subsonic relative discharge flow angle:

\[ \tan \alpha'_3 = \left( r_3 / r_3^h \right) \tan \alpha'_os , \] \hspace{1cm} (3.152)

where

\[ \sin \alpha'_os = b_{o1} \alpha / (s_3 b_3) . \]

The values for the blade pitch are defined using the same equation as for the nozzle; however, for the rotor, it is based on full length blades only.

The optimum (minimal loss) inlet swirl velocity, \( C_{\theta 1}^* \), and absolute flow angle, \( \alpha_1 \), can be calculated using the centrifugal compressor slip factor, \( \sigma \),

\[ C_{\theta 1}^* = \sigma \left[ U_1 - C_{\theta 1} \cot \beta_1 \right] , \] \hspace{1cm} (3.153)
\[ \cot \alpha_1^* = C_{m1} / C_{\theta 1}^* \]  

(3.154)

The basic slip factor, \( \sigma \), applies for most practical cases, however requires an adjustment if the blade solidity is too low. This situation is evaluated by using the slip factor formula below and the impeller radius ratio, \( \varepsilon \).

\[ \sigma = \sin \phi_1 \sqrt{\sin \beta_1 / N^{0.7}}, \]  

(3.155)

\[ \varepsilon = r_3 / r_1. \]  

(3.156)

A simple test is performed to determine if the blade solidity is too low by comparing \( \varepsilon \) with \( \varepsilon_{\text{lim}} \).

\[ \varepsilon_{\text{lim}} = (\sigma - \sigma_o) / (1 - \sigma_o), \]  

(3.157)

where

\[ \sigma_o = \sin(19^\circ + \beta_1 / 5). \]

Thus, if \( \varepsilon > \varepsilon_{\text{lim}} \), then the slip factor is corrected by using the equation below for \( \sigma_{\text{cor}} \).

\[ \sigma_{\text{cor}} = \sigma \left( 1 - \xi \right), \]  

(3.158)

where

\[ \xi = [(\varepsilon - \varepsilon_{\text{lim}}) / (1 - \varepsilon_{\text{lim}})]^{5/10}. \]

The rotor, unlike the nozzles, has more loss sources which need to be defined. Using the absolute angle calculated earlier, one defines the formula for the incidence loss coefficient, \( Y_{\text{inc}} \), below,

\[ Y_{\text{inc}} = \sin^2 \left( \alpha_1 - \alpha_1^* \right) \left[ P_{r1} - P_1 \right] \left[ P_{r3} - P_3 \right]. \]  

(3.159)

The loss coefficient for the blade loading, \( Y_{BL} \), and the hub-to-shroud, \( Y_{HS} \), loading effects are adapted here from the impeller performance analysis that is used for centrifugal compressors as used by Reference [10].

\[ Y_{BL} = \frac{1}{24} \left[ \Delta W / W_3 \right]^2 \]  

(3.160)

where according to Stokes Theorem,

\[ \Delta W = 2\pi r_3 C_{\theta 3} - r_1 C_{\theta 1} / [L(N)], \]  

(3.161)

\[ Y_{HS} = \frac{1}{6} \left[ \frac{\kappa_m b_3 W_2}{W_3 \sin \alpha_3} \right]^2. \]  

(3.162)
The clearance gap loss coefficient, $Y_{CL}$, is calculated by using the average pressure difference across the blade clearance gap, $\Delta P$, which is estimated from the change in angular momentum in the impeller,

$$
Y_{CL} = \frac{\dot{m}_C \Delta P}{\dot{m}_i (P_{r3} - P_3)} \quad (3.163)
$$

$$
\Delta P \left[ \rho_{ave} (rb)_{ave} LN \right] = \dot{m}_i \left[ r_1 C_{\theta1} - r_3 C_{\theta3} \right] \quad (3.164)
$$

The velocity of the leakage flow, $u_{CL}$, across the clearance gap is calculated by,

$$
u_{CL} = \sqrt{2 \Delta P / \rho_{ave}} \quad ,
$$

which then leads to calculating the clearance gap leakage mass flow rate below assuming a gap contraction ratio of 0.816,

$$
\dot{m}_{CL} = 0.816 \rho_{ave} u_{CL} LN \delta_c \quad .
$$

For this rotating component, the “rothalpy” is conserved through the rotor by,

$$
I = H_1 + \Delta H_{DF} - \omega r_1 C_{\theta1} \quad .
$$

Rothalpy in the equation above corrects the inlet total enthalpy for the additional work due to the friction of the rotating disk. Since disk friction parasitic work, $\Delta H_{DF}$, is calculated below for an axial flow turbine, one uses only one-half of the value given, as there is only one side of the disk contributing to this parasitic work.

$$
\Delta H_{DF} = C_M \rho \omega^3 r^5 / \dot{m} \quad ,
$$

where the disk torque coefficient $C_M$, and the torque, $\tau$, are defined below,

$$
C_M = \tau / (\rho \omega^2 r^5) \quad ,
$$

$$
\tau = \dot{m} (r_2 C_{\theta2} - r_1 C_{\theta1}) \quad .
$$

The exit relative enthalpy is defined below, using the variables calculated above,

$$
H'_3 = I + \frac{1}{2} W^2_3 \quad .
$$

Now that all of the loss coefficients are defined, one uses the total loss coefficient, $Y$, and calculates the actual exit relative total pressure at the discharge of the rotor in much the same way that one calculates the relative total pressure at the exit of the nozzle,
\[ Y = Y_P + Y_{inc} + Y_{BL} + Y_{HS} + Y_Q \text{,} \quad (3.172) \]
\[ P_{t3} = \left( P_{t3, id} + YP_3 \right) / \left( 1 + Y \right) \text{.} \quad (3.173) \]

The continuity equation relates the impeller exit mass flow with the flow speed:
\[ \dot{m} = (1 - \Delta)2\pi r_b \rho_3 W_3 \sin \alpha' \text{.} \quad (3.174) \]

The discharge exit static enthalpy is given by,
\[ h_3 = H'_3 - \frac{1}{2} W_3^2 \text{.} \quad (3.175) \]

When the impeller discharge relative flow is known from the subsonic solution as presented thus far, the absolute discharge tangential velocity is given by,
\[ C_{\theta 3} = W_{\theta 3} + U_3 \text{,} \quad (3.176) \]

which leads to the solution for the absolute discharge total enthalpy by,
\[ H_3 = H'_3 + U_3 C_{\theta 3} - \frac{1}{2} U_3^2 \text{.} \quad (3.177) \]

### 3.1.5 Flow Splits

Flow split components in the PDC serve the purpose of splitting a flow into two flows. There is one inlet port and two outlet ports: primary and secondary. The flow fraction, relative to the inlet flow, at the primary outlet port is the only input required by the PDC. The rest of the flow will go to the secondary outlet port.

There is no heat transfer or pressure drop in a flow split. The fluid conditions at both outlet ports are exactly the same those as at the inlet port. Also, for dynamic calculations, there is no volume in the flow splits, so the communication from inlet to outlet is instantaneous,
\[ p_{o1} = p_{o2} = p_i \text{,} \quad (3.178) \]
\[ h_{o1} = h_{o2} = h_i \text{,} \quad (3.179) \]
\[ \dot{m}_{o1} = \dot{m}_{i1} \cdot f_{o1} \text{; } \dot{m}_{o2} = \dot{m}_{i1} \cdot (1 - f_{o1}) \text{,} \quad (3.180) \]

where
\[ i = \text{inlet port,} \]
o1, o2 = primary and secondary outlet ports, respectively, 
fo1 = flow fraction at the primary outlet port (user input).

3.1.6 Mixers

The mixer components serve the reverse purpose to the flow splits. They combine two flows into one. There are two inlet ports, primary and secondary, and a single outlet port. There is no input required for the mixers. The PDC distinguishes primary and secondary inlets only for the purpose of pipe connections.

There is no pressure drop in the mixers and pressures at all three ports are identical. There is no volume or flow accumulation in the mixer, so the outlet flow is equal to the sum of the inlet flows. Also, there is no heat addition, storage, or loss in the mixers, meaning that the total energy outflow is equal to the total energy inflow at two ports:

\[ p_o = p_{i1} = p_{i2}, \quad (3.181) \]
\[ \dot{m}_o = \dot{m}_{i1} + \dot{m}_{i2}, \quad (3.182) \]
\[ \dot{m}_o h_o = \dot{m}_{i1} h_{i1} + \dot{m}_{i2} h_{i2}, \quad (3.183) \]

where
\[ i1, i2 = \text{primary and secondary inlet ports, respectively,} \]
\[ o = \text{outlet port.} \]

3.1.7 Valves

For the purposes of the PDC steady-state calculations, valves only introduce additional pressure drop for the pipe they are located on. In addition to the pipe index, the only other input required for the valve is the valve pressure drop. There are three options for this input:

- Zero pressure drop represents a fully open valve which has no additional flow resistance,
- Any positive number adds that value, in MPa, to the pipe pressure drop,
- If a value of “-1” is provided in the input, the PDC will calculate the valve pressure drop based on the boundary conditions for this pipe and the pipe pressure drop without the valve.

The latter option is to be used for partially closed valves where there is flow but the pressure drop is not known. For example, for the bypass lines, the PDC will calculate required valve pressure drop based on the requested flow rate. In addition, this option needs to be used for fully closed valves, located on the pipes for which the steady-state flow is set to be zero.
There is no heat transfer in the valve, meaning that enthalpy is preserved. However, the fluid temperature can change due to changing pressure at constant enthalpy.

The treatment of the valves in dynamic calculations is described in the dynamic models part of this report in Section 3.2.3.

3.1.8 Pipes

The PDC equations for pipes include heat transfer between the working fluid and the pipe wall and the pressure drop.

3.1.8.1 Heat Transfer in Pipes

The PDC heat transfer equations in pipes include the transfer between the working fluid and the pipe outer surface to the environment (heat loss). The heat loss from the pipe surface is modeled as a combination of convective and radiative heat transfer mechanisms. Convective heat transfer is modeled as natural convection of air around heated cylindrical surfaces. For heat loss calculations, a horizontal pipe arrangement is assumed, and the natural convection heat transfer coefficient for horizontal cylinders provided in the literature [19] is used to calculate heat loss from the pipe:

\[
\frac{HTC_{NC} \cdot D}{k_{air}} = Nu_{NC} = \left\{ 0.60 + \frac{0.387 \cdot Ra^{1/6}_D}{\left[ 1 + (0.559/Pr)^{9/16} \right]^{8/27}} \right\},
\]

where

- \( HTC_{NC} \) = natural circulation heat transfer coefficient,
- \( D \) = pipe outer diameter,
- \( Ra_D = Gr_D \cdot Pr \) = Rayleigh number based on pipe diameter,
- \( Gr_D = \frac{\beta_{air} \cdot g \cdot D^3 \cdot \Delta T}{\nu_{air} \cdot k_{air}} \) = Grashof number,
- \( Pr = \frac{\nu_{air} \cdot Cp_{air} \cdot k_{air}}{\beta_{air} \cdot \rho_{air} \cdot Cp_{air}} \) = air Prandtl number,
- \( \beta_{air}, \nu_{air}, Cp_{air}, k_{air} \) = air coefficient of thermal expansion, kinematic viscosity, specific heat, and thermal conductivity, respectively, calculated at average air temperature, \( \frac{T_s + T_{amb}}{2} \).
- \( \Delta T = T_s - T_{amb} \) = temperature difference between pipe outer surface and ambient air,
- \( g \) = gravitational acceleration.

In steady-state calculations, the heat loss from the working fluid through the pipes to the ambient air due to convection is calculated as:

\[
Q_{HL} = (T_{wf, av} - T_{amb}) \cdot HP \cdot L_{pipe} \cdot N_{pipe},
\]

where

- \( T_{wf, av} \) = average working fluid temperature in the pipe,
\( HP = \) total heat transfer coefficient times perimeter (see below),
\( L_{\text{pipe}} = \) pipe length,
\( N_{\text{pipe}} = \) number of parallel pipe runs, if any.

The total heat transfer coefficient times the perimeter in the above equation is calculated through a sum of thermal resistances of a fluid film, pipe wall, and air film:

\[
\frac{1}{HP} = res_{wf} + res_w + res_{air},
\]

(3.186)

\[
res_{wf} = \frac{1}{HTC_{wf} * \pi * d_i},
\]

(3.187)

\[
res_w = \frac{\ln \frac{d_o}{d_i}}{2 \pi * k_w},
\]

(3.188)

\[
res_{air} = \frac{1}{HTC_{NC} * \pi * d_o},
\]

(3.189)

where
\( d_i, d_o = \) pipe inner and outer diameters,
\( HTC_{wf} = \) heat transfer coefficient on the working fluid side, calculated based on a user-specified heat transfer correlation,
\( k_w = \) pipe wall thermal conductivity,
\( HTC_{NC} = \) natural convection heat transfer coefficient on the air side, calculated using the equation provided above.

The radiative heat transfer from the pipe outer surface is calculated as:

\[
Q_{rad} = \sigma * \epsilon * (T_s^4 - T_{amb}^4) * \pi d_o * L_{\text{pipe}} * N_{\text{pipe}},
\]

(3.190)

where
\( \sigma = \) Stefan-Boltzman constant,
\( \epsilon = \) pipe surface emissivity.

For the 316 stainless steel pipes, the surface emissivity is available at several temperatures [20] (assuming a polished surface) and was fitted with a power law, as shown in Figure 3-33:

\[
\epsilon_{316} = 1 - \frac{1.3685}{T[\degree C]^{0.206}}.
\]

(3.191)

For all other pipe materials, an emissivity of 0.9 is assumed in the PDC.
The total heat loss from the working fluid to air is calculated as a sum of convective and radiative heat losses. At steady-state, the heat loss is used to calculate the working fluid’s enthalpy change in the pipe, which together with the pressure loss will define the properties changes in the pipe.

The PDC does not model the pipe insulation explicitly. However, it includes the provision to account for effects of pipe insulation on the heat loss. In the PDC input, a heat loss multiplication factor, $k_{HL}$, is provided for each pipe. If this factor is set to “1”, then no insulation is assumed to be present on the pipe and there is no modification of the heat loss from the pipe. The pipe heat loss is calculated exactly as described above. In the other extreme, if $k_{HL}=0$, perfect insulation is assumed and there is no heat loss at all for that pipe. Any input between “0” and “1” for a pipe would simulate a less-than-perfect insulation and the heat loss calculated for a bare pipe will be multiplied by that number. Note also that the heat loss multiplication factor can also be used to simulate an enhancement in the heat loss, for example, from the vertical sections of the pipe (as described above, the pipe heat loss is calculated under an assumption of horizontal cylinders). For that, the user needs to provide $k_{HL}$ greater than 1.

3.1.8.2 Pipe Pressure Drop

In the PDC, the pressure drop in pipes consists of a frictional pressure drop along the pipe length, form loss from pipe bends, and the pressure drop in a valve. The latter is described in Section 3.1.7.

The frictional pressure drop in a pipe is calculated based on the average between inlet and outlet pipe conditions, flow rate in the pipe, and the pipe diameter:

$$\Delta p_{fri} = 2\rho V^2 f \frac{L}{D} ,$$

(3.192)
where \( \rho = \) average density in the pipe,
\( V = \) average velocity in the pipe, \( V = \frac{\dot{m}}{\rho A} \),
\( A = \) pipe flow area, \( A = \frac{\pi D^2}{4} \),
\( D = \) inner pipe diameter,
\( f = \) friction factor (see Section 3.4.1),
\( L = \) pipe length.

The pressure drop in the bends is calculated based on the number of bends and the bend radius. These two inputs are supplied by the user. The pipe bends are all assumed to be 90°. The bend pressure drop is calculated in the PDC following Reference [21]:

\[
\Delta p_{\text{form}} = N_{\text{bends}} \frac{\rho V^2}{2} f_{\text{form}} \cdot
\]

The form loss factor is calculated as follows:

\[
f_{\text{form}} = \begin{cases} 
0.00873 \cdot \alpha_{90} \cdot 90^\circ \cdot \frac{1}{R_r} f_c, & \text{if } x < 91 \\
0.0024 \cdot \alpha_{90} \cdot 90^\circ \cdot \frac{1}{R_r^{0.84}} \cdot \frac{1}{Re^{0.17}}, & \text{if } x \geq 91
\end{cases}
\]

where

\[
\alpha_{90} = 0.95 + 17.2 R_r^{1.96},
\]

\[
R_r = \frac{R_{\text{pipe}}}{R_{\text{bend}}} = \frac{1}{2 R_{\text{bend}} D_{\text{pipe}}},
\]

\( R_{\text{bend}} / D_{\text{pipe}} = \) bend curvature (user input),

\[
f_c = \begin{cases} 
0.37 \cdot De^{0.36} \cdot f_{\text{fri}}, & \text{if } Re < Re_{cr} \\
x^{0.05} \cdot f_{\text{fri}}, & \text{if } Re \geq Re_{cr}
\end{cases}
\]

\[
x = Re R_r^2 ,
\]

\[
De = \frac{Re}{2 \sqrt{R_r}} ,
\]

\[
Re_{cr} = 2400 \cdot (1 + 8.6 R_r^{0.45}) \cdot 0.45 ,
\]

\( f_{\text{fri}} = \) friction factor (see above),

\( Re = \) Reynolds number.
### 3.2 Dynamic Models

This section of the report describes the dynamic, i.e., time-dependent, equations in the PDC used to obtain a transient solution. The general approach is to solve partial differential equations with respect to time to obtain the variation of the system parameters, such as pressures, temperatures, and flow rates, for the cycle and individual components as a transient progresses with time. The detailed description of the PDC dynamic equations for the cycle and individual components is provided in the following section of the report. The PDC dynamic model also integrates the various control mechanisms which are also described in the report sections below.

#### 3.2.1 General Formulation of Dynamic Equations in PDC

Since the primary purpose of the PDC is the analysis of supercritical cycles, the dynamic equations in the PDC are generally formulated for the case of a compressible fluid (the simplifications for approximately incompressible flow are described in Section 3.2.9). Consider a flow of a compressible fluid in a heated channel (Figure 3-34).

![Figure 3-34. Flow in a Channel.](image)

The dynamical behavior of a compressible flow in a channel is described by mass (3.195), momentum (3.196), and energy (3.197) conservation equations [22]:

\[
\frac{\partial}{\partial t} \int_V \rho \, dV + \int_S \rho \, \vec{u} \cdot \vec{n} \, dS = 0 ;
\]

\[
\frac{\partial}{\partial t} \int_V \rho \, dV + \int_S \rho (\vec{u} \cdot \vec{n}) \, dS = \int_V \rho \, \vec{g} \, dV + \int_S \vec{n} \cdot \vec{r} \, dS ;
\]

\[
\frac{\partial}{\partial t} \int_V \left( \rho \, e + \frac{1}{2} \rho (\vec{u})^2 - \rho \, \vec{g} \cdot \vec{x} \right) \, dV + \int_S \left( \rho \, e + \frac{1}{2} \rho (\vec{u})^2 - \rho \, \vec{g} \cdot \vec{x} \right) \, \vec{n} \cdot \vec{n} \, dS
\]

\[
= -\int_S \vec{q} \cdot \vec{n} \, dS + \int_S \vec{n} \cdot (\vec{r} \cdot \vec{u}) \, dS .
\]
where \( S = \text{boundary of the volume } V \),
\( \vec{n} = \text{normal to the surface } S \),
\( \rho = \text{density} \),
\( \vec{u} = \text{velocity} \),
\( \vec{g} = \text{gravitational acceleration} \),
\( \tau = \text{stress tensor} \),
\( e = \text{internal energy} \),
\( \vec{q} = \text{heat flux} \).

The following assumptions are made to simplify the dynamic equations.

- Ignore gravitational effects.
- Stress is represented by the friction at the channel wall only. This assumption means that the form losses are neglected compared to the frictional losses, with the exception of the form losses in pipe bends, which are included in the equations. Also, the equations are to be applied to a channel of constant cross-sectional area \((A=\text{const})\). The treatment of the flow through a valve—where form losses are important—is described separately below.
- Ignore acceleration pressure drop.
- Ignore energy loss due to friction.
- The total energy is represented by the specific enthalpy. This assumption means ignoring the kinetic energy of the flow. Since the kinetic energy is important in turbomachinery, this model is to be applied to the flow in heat exchangers and piping; a separate model is used for turbomachinery.
- The flow in the volume is characterized by mean properties and flow rates.

Under these assumptions, the conservation equations can be expressed in the following forms, respectively [23]:

\[
\frac{\partial p}{\partial t} = \frac{m_{\text{in}} - m_{\text{out}}}{A \Delta x}; \tag{3.198}
\]

\[
\frac{\partial m}{\partial t} = \left( p_{\text{in}} - p_{\text{out}} \right) \frac{A}{\Delta x} - 2 f \frac{\bar{m}^2}{A \rho D_h}; \tag{3.199}
\]

\[
\frac{\partial h}{\partial t} = \frac{1}{\Delta x A \bar{p}} \left[ m_{\text{in}} (h_{\text{in}} - \bar{h}) - m_{\text{out}} (h_{\text{out}} - \bar{h}) + q' \Delta x \right]. \tag{3.200}
\]

To apply Equations (3.198) through (3.200) in a computer code, they should be expressed in three variables only—flow rate and two variables that define the fluid state. Since the working fluid properties in the PDC (see Section 3.4.2.1) are originally defined in terms of the temperature and density, selecting these variables would simplify the properties calculations and, therefore, increase the computational speed of the dynamics code. The other parameters (enthalpy and pressure) are expressed in terms of the temperature and density as following:
\[
\frac{\partial h}{\partial t} = \left( \frac{\partial h}{\partial T} \right)_\rho \frac{\partial T}{\partial t} + \left( \frac{\partial h}{\partial \rho} \right)_T \frac{\partial \rho}{\partial t} = h_T \frac{\partial T}{\partial t} + h_\rho \frac{\partial \rho}{\partial t} ;
\]

\[
\frac{\partial p}{\partial t} = \left( \frac{\partial p}{\partial T} \right)_\rho \frac{\partial T}{\partial t} + \left( \frac{\partial p}{\partial \rho} \right)_T \frac{\partial \rho}{\partial t} = p_T \frac{\partial T}{\partial t} + p_\rho \frac{\partial \rho}{\partial t} .
\]

The partial derivatives in Equations (3.201) and (3.202) are derived analytically from the known functions, \( p=p(T,\rho) \), \( h=h(T,\rho) \), and are calculated along the other properties by the properties subroutine.

The fluid conditions (temperature and density) are calculated at the region boundaries (inlet and outlet); the flow rate is calculated between the boundaries (Figure 3-34). In order to calculate the density at the boundary, Equation (3.198) is applied to the region consisting of two halves of the temperature regions from each side of the boundary (Figure 3-35),

\[
\hat{\rho}_i \frac{\Delta x_i}{A} \left( \frac{\Delta x_i}{2} + \frac{\Delta x_{i+1}}{2} \right) \left( \dot{m}_i - \dot{m}_{i-1} \right) = \frac{1}{A} .
\]

The momentum Equation (3.199) applied to the region in Figure 3-35 gives

\[
\hat{m}_i \frac{\Delta x_i}{A} (p_i - p_{i+1}) - \frac{2 f_i \Delta x_i}{M_i D_h} m_i^2 = \frac{A}{\Delta x_i} .
\]
where
\[ M_i = A \bar{\rho} \Delta \chi_i = \text{fluid mass in region } i. \]

To apply the energy Equation (3.200) to the temperature region in Figure 3-35, an assumption of perfect mixing is made. Under this assumption, the enthalpy of the flow leaving the region is the same as the average enthalpy in the region (\( h_{out} \approx \bar{h} \)). The heat flux from the wall is defined by the temperature difference between the wall and average fluid temperature and the thermal resistance between the wall and the flow, similar to the steady-state equations for heat exchangers in Section 3.1.2. The inlet flow rate is calculated as an average between the flow rates adjacent to the inlet boundary,

\[
\frac{\partial h_i}{\partial t} = \frac{1}{M_i} \left( \frac{\bar{m}_i + \bar{m}_{i-1}}{2} \right) (h_i - h_{i-1}) + \frac{\Delta \chi_i N_t}{M_i \text{res}_{w,\text{fluid}}} \left( T_{w,i} - \frac{T_i + T_{i+1}}{2} \right), \tag{3.205}
\]

where
\[ N_t = \text{total number of channels (tubes) for heat transfer}, \]
\[ \text{res}_{w,\text{fluid}} = \text{thermal resistance between the wall and fluid (calculated as described in Equation (3.188) for the steady-state models)}. \]

Equations for the wall temperatures are formulated in a similar manner using the definition of thermal resistances from the steady-state analysis. A single wall temperature, \( T_{w,i} \), in Figure 3-35, is calculated for each fluid node:

\[
\frac{\partial T_{w,i}}{\partial t} = \frac{\Delta \chi_i N_t}{M_{w,i} C_{pw} \text{res}_{w,\text{fluid}}} \left( \frac{T_i + T_{i+1}}{2} - T_{w,i} \right) + \frac{\Delta Q_i}{M_{w,i} C_{pw}}, \tag{3.206}
\]

where
\[ M_{w,i} = \text{wall mass in the region}, \]
\[ C_{pw} = \text{wall heat capacity}, \]
\[ \Delta Q_i = \text{external heat addition or sink, if any (used for electrical heaters and heat loss from pipes)}. \]

If Equation (3.206) is applied to the heat exchanger wall, it has two similar terms for heat transfer with the hot-side and cold-side fluids with corresponding fluid temperatures and thermal resistances.

For the equation solver in the PDC, all previous equations are written in terms of coefficients in front of the functions for which the solution is obtained. For example, Equation (3.205) is being solved in the PDC in the form:

\[
\frac{\partial h_{i+1}}{\partial t} = B_{h,i} \frac{\bar{m}_i + \bar{m}_{i+1}}{2} (h_i - h_{i+1}) + A_{h,w,i} \left( \frac{T_i + T_{i+1}}{2} - T_{w,i} \right). \tag{3.207}
\]

All other equations are written in a similar manner. The notation in the PDC is adopted that the coefficients, \( A \), are those in front of single functions, while \( B \)'s are in front of some multiplication of a function (\( \bar{m} \cdot h \) in Equation (3.207), for example). All those coefficients in Equations (3.203)-(3.207) are calculated in the subroutines, Coef_BC and Coef_BC_HX, at the beginning of
a time step. They are then assumed to be constant during the time step to obtain the solution of the differential equations.

To calculate the other properties derivatives, Relationships (3.201) and (3.202) are used:

\[
\frac{\partial T_{r+1}}{\partial t} = \frac{1}{h_{r,i}} \left( \frac{\partial h_{r+1}}{\partial t} - \frac{\partial h_{r,i}}{\partial t} \right); \\
\frac{\partial p_{r+1}}{\partial t} = p_{r,i} \frac{\partial T_{r+1}}{\partial t} + p_{r,i} \frac{\partial p_{r+1}}{\partial t}. 
\]

(3.208) (3.209)

3.2.2 Flow Branches and Reverse Flow

At the cycle flow merge points, there is more than a single inlet flow. Therefore, Equation (3.203) should have more than one inlet flow term. Also, Equation (3.205) will have more than one term for the heat addition due to inlet flows. Similarly, Equation (3.203) should be modified to include more than one outlet flow for the flow split points. Also, the volumes for Equation (3.203) will include three terms for the merge and split point. Therefore, Equations (3.203) and (3.205) are modified as follows.

Before the dynamic calculations, the volumes for each density point are calculated. These volumes include two adjustment region halves for the regular point and three halves for flow split/merge points. Then, in the dynamic calculations, the derivative of the density is calculated as a sum of all of the inlet flow rates minus the sum of all outlet flow rates divided by the volume:

\[
\frac{\partial \rho_j}{\partial t} = \frac{1}{V_{\rho,i}} \left[ \sum_{i=\text{in}} m_i - \sum_{i=\text{out}} m_i \right]. 
\]

(3.210)

The subscript, \(\rho\), is used for the volume to distinguish it from the volumes for the enthalpy equations.

The same approach is used for Equation (3.205) to account for several inlet flows. This approach is combined with the treatment of negative (reversed) flows as described below.

A solution of the flow equation may result in a reversed flow, i.e. negative values of flow rates. The reversed flow would exchange the inlet and outlet points in Equations (3.203)-(3.205). To account for reversed flows and their effect on the equations, the following approach is used.

Before the dynamic calculations, two arrays are generated which define inlet and outlet nodes for each flow rate in the system (including flows in the heat exchangers) under steady-state (positive flow) conditions. If, during a transient, the flow is positive, then the outlet node for this flow as the same as at steady-state; if the flow is negative, then the outlet node is the steady-state inlet node. At the beginning of a time step, the density and enthalpy derivatives for each point are set to zero. Then, for each flow rate, the value of the density derivative is increased at the outlet node.
and decreased at the inlet node. Also, the value of the enthalpy derivative is increased for the outlet node.

\[
\frac{\partial \rho_{i-out}}{\partial t} = \frac{\partial \rho_{i-out}}{\partial t} + \frac{1}{V_{i-out}} \dot{m}_i, \tag{3.211}
\]

\[
\frac{\partial \rho_{i-in}}{\partial t} = \frac{\partial \rho_{i-in}}{\partial t} - \frac{1}{V_{i-in}} \dot{m}_i, \tag{3.212}
\]

\[
\frac{\partial h_{i-out}}{\partial t} = \frac{\partial h_{i-out}}{\partial t} + \frac{1}{M_i} \dot{m}_i \left( h_{i-in} - h_{i-out} \right) + \frac{\Delta x_i N_i}{M_{res_{w, fluid}}} \left( T_{w,j} - \frac{T_j + T_{res}}{2} \right) \tag{3.213}
\]

where

\( i-in \) and \( i-out = \) indices for the inlet and outlet nodes for flow, \( \dot{m}_i \),

the heat transfer term is omitted for the pipes.

In a similar fashion, the flow equation is modified to account for negative flow:

\[
\frac{\partial \dot{m}_i}{\partial t} = \frac{A}{\Delta x_i} (p_i - p_{in}) - \frac{2 f_i \Delta x_i}{M_i D_h} \dot{m}_i |\dot{m}_i|, \tag{3.214}
\]

In order to fully implement the reversed flow treatment, the enthalpy Equation (3.213) is further modified in the PDC to calculate the enthalpy change based on the flow rate inside each node, rather than the average flow rate at the inlet border. With the possibility of flow going in different directions, the meaning of the average inlet flow is not clear and replacing it with the flow rate inside each node is a more accurate representation of energy transfer with the flow in this node:

\[
\frac{\partial h_{i-out}}{\partial t} = \frac{\partial h_{i-out}}{\partial t} + \frac{1}{M_i} \dot{m}_i \left( h_{i-in} - h_{i-out} \right) + \frac{\Delta x_i N_i}{M_{res_{w, fluid}}} \left( T_{w,j} - \frac{T_j + T_{res}}{2} \right). \tag{3.215}
\]

The treatment of flow splits and flow mixers in dynamics is different from that in the steady-state. Because of the possibility of reversed flow, there is no clear distinction of flow splits and flow mixers anymore. Depending on the flow direction, a split can be acting as a mixer if more flows are coming in than going out of that component. There could even be a situation when all flows would be leaving from the component or all flows coming into the component, so the component could not be characterized as either a split or mixer anymore. Similarly, there would not be a clear definition of the inlet and outlet ports for these components in a transient.

To account for these situations, a new treatment of flow splits and mixers is implemented in the PDC dynamic equations as shown in Figure 3-36. The component is still treated as being a zero-volume component and the fluid conditions at all ports (called inlet and outlet at steady-state) are set to the common conditions (for example, the common enthalpy, \( h_i \), in Figure 3-36). That common enthalpy is calculated from the energy influx from all the flows coming to that node as shown in the equations in Figure 3-36. The outwards flows do not affect the enthalpy change in
the node. Note that the dynamic enthalpy equation is shown in Figure 3-36 in a simplified form, while in the code, there would be an extra term for the heat transfer with the pipe wall as described in Section 3.2.5. The change in density is calculated from all flow rates, both inlet and outlet.

Figure 3-36. Flow Splits and Mixers in Dynamics.

Figure 3-36 describes a general concept of treating flow branches in the PDC dynamic equations. For the actual equations implemented in the code, there are still split and mixer components and the designation of the inlet and outlet ports exists as in the steady-state model. So, the derivatives described in Figure 3-36 are combined in the code to obtain the common derivative for all ports as described below.

For example, for a mixer with two inlet flows, \( i_1 \) and \( i_2 \), and one outlet flow, \( o_1 \), all enthalpies are set to be equal to the outlet enthalpy at the dynamics initialization step:

\[
h_{i1} = h_{i2} = h_{o1}.
\]  

During the dynamic calculations, the changes in enthalpy are calculated only for flows which enter the mixer. For example, if flows are still in the same direction as in steady-state, then the derivatives for \( h_{i1} \) and \( h_{i2} \) are calculated:

\[
\frac{\partial h_i}{\partial t} = \ldots + \dot{m}_{i1}(h_{i1-1} - h_{i1});
\]  

\[
\frac{\partial \rho_i}{\partial t} = \frac{1}{V_i} \left[ \sum_{\text{in}} \dot{m}_j(h_j - h_i) - \sum_{\text{out}} \dot{m}_i \right].
\]
\[
\frac{\partial h_{i2}}{\partial t} = \cdots + \dot{m}_{j2}(h_{i2-1} - h_{i2}) ;
\]

\[
\frac{\partial h_{o1}}{\partial t} = \cdots + 0 ;
\]

where \( j_1 \) and \( j_2 \) correspond to the inlet flow nodes for nodes \( i_1 \) and \( i_2 \), respectively.

As stated above, there would be other components in enthalpy Equations (3.217)-(3.219) for the heat transfer to the wall, which are omitted from the above equations for simplicity and replaced with “...”.

When all changes from the inlet flows are calculated, then the derivatives are added to insure the same properties for all nodes:

\[
\frac{\partial h_{o1}}{\partial t} = \frac{\partial h_{i1}}{\partial t} + \frac{\partial h_{i2}}{\partial t} + \frac{\partial h_{o1}}{\partial t} ;
\]

(3.220)

\[
\frac{\partial h_{i1}}{\partial t} = \frac{\partial h_{o1}}{\partial t} ;
\]

(3.221)

\[
\frac{\partial h_{i2}}{\partial t} = \frac{\partial h_{o1}}{\partial t} .
\]

(3.222)

Since the enthalpies are set to be equal at the first time step and all the derivatives of the enthalpies are equalized at each time step, the enthalpies for all mixer ports will be equal at each time step.

A similar approach is applied to the density equations as well as for the splitters. When the derivatives for the enthalpies and densities are calculated, the derivatives for other properties, - temperature and pressure, - are calculated using the partial derivative definitions in Equations (3.201) and (3.202).

The main advantage of this approach is that it applies the common treatment to the mixers and flow splits and no complicated checking is required to see if, for example, a split is acting as a mixer with reversed flows. It preserves the energy balance in all flow branches under all possible flow directions and combinations. The only drawback of this approach is that the information on the incoming temperatures for the mixers and splitters is lost. For example, for the turbine bypass mixing location, the new approach does not allow tracking of the temperature coming in from the bypass line. The inlet temperature from the main line is very close to that at the turbine outlet. However, the bypass line usually involves a significant pressure drop through the bypass valve, such that the temperature downstream of the valve could be significantly different from that on the upstream side of the valve. It is noted, however, that the incoming temperatures are not used in the dynamic equations, which are based on the enthalpies. As described above, the enthalpy equations would still account for the differences between the enthalpies in the incoming flows in the new mixer treatment.
3.2.3 Valves

Valves are used in the PDC cycle model for control purposes. The valves are used to regulate flow by adding a resistance to the flow. In order to model the hydraulic resistance presented by a valve, a momentum Equation (3.214) is modified to account for the pressure losses in the valve. The valve is simulated in the PDC as a sudden flow area contraction followed by a sudden flow area expansion. The total pressure loss is represented by the sum of the form losses from contraction and expansion:

$$\Delta p_v = \frac{1}{2} K_{\text{contr}} \rho u_{\text{small}}^2 + \frac{1}{2} K_{\text{exp}} \rho u_{\text{small}}^2,$$  \quad (3.223)

where

$$K_{\text{contr}} = \frac{1}{2} \left(1 - \frac{A_{\text{open}}}{A_{\text{total}}}\right) = \text{contraction loss coefficient},$$

$$K_{\text{exp}} = \left(1 - \frac{A_{\text{open}}}{A_{\text{total}}}\right)^2 = \text{expansion loss coefficient},$$

$A_{\text{open}} = \text{flow area open to the flow (flow area inside a valve)},$

$A_{\text{total}} = \text{total flow area (flow area outside a valve)},$

$\rho = \text{density},$

$u_{\text{small}} = \text{flow speed at the opening}.$

The following variables are introduced to simplify Equation (3.223):

- The ratio of the open area to the total area is defined as the valve open area fraction. The fraction is either user-defined or a result of the control calculations,

$$f_{\text{open}} = \frac{A_{\text{open}}}{A_{\text{total}}},$$ \quad (3.224)

- Two loss coefficients are combined to form a valve loss coefficient:

$$K_v = K_{\text{contr}} + K_{\text{exp}} = \frac{1}{2} \left(1 - f_{\text{open}}\right) + \left(1 - f_{\text{open}}\right)^2 = \frac{1}{2} \left(1 - f_{\text{open}}^2\right) + 1 - 2f_{\text{open}} + f_{\text{open}}^2$$

$$= \frac{1}{2} - \frac{1}{2} f_{\text{open}} - f_{\text{open}} + f_{\text{open}}^2 = \frac{1}{2} \left(1 - f_{\text{open}}\right) - f_{\text{open}} \left(1 - f_{\text{open}}\right)$$

$$= \left(1.5 - f_{\text{open}}\right) \left(1 - f_{\text{open}}\right) \quad (3.225)$$

- The flow speed is calculated based on the continuity equation:

$$u_{\text{small}} = \frac{\dot{m}}{\rho A_{\text{open}}}.$$ \quad (3.226)
- The density is calculated as the average density between inlet and outlet conditions:

\[ \rho = \frac{\rho_{\text{in}} + \rho_{\text{out}}}{2} \]  \hspace{1cm} (3.227)

Using the above definitions, the pressure drop across the valve becomes:

\[ \Delta p_v = \frac{1}{2} K_v \frac{1}{\rho} \frac{1}{A_{\text{open}}} \dot{m}^2 = \frac{1}{2} K_v \frac{1}{\rho} f_{\text{open}}^2 \frac{1}{A_{\text{val}}} \dot{m}^2 \]  \hspace{1cm} (3.228)

The open area fraction in the denominator is added to the valve loss coefficient to collect valve openings in one function:

\[ K'_v = K_v \frac{f_{\text{open}}^2}{f_{\text{open}}^2} = \left(1.5 - f_{\text{open}}\right) \left(1 - f_{\text{open}}\right) \]  \hspace{1cm} (3.229)

After the derivatives for all flow rates in the cycle are calculated using Equation (3.214), the derivatives of the flow rates through valves are corrected to add the valve resistance (Equation (3.228) is corrected to allow for a negative flow):

\[ \frac{\partial \dot{m}_{i-v}}{\partial t} = \frac{\partial \dot{m}_{i-v}}{\partial t} - \frac{A_{i-v}}{2 \rho A_{i-v}^2} K'_v \dot{m}_{i-v} \] \hspace{1cm} (3.230)

where

\[ i\cdot v = \{2, 25, 28, 29, 30, 31\} = \text{indices for the valves locations.} \]

### 3.2.4 Critical Flow Limitation

According to the momentum Equation (3.214), the flow between two points is determined by the pressures at those points. Pressure waves travel through a fluid at the sound speed. If the flow rate is high enough that the local speed reaches the sonic speed, the conditions downstream of this point could not be communicated upstream any more. Therefore, the flow rate cannot increase even if outlet pressure decreases. This condition is called critical flow.

Critical flow occurs when the local speed reaches the speed of sound. According to the continuity equation, speed is reciprocal to the flow area, so that the maximum speed is achieved at the minimum flow area. In the cycle, the minimum flow areas occur at valve openings. Therefore, it is expected that the flow in a valve could reach critical flow. The flow could not be increased beyond the critical flow no matter how low the outlet pressure is, even if Equation (3.214) allows for that. So, the critical flow rate should be calculated for the conditions of each valve and the limitation of the critical flow should be applied to the flow.
Consider flow through a valve (Figure 3-37). The conditions of the flow before the valve (Point 1) are given. At critical flow, the flow speed in the opening is equal to the sound speed defined by local properties.

\[ u_0 = V_{s,0} = V_s(h_0, s_0), \]  

(3.231)

where \( V_s \) = sound speed.

![Figure 3-37. Flow Through a Valve Opening.](image)

The critical flow rate is defined from the continuity equation.

\[ \dot{m}_c = \rho_0 u_0 A_0 = \rho_0 u_0 A_{\text{open}}, \]  

(3.232)

where

\[ f_{\text{open}} = \frac{A_0}{A_1} = \text{valve open area fraction}. \]

To find the conditions at the opening and the local sound speed, an iterative process is applied. It is assumed that the flow through the valve is isentropic, i.e. \( s_0 = s_1 \). Suppose that the density and enthalpy at the opening are known (for the first approximation, the inlet parameters could be taken). Then the continuity equation defines the flow speed before the valve:

\[ u_1 = \frac{\dot{m}_c}{\rho_1 A_1}. \]  

(3.233)

The enthalpy at the opening is found from the total energy conservation equation:

\[ h_1 + \frac{u_1^2}{2} = h_0 + \frac{u_0^2}{2}; \]  

(3.234)

\[ h_0 = h_1 + \frac{u_1^2}{2} - \frac{u_0^2}{2} = h_1 + \frac{1}{2} \left( \frac{\dot{m}_c}{\rho_1 A_1} \right)^2 - \frac{V_{s,0}^2}{2} = h_1 + \frac{1}{2} \left( \frac{\rho_0 A_1 V_{s,0}}{\rho_1 A_1} \right)^2 - \frac{V_{s,0}^2}{2} \]  

(3.235)
When the enthalpy and entropy at the opening are known, the density and the sound speed are recalculated based on the fluid properties,

\[
\rho_0 = \rho(s_0, h_0),
\]

\[
V_{s,0} = V_v(s_0, h_0).
\]

The iterations through Equations (3.232)-(3.238) are continued until convergence on the flow rate is achieved. Then the critical flow limits are applied to the flow rate calculated by Equations (3.214) and (3.230); i.e., the flow rate is not allowed to exceed the critical flow rate.

Note that the critical flow rate does not depend on the conditions downstream of the valve (Point 2 in Figure 3-37) as it should be, since, at critical flow, the downstream conditions are not communicated back to the inlet point.

Although the critical flow algorithm is developed for the flow through a valve, it is also applied to every flow in the cycle. Indeed, if a flow doesn’t go through a valve, then \( f_{\text{open}} = 1 \), and conditions at point 0 are the same as those at point 1. Therefore, the iterative process will automatically converge after just one iteration. So, the critical flow is calculated and limitations are applied to every flow in the cycle.

Because of the possibility of reversed flow, the critical flow rate is calculated for both directions. The critical flow in the reversed direction, \( \dot{m}_{c}^{-} \), is defined by the conditions which are outlet conditions for normal flow (Point 2 in Figure 3-37). The critical flow in the reversed direction is negative and the flow rate should always be between those two critical flows:

\[
\dot{m}_{c}^{-} \leq \dot{m} \leq \dot{m}_{c}.
\]

According to Equations (3.237) and (3.238), the iterative scheme for the finding the critical flow rate requires calculating the density and sound speed as functions of enthalpy and entropy. Since the working fluid properties in the PDC are defined as functions of temperature and density, using Equations (3.237) and (3.238) requires multiple iterations on the fluid properties. Because of the complicated properties calculations, these iterations are too slow to be used in the dynamics code. Therefore, the following approach has been taken to eliminate iterations on properties. Tables of working fluid properties have been generated to provide pressure, temperature, density, and sound speed as a function of enthalpy and entropy (called “h-s tables”). The h-s tables cover the entire possible range of operating conditions for the cycle (temperatures from 230 K to 1100 K, pressures from 0.05 MPa to 50 MPa). The tables provide the properties at fixed \((h_i, s_j, i,j=1..500)\) points; linear interpolation is used between the points. In all regions, except the two-phase region, the properties are defined by the properties subroutines. In two-phase region, Henry’s formula [24] is used to calculate the sound speed:
\[ V_s = \left( \frac{[(1-x)\rho^* + x\rho']^2 + x(1-x)(\rho' - \rho^*)^2}{x(\rho')^2 + (1-x)(\rho^*)^2} \right)^{1/2} \]  \hspace{1cm} (3.240)

\[ h = xh'' + (1-x)h' \]  \hspace{1cm} (3.241)

\[ s = xs'' + (1-x)s' \]  \hspace{1cm} (3.242)

\[ \frac{1}{\rho} = \frac{x}{\rho''} + \frac{1-x}{\rho'} \Rightarrow x = \frac{1}{\rho} \frac{1}{\rho'' - \rho'} \]  \hspace{1cm} (3.243)

where \( y' \) and \( y'' \) denote liquid and gas properties, respectively.

The \( h-s \) tables are based on the properties only and need to be generated only once. They are stored in a file and are read before the calculations start. The tables have also proved to be useful as a first guess for iterations in turbomachinery calculations which frequently employ calculations of the properties based on the specific enthalpy and entropy.

The \( h-s \) tables are only used in the critical flow calculations. Other properties calculations, such as for Equations (3.211)-(3.214), are based on the exact properties subroutines and do not use the tables. Although using the tables instead of the exact calculations will result in some error, that error is not expected to be significant for system performance for the following reasons. Critical flow is expected to occur in valves. The PDC valve model described in Section 3.2.3 is an approximation itself since the valves are simulated by the sudden contraction/sudden expansion process. Also, the valves themselves are regulated by the cycle control system. The control mechanisms monitor the system parameters and adjust the valve openings accordingly. However, valve opening itself does not affect the system performance – it is the flow rate through the valve that is important. So, the control mechanisms effectively adjust the flow rate through the valves. Therefore, if there is an error in the critical flow rate calculation, the flow rate will be slightly different from the actual value, but the control system will still be adjusting the flow rate to a required value so that the resulting valve opening calculated by the control system may differ slightly from the actual value. Thus, the reported valve opening may not be exact due to utilization of the properties tables, but the flow rate still will be accurate such that the system performance is not affected.

Even with the properties tables, calculation of critical flow requires iterations on Equations (3.232)-(3.238). So, the critical flow rate is calculated only at the beginning of the time step. However, it is found that smooth variation of a valve open area is beneficial to the stability of the control system action. Therefore, the critical flow rate should also change smoothly during the time step. It is assumed that during the time step, the parameters of the flow in the opening are constant and the critical flow rate is proportional to the valve open area fraction according to
Equation (3.232). The flow parameters and the critical flow rate are recalculated at the beginning of the next step.

Implementing Equations (3.229)-(3.230) will result in a numerical singularity when a valve approaches the fully closed position \((f_{\text{open}} \rightarrow 0 \Rightarrow K_v' \rightarrow \infty)\). To avoid this problem, a threshold value for a valve opening is introduced. If the opening is below this threshold value, then the flow is assumed to be critical, and calculations of Equations (3.229) and (3.230) are skipped. A 1% open area is assumed for this threshold in the code.

### 3.2.5 Pipes

The equations derived so far in this chapter are applied to the flows in the pipes. They include:

- The equations for the fluid enthalpy and density change at each end of the pipe, with the equations for flow branching when needed;

- The flow rate equation, including frictional and pipe bend pressure losses, the effects from the valves, and subject to critical flow limitations,

- The equation for the pipe wall temperature.

The volumes for the dynamic equations are calculated by splitting the pipe length in half. One half is added to the volume for the inlet point (in steady-state terms), while the other half is added to the outlet volume. When a pipe is connected to a heat exchanger, the volume for this node consists of one-half of the pipe volume, one-half of the first (or last, depending on the connection) heat exchanger region volume, and the user-specified volume at the heat exchanger inlet/outlet (such as for an inlet/outlet header).

The pipe wall temperature is calculated as shown in Equation (3.206). The heat loss term, \(\Delta Q_i\), is calculated at the beginning of each time step as described in the steady-state model (see Section 3.1.8.1). It is assumed that the heat loss rate from the pipe to the environment is fixed during a time step, so the \(\Delta Q_i\) term in Equation (3.206) is treated as a constant for the solution of the dynamic equation during a time step.

### 3.2.6 Heat Exchangers

#### 3.2.6.1 Counter-Flow Heat Exchangers

Equations (3.203)-(3.209) are readily applied to the flow in counter-flow heat exchangers. This type of heat exchanger is used for the majority of the heat exchangers in the PDC. Only the cross-flow heat exchanger options for the cooler require a special approach for formulation and solution of dynamic equations, as is described in the next section.
For counter-flow heat exchangers, the same one-dimensional treatment with several nodes along the heat exchanger length is used for the dynamic part of the PDC as it is in the steady-state models. The same number of nodes along the heat exchanger length is used in dynamics as in the steady-state models. For the boundary nodes (HX inlet or outlet), the parameters of the connecting pipes (Δx and m) are used in Equations (3.203) and (3.205), if the index is beyond the heat exchanger (e.g. m_{i-1} is equal to the flow rate in the inlet pipe for region i=1).

The wall temperature Equation (3.206) does not include additional heat transfer terms but includes the heat transfer to both the hot- and cold-side fluids:

\[
\frac{\partial T_{w,i}}{\partial t} = \frac{\Delta x_i N_t}{M_{w,i} C_{pw}} \left[ \frac{1}{r \text{e}_{w,h}} \left( \frac{T_{i+1}^h + T_i^h}{2} - T_{w,i} \right) + \frac{1}{r \text{e}_{w,c}} \left( \frac{T_{i+1}^c + T_i^c}{2} - T_{w,i} \right) \right]
\]

(3.244)

where

- \( \Delta x_i \) = region length,
- \( N_t \) = number of parallel channels (tubes),
- \( M_{w,i} \) = wall mass in the region,
- \( C_{pw} \) = wall heat capacity,
- \( r \text{e}_{w,h} = r \text{e}_h + r \text{e}_w/2 \),
- \( r \text{e}_{w,c} = r \text{e}_c + r \text{e}_w/2 \),
- \( r \text{e}_h, r \text{e}_c, r \text{e}_w \) = thermal resistances for hot side, cold side, and wall, respectively, calculated the same way as for the steady-state models (Section 3.1.2).

The wall mass is calculated for each node prior to a transient based on the room temperature density, cross-sectional area of the HX wall structure (which depends on the HX type), and the node length. This mass is fixed during the entire transient.

### 3.2.6.2 Cross-Flow Heat Exchangers for the Cooler

The cross-flow heat exchanger configuration unavoidably requires solution of a two-dimensional temperature field (Figure 3-38) to accurately track the properties variations, – a necessity near the critical point where the coolers operate.
For the steady-state solution in the PDC, there is a separate subroutine specifically for cross-flow heat exchangers, in order to avoid mixing one-dimensional (for counter-flow heat exchangers) and two-dimensional temperature arrays in the same subroutine. A similar approach could not be easily applied to the dynamic solver, since this subroutine seeks the solution of all cycle differential equations simultaneously and, therefore, does not have a separate subroutine to solve just the cooler equations. Thus, to include the possibility to solve two-dimensional temperature fields in the cooler, all arrays related to the cooler, including temperature, density, pressure, enthalpy, and flowrate, have an extra dimension. Since this extra dimension is not needed for counter-flow heat exchangers, the number of nodes in this direction is set to one for all heat exchanger options, except for cross-flow HXs.

To simulate the flow of two fluids flowing in different directions, the arrays which specify inlet and outlet temperature nodes for each heat transfer (HT) region include an extra dimension. There are two arrays that specify inlet/outlet temperature nodes in the “horizontal” and “vertical” directions. For the example in Figure 3-38 with a normal (not reversed) flow direction in the cooler, the inlet/outlet nodes for HT region \([i,j]\) are specified as follows:

\[
\begin{align*}
\text{Hot side:} & & i_{\text{in hot}}[i,j] &= i & j_{\text{in hot}}[i,j] &= j \\
& & i_{\text{out hot}}[i,j] &= i + 1 & j_{\text{out hot}}[i,j] &= j \\
\text{Cold side:} & & i_{\text{in cold}}[i,j] &= i & j_{\text{in cold}}[i,j] &= j \\
& & i_{\text{out cold}}[i,j] &= i & j_{\text{out cold}}[i,j] &= j + 1
\end{align*}
\]

(3.245) (3.246)
For counter-flow HXs, the second dimensions is not used, such that $j_{in/out_{hot/cold}} = j = 1$ always.

In the case of the hot side flow reversal, only $i_{in/out_{hot}}$ will be changed (they will be switched). All other indices remain the same. Flow reversal on the cold side is not currently supported by the code and air is always assumed to flow from the nominal inlet to nominal outlet locations.

The equations solved by the code are still the same as described in the previous sections. There are only two differences for a cross-flow HX. First, the heat transfer area is calculated for each node according to Figure 3-38 using the same approach as in the steady-state models in Section 3.1.2.6. Second, the equations are solved in different directions as shown in Figure 3-38 and Equations (3.245) and (3.246): “$i$” direction for hot side flow and “$j$” direction for cold side flow.

As in the steady-state model, the PDC dynamic model for the cooler supports the multi-pass heat exchanger arrangement with flow turns either in headers or in tubes (see Figure 3-17 in Section 3.1.2.6). The multi-pass sections of the same heat exchanger are still treated as separate heat exchangers, since these sections are independent with regard to air temperatures and flow. The headers, if present, are used simply to average hot side conditions, -enthalpy and pressure, between the sections. The same approach is retained for the dynamic calculations: the sections are independent of each other and the enthalpies and pressures are averaged at each header’s outlet at each time step to provide boundary conditions for the next section. One extra assumption in the dynamic calculation is made to neglect the hot side mass in the headers (in comparison to the mass in the tubes) and its effect on the time derivatives in a transient. It is assumed that the averaging in headers is instantaneous.

To maintain a reasonable number of the equations for a cross-flow cooler, the incompressible flow treatment (see Sections 3.2.6.3 and 3.2.9) is always used for this type of cooler for both hot- and cold-side fluids.

### 3.2.6.3 Incompressible Flow Equations for Fluids outside the Cycle

The equations for the flow rate for the working fluid described above assume a compressible treatment, i.e., the flow rate is could be different in adjacent cells to redistribute the working fluid mass between the regions. These equations, however, were found to be not applicable to incompressible fluids, such as water on the cold side of a cooler. In particular, the derivative of density with respect to pressure (compressibility) is so small for incompressible fluids such that a very small time step would be required to properly resolve the compressible flow equations for such fluids. For these reasons, the incompressible flow equations are always applied in the PDC to the fluids other than the cycle’s working fluid, such as:

- Hot-side fluid for the heat addition heat exchangers; and
- Water or air on the cold side of a cooler.

The PDC incompressible flow equations are described below for the example of water flow in the cooler. The equations are similar for other fluids and listed above. A single water flow rate is
calculated for the entire cooler. Since the water properties are weak functions of pressure over the considered range of pressures and temperatures, only temperatures are calculated on the water side at each node. The pressure drops in each region are calculated for the water side, but they are not used for properties calculations. The individual pressure drops are added up to calculate the total pressure drop through the water circuit (which is assumed to be equal to the pressure drop through the cooler).

Water enthalpy (each cooler node):

$$\frac{\partial h_{H,O,i}}{\partial t} = \frac{1}{M_{H,O,i}} \dot{m}_{H,O}(h_{H,O,i} - h_{H,O,i+1}) + \frac{\Delta x_i N_i}{M_{H,O,i} \rho_{H,O}} \left( T_{w,i} - \frac{T_{H,O,i} + T_{H,O,i+1}}{2} \right) . \quad (3.247)$$

Water flow rate (a single value for the entire cooler):

$$\frac{\partial \dot{m}_{H,O}}{\partial t} = \frac{\Delta p_{pump}}{I_1} - \frac{2S_1}{I_1 A_{H,O} D_{H,O}} \dot{m}_{H,O}^2 , \quad (3.248)$$

where

$$I_1 = \sum_{i=1}^{N_{reg}} \frac{\Delta x_i}{A_{H,O}} ,$$

$$S_1 = \sum_{i=1}^{N_{reg}} \frac{f_i \Delta x_i}{\rho_{H,O,i}} .$$

Water temperature:

$$\frac{\partial T_{H,O,i}}{\partial t} = \frac{1}{c_{H,O}} \frac{\partial h_{H,O,i}}{\partial t} . \quad (3.249)$$

The water pump pressure head, $\Delta p_{pump}$, in Equation (3.247) is considered to be an external controllable parameter. The water flow rate automatic control adjusts the pumping head according to the action that is required. (The water flow rate control and pump models are discussed in Section 3.3.2).

3.2.7 Electrical Heater

The dynamic equations for the electrical heater are similar to those for the heat exchanger described in the previous section. There are only two differences. First, there is no hot-side fluid. Second, the external heat is added directly to the tubes (wall). Therefore, Equation (3.206) is used for the wall temperature with the $\Delta Q_i$ term calculated by scaling the total external heat input with the region lengths. That heat input is either supplied by a user or is calculated by the control system.
3.2.8 Turbomachinery

A common approach in turbomachinery modeling, an instantaneous response assumption [23], is used in the PDC to characterize turbine and compressor behavior in a transient. Under this assumption, the flow rate and outlet parameters react instantaneously to changes in the inlet and outlet pressure and/or rotational speed. The steady-state off-design performance models, described in Section 3.1.4, are used to calculate the turbomachinery behavior under this approach. However, those off-design models usually involve multiple layers of iterations on fluid properties, speeds, and losses and, therefore, are much too slow to be directly used in dynamic calculations. The iterations could be very slow for supercritical fluids due to rapid properties variations.

3.2.8.1 Turbomachinery Maps

Performance maps are generated for each turbomachinery component before the dynamic calculations are performed. The maps are then used in the dynamic model. The maps should cover the whole possible range of parameter variations to avoid extrapolation. The parameters which define the turbomachinery state are:

- Inlet temperature;
- Inlet pressure;
- Outlet pressure; and
- Rotational speed.

Based on these parameters, the steady-state off-design performance model calculates all other parameters and conditions. Of the calculated parameters, the mass flow rate though the turbomachinery and outlet temperature (or specific enthalpy) are used in the dynamics model. So, the goal of the performance maps is to generate a behavior law for flow rate and outlet temperature for variations in each of the four parameters listed above. The traditional approach for ideal gas cycles has been to reduce the number of varying parameters to two (usually, pressure ratio and temperature-corrected rotational speed) using the fact that the fluid follows the ideal gas law. Therefore, the turbine and compressor maps are usually generated as functions of two variables in traditional approaches.

It is known, however, that supercritical fluids do not follow the ideal gas law, especially near the critical point where compressors could be operating. Table 3-4 demonstrates why ideal gas scaling laws are not necessarily applicable to supercritical compressors. The table shows the example of CO₂ conditions near the critical point. The usual practice for an ideal gas is to reduce turbomachinery performance to a parameter shown in the fourth column in Table 3-4. However, the table demonstrates that even for CO₂ conditions different by just 1 °K, the same value for this parameter can result in significant differences in densities, depending on pressure conditions. That difference in density would result in significantly different velocities and, therefore, velocity triangles, such that the same compressor performance cannot be expected. For these reasons, the
turbomachinery maps in the PDC do not rely on any simplifications using the ideal gas laws and use four-dimensional maps, instead of commonly-used two-dimensional maps.

Table 3-4. Example of Scaling with Idea Gas Law

<table>
<thead>
<tr>
<th>Conditions</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>$p_{01}$, MPa</td>
<td>$T_{01}$, K</td>
</tr>
<tr>
<td>7.775</td>
<td>307</td>
</tr>
<tr>
<td>7.762</td>
<td>306</td>
</tr>
</tbody>
</table>

Four-dimensional performance maps are generated for all the turbines and compressors. These maps provide the flow rate, outlet temperature, maximum Mach number (for checking choke conditions), and stall parameter (for checking compressor stall conditions) for each value of rotational speed, inlet temperature, and inlet and outlet pressures.

The parameters between the map points are obtained in the dynamic model using cubic spline interpolation [25] between the map points. The coefficients for the spline interpolation are calculated by the code in the map generation subroutine and are stored in the turbomachinery maps. This allows for fast and smooth application of the turbomachinery maps in the dynamic calculations. The cubic spline interpolation is applied to the pressure-versus-flow curves only. For other map dimensions, such as inlet temperature and shaft speed, linear interpolation between the points is used.

The PDC allows one to generate and use two types of turbomachinery maps: general and synchronous. The difference is that the synchronous maps assume a fixed shaft speed at the design value. The general maps, which cover changing shaft speed, can be used in all calculations. However, using synchronous maps for transients where the shaft speed would not change (such as for synchronous connection to the grid), allows an increase in accuracy of the maps for the remaining three dimensions for the same map file size.

The turbomachinery maps are generated by the PDC in a text format, so the user can check the maps, if needed. The maps are used in the PDC dynamic calculations in the binary format to reduce the file size. Therefore, the maps need to be converted from the text to binary format using either the PDC GUI or the map conversion utility, as described in Sections 2.3.4.5 and 2.4.3. Once converted, the text version of the maps is no longer needed by the code and can be deleted. If needed, there is a reverse utility to convert maps from binary back to text files.

Since using the turbomachinery maps in transient calculations unavoidably results in approximations from the interpolation between map points, the PDC has an option to verify turbomachinery maps with the actual performance subroutines. If this option is used (which is triggered by the corresponding input for the map dynamic input in Figure 2-32), the maps are used only as a first guess for iterations. Then, the performance subroutines are used to obtain the turbomachinery performance for the actual inlet and outlet conditions on each time step. Because the turbomachinery performance subroutines require several layers of iterations, including those on properties, this map verification option significantly reduces the computational speed of the
code. However, it increases the accuracy of the code. There are two options to use map verification in the PDC: always and only when the shaft speed is changing.

3.2.8.2 Turbomachinery Shaft Dynamics

The turbomachinery rotor dynamics equation defines the change in the turbomachinery rotational speed [23]:

\[
\frac{\dot{\omega}}{I} = \frac{W_{\text{gen}} - W_{\text{grid}}}{I \omega}, \quad (3.250)
\]

where

- \( \omega = 2\pi n_r \) = rotational speed,
- \( W_{\text{gen}} \) = generator power (see below),
- \( W_{\text{grid}} \) = demand from the grid,
- \( I \) = total moment of inertia.

As for the steady-state calculations in Equation (3.47), the generator power is defined as the difference between the power produced by all turbines (\( \Sigma W_{\text{turb}} \)) and power consumed by all compressors (\( \Sigma W_{\text{comp}} \)) with accounting for the mechanical losses (\( W_l \)), generator efficiency (\( \varepsilon_{\text{gen}} \)), and power input for the pump for the cooling water or air provided to the cooler:

\[
W_{\text{gen}} = \left( \sum_{\text{All turb}} W_{\text{turb}} - \sum_{\text{All comp}} W_{\text{comp}} - W_l \right) \varepsilon_{\text{gen}} - W_{\text{pump}}. \quad (3.251)
\]

The turbine and compressor power is calculated as the flow rate through the component times the change in specific enthalpy across the component.

Note that unlike the steady-state Equation (3.47), the mechanical losses in Equation (3.251) are calculated in dynamics separately from the turbine and compressor power. This is done to account for the fact that the mechanical losses scale with the shaft speed. In PDC calculations, the loss is assumed to be proportional to the square of the rotational speed. The steady-state value for the total mechanical loss is calculated prior to the transients and is re-calculated at each time step with the square of the shaft rotational speed.

The grid demand in Equation (3.250) is given as a function of time. The total moment of inertia is a sum of the moments for the turbine, compressors, and generator rotors. The moment of inertia is defined as [26]:

\[
I = \int r^2 dm. \quad (3.252)
\]

For a solid cylinder of radius \( r \), length \( L \), mass \( m \), and density \( \rho \), it is equal to:
\[ I_{\text{cyl}} = \frac{1}{2}mr^2 = \frac{1}{2}\pi \rho Lr^4. \]  \hspace{1cm} (3.253)

Equation (3.253) is used to obtain the moment of inertia for each stage of the turbine and compressor. For example, the moment of inertia of an axial compressor stage is a sum of moments for each rotating part\(^1\) as shown in Figure 3-39.

\[ I_{\text{comp}} = \sum_{i=1}^{N_i} (I_{\text{shaft}}^{\text{rot}} + I_{\text{hub}}^{\text{rot}} + I_{\text{blades}}^{\text{rot}} + I_{\text{stat}}^{\text{rot}}), \]  \hspace{1cm} (3.254)

\[ I_{\text{shaft}}^{\text{rot}} = \frac{1}{2}\pi \rho_{\text{shaft}} \text{Chord}_{i}^{\text{rot}} r_{\text{shaft}}^4, \]  \hspace{1cm} (3.255)

\[ I_{\text{shaft}}^{\text{stat}} = \frac{1}{2}\pi \rho_{\text{shaft}} \text{Chord}_{i}^{\text{stat}} r_{\text{shaft}}^4, \]  \hspace{1cm} (3.256)

\[ I_{\text{hub}}^{\text{rot}} = \frac{1}{2}\pi \rho_{\text{hub}} \text{Chord}_{i}^{\text{rot}} (r_{\text{hub}}^4 - r_{\text{shaft}}^4), \]  \hspace{1cm} (3.257)

\[ I_{\text{blades}}^{\text{rot}} = \frac{1}{2}\pi \rho_{\text{blade}} K_{\text{blade}} \text{Chord}_{i}^{\text{rot}} (r_{\text{tip}}^4 - r_{\text{hub}}^4), \]  \hspace{1cm} (3.258)

where
\[
\begin{align*}
\rho &= \text{material density}, \\
r &= \text{radius}, \\
K_{\text{blade}} &= \text{blade row “porosity” (see below)}.
\end{align*}
\]

The blade row “porosity” is a ratio of the volume occupied by the blades to the total volume between the hub and tip. The blade’s total volume is calculated under the assumption that the blades are arcs with an average thickness equal to half of the maximum thickness.

\[ K_{\text{blade}} = \sigma \frac{t_b}{2c} \frac{\theta}{2\sin \frac{\theta}{2}}, \]  \hspace{1cm} (3.259)

where (see figure to the right)
\[
\begin{align*}
\sigma &= \frac{c}{s} = \text{blade solidity}, \\
c &= \text{blade chord}, \\
s &= \text{blade spacing},
\end{align*}
\]

\(^1\) Depending on the turbomachinery design, the stator row hub may or may not be included into rotating parts. It is expected though that the moment of inertia of this part will be much smaller than for the other components, such as for the generator, so the effect of including or not including the stator hub is not significant for the total moment of inertia.
\( t_b \) = maximum blade thickness,  
\( \theta \) = blade angle.

![Figure 3-39. Compressor Stage for Moment of Inertia Calculations.](image)

3.2.8.3 Grid Connection Modes

The PDC supports three connection modes between the turbomachinery shaft and the electrical grid.

In *Synchronous* mode, the shaft speed is fixed by the grid frequency. Its value is provided in the input for the shaft and is not allowed to change in a transient (unless a grid disconnection transient is simulated, as described below). Equation (3.251) is used to calculate the power provided by the plant to the grid. This power, along with the user-specified grid demand, are used for reporting purposes only, as they do not affect any other variables. Equation (3.250) is not used in this mode.

In *Asynchronous* mode, the shaft is connected to the grid, but the shaft speed is allowed to change according to Equation (3.250). The user provides the grid demand in the input as a function of time, while the net generator power is calculated using Equation (3.251) at each time step.

In *Not Connected* mode, there is no grid connection. The shaft speed Equation (3.250) is used to calculate speed, but the grid demand is assumed to be zero (the user input for this is ignored). This mode is to be used, for example, for the shaft configuration where a turbine drives a compressor directly. It is also used for grid disconnection transients, when the grid demand is set.
to -100% in the input, regardless of whether synchronous or asynchronous mode is selected for the shaft.

### 3.2.9 Incompressible Flow Treatment Option

The PDC dynamic equations described in Section 3.2.1 solve the compressible flow equations. For these equations, the flow rate is found from the momentum equation as a function of the pressure difference. The flow rate is allowed to change from cell to cell and the difference in the flow rates in two adjacent cells defines the density change at the borders of the cell. To relate the density with the pressure needed to solve the momentum equation, a partial derivative of the pressure with respect to density is calculated, as following:

\[
\frac{\partial \hat{m}_i}{\partial t} = \frac{A}{\Delta x_i} \left( p_i - p_{i+1} \right) - \frac{2 f_i \Delta x_i}{M_i D_h} \hat{m}_i \left| \hat{m}_i \right| ;
\]

\[
\frac{\partial \rho_i}{\partial t} = \frac{1}{A \left( \frac{\Delta x_i}{2} + \frac{\Delta x_{i-1}}{2} \right)} \left( \hat{m}_i - \hat{m}_{i-1} \right) ;
\]

\[
\frac{\partial p_{i+1}}{\partial t} = p_{r,i} \frac{\partial T_{j+1}}{\partial t} + p_{\rho,i} \frac{\partial \rho_{i+1}}{\partial t} ;
\]

where \( p_{\rho,i} = \left( \frac{\partial p}{\partial \rho} \right)_{T,j+1} = \frac{1}{\left( \frac{\partial p}{\partial \rho} \right)_{T,j+1}} \) = partial derivative of the pressure with respect to density.

For an assumed incompressible fluid, like water, density is almost independent of the pressure, such that

\[
\left( \frac{\partial \rho}{\partial p} \right)_{T,j+1} \to 0 .
\]

The derivative would be equal to zero for a perfectly incompressible fluid.

It has been observed during previous calculations with the PDC that the time step size for the transient calculations of a supercritical cycle is mostly controlled by the momentum equation in the cooler, i.e. close to the critical point. That feature of the PDC can be explained by Figure 3-40 which plots the CO₂ compressibility around the traditional recompression sCO₂ cycle, such as that shown in Figure 3-1. The compressibility is defined as:

\[
z = \frac{p}{\rho RT} .
\]
Near the top part of the cycle (RHX, turbine, HTR), the compressibility is close to unity meaning that CO$_2$ behaves like an ideal gas. However, around the cooler and the main compressor, the compressibility approaches very low values, typical for an incompressible liquid.

Since CO$_2$, like other supercritical fluids, shows liquid-like behavior near the cooler and compressor, the derivative of density with respect to pressure becomes very small in this region such that the derivative of pressure with respect to density becomes very large. As a result, a transition from the density (mass) equation to pressure for the momentum equation is done by multiplying by a very large number. In order to compensate for this multiplication, a very small time step ($<10^{-3}$ sec) would be needed to solve the equations even at the steady-state (i.e., not changing) conditions.

To accelerate the PDC calculations, an option for an incompressible flow treatment in the heat exchangers has been added. To trigger this option, a user defines thresholds for the compressible flow treatment in the general section of the PDC dynamic input file (see Figure 2-23). At the beginning of each time step, the code calculates the maximum compressibility of the working fluid according to Equation (3.264) for each flow in each heat exchanger. If this compressibility is greater than the user-defined threshold, then the compressible flow equations, as described above, are still applied to that flow. If, however, the compressibility is less than the threshold value, then an incompressible flow treatment is applied to that particular flow. The threshold check is carried out independently for each heat exchanger at each time step.

Figure 3-40. CO$_2$ Compressibility in the sCO$_2$ Cycle.
To avoid frequent switching between compressible and incompressible flows, two thresholds are provided in the PDC input file. The first value defines the $z$-value below which the flow treatment should switch to incompressible flow. The second input defines the $z$-value above which the treatment switches back to compressible flow. It is recommended that the second input be slightly higher than the first one to provide a margin. For example, if 0.8 and 0.85 are used for these inputs, PDC will switch to compressible flow if the compressibility falls below 0.8, but will not switch back to the compressible flow treatment until the compressibility increases above 0.85.

The incompressible flow treatment is similar to Equations (3.247)- (3.249) for the water side on the cooler in Section 3.2.6.3. It is assumed that the flow rate is the same for all cells of the heat exchanger, and the momentum equation above is integrated over the heat exchanger length to calculate the flow rate:

\[
\frac{\partial \dot{m}}{\partial t} = \frac{A}{L} (p_{in} - p_{out}) - \frac{2}{D_h} \frac{m \Delta \dot{h}}{\sum_{i=1}^{n} f_i \Delta x_i}, \tag{3.265}
\]

where the friction coefficients and masses are calculated for each region at the beginning of each time step and the sum is assumed to be constant during the time step. The pressures inside of the heat exchanger are calculated from the pressure drop for a given flow rate:

\[
p_{i+1} = p_i - \frac{2 f_i \Delta x_i^2}{A M_i D_h} \dot{m}^2. \tag{3.266}
\]

Then, the densities needed for the properties calculations are computed from pressure and temperature through the partial derivatives.

A sensitivity study for the incompressible flow treatment threshold was carried out for an sCO$_2$ cycle. The tradeoff between the computational time and the calculational error was investigated for an example of a transient defined by a ramp load change from 100 % to 50 % nominal load. The computational times were recorded and the accuracy of the incompressible flow was defined as a maximum error in the transient between the calculated values of the cooler-outlet temperature and pressure and those calculated by the fully compressible flow treatment. The cooler outlet conditions were selected since the accurate calculations of the CO$_2$ conditions near the critical point is important for the transient behavior of the entire cycle. Table 3-5 shows the results of the sensitivity study. When a threshold is selected such that the incompressible flow treatment is applied only in the cooler, the computational time is reduced significantly while the maximum errors in temperature and pressure are very small. When the threshold is increased to add the low and high temperature recuperators, the computational time continues to decrease but at the expense of less accurate cooler outlet conditions. Since the CO$_2$ properties are strong functions of temperature and pressure near the critical point, the difference of 0.5 °C, for example, is considered to be significant. From Table 3-5, it is recommended to set the compressibility threshold to 0.8 or below in the PDC calculations, at least for the sCO$_2$ cycles.
### Table 3-5. Effect of the Incompressible Flow Treatment for sCO	extsubscript{2} Cycle

<table>
<thead>
<tr>
<th>Incompressible Flow Treatment in</th>
<th>Simulation time*</th>
<th>Maximum transient error in cooler outlet conditions</th>
</tr>
</thead>
<tbody>
<tr>
<td>- (compressible)</td>
<td>4 hr 10 min</td>
<td>-</td>
</tr>
<tr>
<td>Cooler</td>
<td>1 hr 3 min</td>
<td>0.06, 0.019</td>
</tr>
<tr>
<td>Cooler + LTR cold side</td>
<td>47 min</td>
<td>0.57, 0.176</td>
</tr>
<tr>
<td>Cooler + LTR + HTR</td>
<td>25 min</td>
<td>0.89, 0.275</td>
</tr>
</tbody>
</table>

*Computational times in this table were obtained with an earlier version of the code on an older computer. Therefore, these times may not be representative of the modern run times for the PDC.

The incompressible flow treatment, described here is only applied to the cycle heat exchangers. The flow in pipes is resolved with a single node and there would be no difference between a compressible and incompressible flow treatment. The flow rate in turbomachinery is calculated from the turbomachinery maps such that neither compressible nor incompressible flow equations are needed.

As described in Section 3.2.6.3, the incompressible flow treatment is always applied in the PDC to fluids other than the cycle working fluid for the heat addition heat exchangers and coolers.

### 3.2.10 Solution Algorithm

#### 3.2.10.1 Numerical Solution of Differential Equations

The equations described above for time-dependent temperatures, densities, and flow rates are combined into a system of differential equations. The total number of equations required to be solved in an entire cycle can be in the few-hundred range, depending on the number of components and nodalization for each component. The resulting system has three major characteristics important for the solution scheme.

First, the system is highly-coupled meaning that the system could not be divided into independent sub-systems. For example, the equations for enthalpy need flow rate and wall temperature. The flow rate is obtained from the momentum equation which requires pressures. The pressures are obtained from mass conservation equations, but it turn require the flow rates. Likewise, the wall temperature equations needs the fluid temperatures and flow rates (for heat transfer coefficients). Therefore, the whole system of differential equations has to be solved simultaneously.
Second, the majority of the differential equations are non-linear. For example, Equation (3.213) for the specific enthalpy derivative has the term, $\dot{m}h$, where both variables are found as a solution of separate differential equations. Therefore, linear solution schemes cannot be applied to this system.

Third, it is found that the system is a stiff system of differential equations. A stiff system means that the time constants of the equations in the system differ significantly. For example, time constants for the flow rate equations are very small, especially near the critical point. The time constant for some structures, such as a heat exchanger wall, can be large. Traditional methods (such as Euler or Runge-Kutta) could be applied to the stiff system; however, the time step would be selected by the smallest time scale of the system resulting in a significant amount of computation.

In order to address these specific features of the system, a special solution technique has been developed for the PDC dynamic equations. The numerical scheme is based on Taylor series methods [25] with accounting for different time scales and a dynamically-controlled time step.

It is noticed that all of the equations can be described by the general form:

$$y_i' = \frac{\partial y_i}{\partial t} = A y_i + B y_i y_j + C y_k + D,$$  \hspace{1cm} (3.267)

where $i$ could be equal to $j$ (to produce $y_j^2$) and some of the coefficients, $A, B, C, \text{ or } D$, could be zero.

The coefficients in Equation (3.267) include properties of the materials and structures (such as specific heat, thermal resistance, pressure derivatives with respect to temperature and so on). Assuming that the time step is small enough that those coefficients could be considered constant during the time step, the higher order derivatives can be calculated:

$$y_i^{(n+1)} = \frac{\partial}{\partial t} y_i^{(n)} = A y_i^{(n)} + B \left( y_i y_j \right)^{(n)} + C y_k^{(n)} \quad n=1,2,3,...$$  \hspace{1cm} (3.268)

The derivative of the product is calculated using the Leibniz identity [27]:

$$\left( y_i y_j \right)^{(n)} = \sum_{k=0}^{n} nCk y_i^{(k)} y_j^{(n-k)} \quad ,$$  \hspace{1cm} (3.269)

where $nCk = \frac{n!}{(n-k)!k!} = \text{binomial coefficient}$.

Note that in equations of the form of Equation (3.267), the derivatives are expressed in terms of parameter values such as temperature, density, and flow rate and they are known at the beginning of the time step. The derivatives in Equation (3.268) are expressed in terms of lower-order
derivatives only, which have been calculated before. So the derivatives of any order can be calculated for the developed system using Equations (3.266)-(3.268).

This fact is used to apply the Taylor series method to find the solution for the dynamic equations. The method is based on the fact that the value of a function at the end of a time step can be represented using the Taylor series [25]:

\[
y(t + h) = y(t) + y'(t) \frac{h}{1!} + y''(t) \frac{h^2}{2!} + y'''(t) \frac{h^3}{3!} + ... \tag{3.270}
\]

The representation is exact, if an infinite number of terms is used. In practice, the required number of terms is included until the next one is less than a pre-specified error:

\[
\left| y^{(n+1)}(t) \frac{h^{n+1}}{(n + 1)!} \right| < \varepsilon. \tag{3.271}
\]

As follows from Equation (3.271), the accuracy of the Expansion (3.270) can be controlled by both the number of terms, \( n \), and the time-step, \( h \). This fact is used in the code. The minimum number of terms for the Expansion (3.270) is specified by the user in the input file (“Order” parameter). This number is used for the most slowly-changing variables, such as the heat exchanger wall temperatures. For the faster-changing variables, more terms are used. Experience has shown that the smallest time scale in the system is for the working fluid flow rate equations. So, the largest number of terms is used for the flow rates. At the same time, the \( n \)-th derivative of the flow rate requires knowledge of the \( (n-1) \) derivatives of the fluid temperatures and densities. Thus, the equations for these variables require one-order fewer calculations. This approach allows saving of computational effort by not calculating unnecessary derivatives. The accuracy is controlled by the time step as described below.

Equation (3.268) can be readily applied to most of the differential equations described previously. Once the derivatives of enthalpy and densities are know from Equations (3.211)-(3.213), derivatives of temperatures and pressures are calculated using Relationships (3.208) and (3.209).

### 3.2.10.2 Convergence Criteria and Accuracy Control

The PDC supports two approaches for satisfying the user-specified convergence criteria, “Halving time step” and “Based on derivatives.” Selection of which approach to use is a user choice in the General section of the PDC dynamic input, field “Convergence option” in Figure 2-23. For both methods, the system parameters (flow rates, temperatures, and densities) are known and the coefficients for each differential equation are calculated at the beginning of a time step. The differential equations, as derived above, are used to calculate first derivatives of each parameter. The higher derivatives are calculated at the beginning of a time step using Equation (3.268). Equation (3.270) is then used to calculate the values of each parameter at the end of the time step.
For the “Halving time step” method, these values for all calculated variables are stored in a common array, $Y$. The time step is then divided into two time sub-steps. Equation (3.270) is used to calculate the parameters at the end of first sub-step. Based on new values of the system parameters at the end of a sub-step, the derivatives are updated in the same way as described above. These derivatives are used to calculate the system parameters at the end of the second sub-step, i.e., at the end of the original time-step. Again, all parameters are stored in array, $Y$, and compared with values obtained with a single time step. The calculations stop if the difference between the parameters at the end of the time step does not exceed the specified accuracy for each parameter, i.e., the following condition is satisfied:

$$\max \left\{ \frac{Y_i - Y_{i,\text{iter}}}{Y_i} \right\}_{i = 1 \ldots N} \leq \varepsilon,$$  \hspace{1cm} (3.272)

where

- $Y$ = array of parameters obtained with current sub-step,
- $Y_{i,\text{iter}} = Y$ on previous iteration (with larger sub-step),
- $N$ = total number of system parameters (equations),
- $\varepsilon$ = convergence criteria (user-defined in an input file).

If Condition (3.272) is not satisfied, then the current sub-step is divided in half and the process is repeated to calculate the values at the end of the original time step. The iterations continue until Condition (3.272) is satisfied.

At each convergence check, the index for the variable with the largest difference from the previous iteration step is stored. This index is then reported in an output file to allow the user to determine which variables have the slowest rate of convergence. This approach has been used to determine that the flow rates are the fastest-changing variables in the system.

Again, it is assumed in the process described here that the coefficients in the differential equations (such as mass or specific heat) are constant during the time step. Meanwhile, this solution method will converge for any time step (when the number of sub-steps is large and the sub-step is small). If the time step is large, then the properties could change significantly. In this case, the assumption of constant coefficients would not hold. Therefore, special arrangements are required to avoid this situation. This is done through a dynamic time step control, as described below.

The number of the sub-steps required to achieve a given accuracy is stored in a public variable. On the next time step, the calculations start with this number divided by 4. Division by 4 is introduced to check if convergence is improved and the number of the sub-steps could be decreased. At least two iterations are required to check the accuracy according to Equation (3.272). The number of the sub-steps on the second iteration step is twice that on the first iteration step. Therefore, convergence is first checked with the number of the time steps equal to twice what was selected for the first iteration step. Thus, if for the first iteration step, the number of the sub-steps is selected to be four times smaller than that on the previous time step, the convergence will be checked with a number of the sub-steps two times smaller than what was needed on the previous time step. So, if convergence has improved, the number of the sub-steps will be reduced.
At the same time, this approach avoids unnecessary calculations by starting with approximately the same time sub-step as before.

For the “Based on derivative” method, the size of the time sub-step is selected based on the contribution of each term in the Taylor series expansion as follows:

$$\left| \frac{y^{(k)}_i h^k}{y_i k!} \right| \leq \epsilon,$$

(3.273)

where $y^{(k)}_i$ = $k$-th derivative of the calculated value $y_i$ (such as a flow rate or temperature), $h$ = the time sub-step.

In the solution scheme with Taylor series, several time-derivatives are calculated for each variable. These derivatives are all calculated at the same time. That is, the first derivatives are calculated for all variables, then the second derivatives are calculated, and so on. In this time step control approach, Equation (3.273) is applied to all calculated values and all calculated derivatives at each sub-step. For example, when the $k$-th derivatives are calculated, the time sub-step, $h$, is determined such that the $k$-th term in the series expansion is less than the specified accuracy, using the above equation. Then, the smallest value of $h$ determined for all variables is selected as the current sub-step. Then all variables at the end of the selected time sub-step are calculated. After that, all derivatives are calculated again, and a new sub-step size is calculated, until the end of the main time step is reached.

The calculations have shown that the sub-step size determined by this approach is about the same as that from the “halving time step” scheme. However, the derivatives are calculated only once (in the approach with halving the time sub-step, the derivatives were effectively calculated twice per sub-step). Thus, the “based on derivative” approach improves the computational time by as much as 50% without compromising the accuracy. Still, the selection of which scheme to use remains a user’s choice in the PDC.

### 3.2.10.3 Dynamic Time Step Control

The PDC dynamic solver user the concept of a main (or “physical”) time step and a sub-step (or “mathematical”). As described above, the main assumption of the implemented solution scheme in the PDC is that the coefficients in the differential equations are constant during a main time step. Therefore, the “physical” time step defines the time interval over which the coefficients of the differential equations, such as heat transfer coefficients, partial derivatives of properties, etc., are assumed to be constant.

For slow transients (when conditions change slowly), the coefficients could be considered approximately constant during a relatively long time. In this case, a large time step is beneficial to reduce the computational effort needed to recalculate those coefficients. For fast transients, however, large time steps cannot be used since the conditions could vary significantly over a large time step. The following approach is implemented in the code to determine how fast the transient is and which main time step to use.
For each main time step, convergence is achieved by increasing the number of sub-steps over which the differential equations are solved as described in the previous section. These time steps are smaller than the main time step and are used to find the converged “mathematical” solution of the system of the differential equations. High and low limits are imposed on the number of sub-steps. If the number of sub-steps exceeds its high limit and convergence is still not achieved, then the transient is considered to be too fast for the current time step. The time step is decreased by a factor of 10 in this case and the solution is repeated for the new time step. (Note that the coefficients in the differential equations are not recalculated, since they are determined at the beginning of the time step; however, the time interval over which these coefficients are considered to be constant is reduced). If convergence is achieved with a small number of steps (less than the lower limit), then the time step is increased by a factor of 10 for the next time-step calculations. Sixteen and 512 sub-steps are somewhat arbitrarily selected as lower and upper limits on the number of sub-steps.

This dynamic control of the time step enables the calculation of slow transients (or part of a transient) with large time steps increasing the computational speed while fast transients (or the fast part of a transient) are calculated with smaller time steps for greater accuracy.

3.2.10.4 Separate air side cooler calculations

In the solution method described so far in this chapter, it is assumed that all of the differential equations are solved simultaneously. However, an exception from this rule is made in the PDC for the dynamic treatment of a cooler. Due to the possibility of a large number of differential equations in a cross-flow cooler (see Section 3.2.6.2), solving all of the cycle equations at the same time with all of the cooler equations may be too time consuming.

At the same time, an observation is made that the equations for the cycle and the water/air sides of a cooler only affect each other through the heat exchanger (tube) wall temperature. This heat exchanger wall is usually a large mass of metal, such that its temperature is not expected to change much or fast during a time step. Therefore, an assumption is made in the PDC that the behavior of the cooler wall temperature can be described with a first derivative only; all higher derivatives are assumed to be zero.

According to Equation (3.244), the first derivative of the wall temperature (for all nodes) can be calculated at the beginning of each time step using the current values for the wall temperatures and the temperatures of the fluids on the two sides. That is, no knowledge of higher-order derivatives is needed to calculate the first derivative of the tube wall temperature. Since all higher order derivatives of this temperature are assumed to be zero, the first derivative, as calculated at the beginning of a time step, is assumed to be constant during that time step. This effectively means that the cooler wall temperature will be known for each sub-step inside the main time step.

These assumptions on the wall temperature allow separation of the cycle and cold-side equations for the cooler. For example, the hot-side (cycle) equations can now be solved without any knowledge of the parameters on the cold side. Likewise, the cold-side equations can be solved
independently of all other equations in the code. Therefore, the PDC employs two independent solver subroutines – one for the cycle and the other for the cooler cold side. The only common link between these two solvers is the initial value and the first derivative of the wall temperature, which are calculated prior to calling the solver subroutines. This approach solves two smaller systems rather than one large system, which improves the computational speed of the code. Moreover, the two smaller systems can be solved on different time scales (i.e., a different number of sub-steps), which further improves the computational time.

The derivative of the cooler wall temperature will then be recalculated at the next time step to reflect the changes in the hot and cold side conditions during prior time step.

3.2.11 Initial and Boundary Conditions for Transient Calculations

The dynamic (transient) calculations in the PDC always start from the steady-state conditions\(^1\). Before the transient calculations are run, the PDC calls the dynamic initialization subroutines, \textit{initial\_cond\_BC} and \textit{initial\_cond\_RHX}, where the parameters and arrays required for the PDC transient models are calculated and initialized.

The transient calculations in the PDC are divided into two stages. At the first stage, the steady-state solution is verified using the dynamic equations. There is no transient initiator at this stage. The goal here is to obtain a stable and converged transient solution for the steady-state conditions before the actual transient begins. The PDC provides the user with an option to “accelerate” this stage by artificially reducing the heat capacity for all structures in equations such as Equation (3.244) for the heat exchanger wall temperature. The input for the “Heat capacity reduction factor in Get\_SS” in the general section of the PDC dynamic input defines this factor.

The boundary conditions for the PDC transient calculations are defined for the hot-side fluid in the heat addition heat exchanger(s) and for the cold-side fluid in the cooler(s).

The HAHX hot side fluid conditions at the HAHX inlet, - temperature, pressure, and flow rate, - are provided directly by the user in the table forms as a function of time in the GUI form in Figure 2-25 or in the “RPF\_....\_dat.txt” input files. The pressure and flow rate are provided as fractions of the steady-state values, while the temperature is entered in the absolute (not normalized) sense. As an alternative to the direct input, the HAHX hot-side conditions can be calculated by the SAS4A/SASSYS-1 code, if the PDC-SAS4A/SASSYS-1 coupling option (see Section 2.6) is used. In this case, the values in the table input files are not used by the code.

The water/air inlet temperature at the cooler inlet is directly provided in the PDC GUI form (Figure 2-31) or in the “H2O\_T\_in\_dat.txt” input file. Again, the input here is a table of values versus time. Atmospheric pressure is assumed to be always maintained for the cooling fluid. The water/air flow rate is calculated by the PDC control system, as described in Section 3.3.2.

\(^1\) The PDC restart capability described in Section 2.5 allows running dynamic calculations without first running the steady-state calculations on the same run. However, to create the restart file, steady-state calculations are still required.
3.2.12 Transient Definitions

In general, a transient in the PDC is initiated by any entry in the PDC input which is different from the steady-state value. Below are listed some of the most common transient initiators for the PDC. There is no requirement that a single transient initiator should be used such that any reasonable combination of the examples listed below can be used in the PDC.

3.2.12.1 Change in Boundary Conditions

A transient can be initiated by any change in the boundary conditions described in Section 3.2.11. This includes the conditions for the HAHX hot-side fluid, including those calculated by external code, as well as cooling fluid cooler-inlet temperature. These inputs are provided in the Heat Addition and Heat Removal sections of the PDC dynamic input.

3.2.12.2 Load Following

The PDC automatic control system (Section 3.3) is set up to match the generator output to the grid demand. The grid demand table, in terms of values normalized to the steady-state cycle output, is provided by the user in the General section of the PDC dynamic input. This table should be used to specify the load following transient.

3.2.12.3 Grid Disconnection/Loss of Load

As a variant of load following, a complete disconnection from an electrical grid (loss of electrical load) can be simulated using the grid demand table. To start such a transient, an entry of “-100” needs to be provided in the table. The grid disconnection transient can be started at any time. When it is initiated, the grid demand will be set equal to zero. In addition, if synchronous mode with fixed shaft speed is used for a shaft, the shaft will be switched to asynchronous mode with the variable shaft speed.

3.2.12.4 Pipe Break

The General section of the PDC dynamic input includes the input for simulating a pipe break. The input includes the equivalent break diameter (for a circular break) and the break location. If any positive value for the break diameter is entered, the PDC will simulate the pipe break at the corresponding location. The break is assumed to happen instantaneously at time=0.

If zero break diameter is entered, there is no break and the break location input is ignored.
3.2.12.5 Control Action

The plant control system described in Section 3.3 can be used to initiate a transient. A transient can be initiated by a manual control action (see Section 3.3.1.2). In addition, any entry in the target tables for any of the controls which is different from the corresponding steady-state value will automatically initiate a transient.
The dynamic model in the PDC includes the simulation of control mechanisms for the cycle itself, the HAHX hot-side fluid, and the cooling media on the cold side of a cooler. The control action is implemented in the PDC as a combination of proportional (P), integral (I), and differential (D) controls:

\[
\text{Control Action } (t) = K_P \cdot E(t) + K_I \cdot \int_0^t E(\tau) d\tau + K_D \cdot \frac{dE(t)}{dt}
\]  \hspace{1cm} (3.274)

where

\[K_P, K_I, \text{ and } K_D = \text{PID control coefficients (user input)},\]

\[E(t) = \text{deviation in controlled variable, i.e., difference between the target value and the actual value, at time } t,\]

\[\text{Control Action} = \text{Action depending on the control type. For valves, Action is the rate of opening and closing the valve.}\]

The derivative of the deviation is calculated as the difference between the current value and the value at the previous time step divided by the time step,

\[
\frac{dE(t)}{dt} = \frac{E(t) - E(t-\Delta t)}{\Delta t}.
\]  \hspace{1cm} (3.275)

The deviation integral is calculated as a sum of error values multiplied by the time step for all time steps from the beginning of a transient,

\[
\int_0^t E(\tau) d\tau = \sum_i E_i \Delta t_i
\]  \hspace{1cm} (3.276)

For most of the cycle controls the deviation, \(E\), can be averaged over a number of previous time steps to improve the stability of the control action, if needed. The number of time steps over which the deviation is averaged is the user input for each control. In no averaging is needed, then “1” should be used for this input.

The coefficients for the proportional, differential, and integral parts of the control are defined by the user in the input file for each control mechanism. They should be selected to achieve a satisfactory response from the control system.

The control action calculated using Equation (3.274) is used in the PDC to adjust the controllable variable. If the control mechanism is a valve, then the action is the rate of valve opening and closing, \(f'\), and the valve open fraction at the end of the time step is calculated based on the value at the beginning of the time step and the opening or closing rate:

\[
f_{\text{open}}(\Delta t) = f_{\text{open}}(0) + f' \Delta t
\]  \hspace{1cm} (3.277)
The limitations on the open area fraction (between 0 and 1) and valve opening and closing rates (defined by the user) are applied to the results obtained from Equations (3.274) and (3.277).

### 3.3.1 Cycle Controls

The cycle control system usually simulates the movement of the control valves to regulate flows in the cycle to achieve the control system’s objectives. Figure 3-41 shows the cycle control mechanisms supported by the PDC. Notice that this figure only lists the available controls, the location of the control valves as well as the choice of how to use the controls is defined by the user though the PDC input. For example, the turbine bypass control in Figure 3-41 can be used to regulate flow around a compressor, but it will still be referred to as “turbine bypass” in the PDC input and in this report. Also, it is not necessary to use all controls for a particular system.

Each control mechanism in the PDC will have a target value, which the automatic control system will try to match by adjusting the control valve position to minimize the error (difference) between the current and the target values for the controlled parameter. The target values for each control are usually provided by the user in the PDC input files in tables as a function of time. These inputs, along with other specifics for each control, are described below.
3.3.1.1 Options for Scaling of Control PID Coefficients

The PDC supports the input of two sets of PID coefficients for each control in the input file – one for the synchronous and one for the asynchronous generator connection modes. The switching
between these sets automatically occurs when the generator mode is switched between the synchronous and asynchronous modes. If distinction between these modes is not needed, then the same sets of the PID coefficients need to be provided in the input.

For the asynchronous mode, the PID coefficients can also be scaled with the shaft speed. The following scaling of the control coefficients is implemented according to the power law is implemented in the PDC:

\[ k_x = k_{x0} \left( \frac{N_r}{N_{r0}} \right)^c, \quad (3.278) \]

![](Image)

where \( x = \{P, I, \text{or } D\} \),

- \( k_{x0} = \) value at design (100\%) shaft speed, \( N_{r0} \),
- \( N_r = \) shaft speed,
- \( c = \) scaling power exponent (user input).

For this scaling, the target (rather than actual) shaft speed is used to avoid local variations.

Depending of the value of the scaling power exponent, several laws could be simulated using Equation (3):

- \( c = 0 \), \( k_x \) is constant at \( k_{x0} \) value, i.e. no scaling is implemented,
- \( c = 1 \), \( k_x \) is scaled linearly with \( N_r \),
- \( c = -1 \), \( k_x \) is reversely proportional to \( N_r \),
- \( c = 2 \), \( k_x \) is scaled squarely with \( N_r \), etc.

### 3.3.1.2 Manual Control Overwrite

The PDC automatic control system calculates the required control action for all control mechanisms described below. However, the PDC also supports manual overwrite of that automatic control. In the manual mode, the user provides the valve position in the value-versus-time table. The manual overwrite is triggered, if the number of entries in that manual control table is more than one.

### 3.3.1.3 Turbine Bypass Control

The common practice for gas Brayton cycles is to use turbine bypass for turbomachinery speed or power control. The same approach is used in the PDC. If the generator power exceeds the grid demand, the turbine bypass valve opens reducing the flow rate through the turbine and, therefore, decreasing the turbine work. The turbine bypass automatic control calculates the difference between the actual rotational speed or power and its specified value. It also calculates the derivative and integral value of this difference. The bypass valve action, valve opening or closing, is calculated based on the three parameters representing proportional, differential, and integral control as defined by Equation (3.274):
\[ f''_{\text{TBP}} = k_{p}^{\text{TBP}} E_{\text{TBP}} + k_{d}^{\text{TBP}} E'_{\text{TBP}} + k_{i}^{\text{TBP}} \int_{0}^{t} E_{\text{TBP}}(t) dt , \] (3.279)

where

\[ f''_{\text{TBP}} = \text{rate of change of open area fraction, } f'_{\text{open}}, \text{ or speed at which the valve is opening or closing,} \]

\[ E_{\text{TBP}} = \frac{n_r(t) - n_r^{\text{spec}}}{n_r^{\text{spec}}} = \text{deviation from its specified value (see below),} \]

\[ k_d, k_p, k_i = \text{user-defined control coefficients.} \]

Depending on the grid connection mode, the turbine bypass automatic control monitors the rotational speed or the net power of the turbomachinery shaft. In asynchronous and “not connected” modes, the control monitors the shaft speed, and the deviation for Equation (3.279) is calculated based on the shaft speed:

\[ E_{\text{TBP}}^{\text{Asynch}} = \frac{n_r(t) - n_r^{\text{target}}}{n_r^{\text{target}}} . \] (3.280)

In the synchronous mode, the shaft speed is fixed so the turbine bypass control action is based on the shaft power:

\[ E_{\text{TBP}}^{\text{Synch}} = \frac{W_{\text{gen}}(t) - W_{\text{grid}}(t)}{W_{\text{grid}}(0)} . \] (3.281)

The target shaft rotational speed and the grid demand for the turbine bypass control are provided by the user in the PDC input.

The turbine bypass control is a fast control mechanism which allows to change power output from a generator very quickly. At the same time, this control leads to the least efficient operation of the cycle since it simply reduces the useful turbine work (while also increasing the compressor work).

### 3.3.1.4 Inventory Control

The inventory control works by removing a fraction of the working fluid mass from the cycle. Lower working fluid inventory leads to lower cycle densities and pressures, which in Brayton cycles leads to reduced flow rate delivered by the compressors. In an ideal cycle, the flow rate reduction would not affect cycle temperatures. Also, since the flow rate is reduced uniformly everywhere in the cycle, the ratio between the compressor work and turbine work is preserved. Therefore, in an ideal cycle, the inventory control would reduce the power production by the cycle while maintaining the same level of cycle efficiency. In real cycles, though, there would always be a reduction in cycle efficiency since the turbomachinery would be operating away from its design point. The inventory control is also a slow control and should be applied carefully. A
fast removal or addition of the working fluid would affect one side of a compressor faster than the other, potentially leading to surge or stall of that compressor.

The inventory control system in the PDC requires an inventory tank/vessel and inlet and outlet valves, as shown in Figure 3-41. The action of the inventory control is based on the user-specified table of mass addition to the inventory tank as a function of grid demand. That table needs to be pre-calculated by the user and can be adjusted to provide the desired inventory control action.

The automatic inventory control system monitors the mass in the inventory tank and opens and closes inlet and outlet valves by an approach similar to Equation (3.274), in order to match the required mass obtained from the control table. Since opening an inlet or outlet valve adds or removes inventory from the tank (acting as a derivative of the inventory), the inventory control system calculates valve openings (not their derivatives).

\[
f_{\text{INV}} = k_p^{\text{INV}} E_{\text{INV}} + k_q^{\text{INV}} E_t^{\text{INV}} + k_i^{\text{INV}} \int_0^t E_{\text{INV}}(t) dt \quad (3.282)
\]

where

\[
f_{\text{INV}} = \text{total action from inlet and outlet valves (see below)},
\]

\[
E_{\text{INV}} = \frac{\Delta M_{\text{spec}} - \Delta M_{\text{INV}}(t)}{M_{t,t=0}} = \text{deviation of the mass addition to the inventory tank, } \Delta M_{\text{INV}} \text{ from its specified value.}
\]

The deviation derivative and integral are calculated as in Equations (3.275) and (3.276).

If the inventory control action calculated by Equation (3.282) is positive (\(\Delta M_{\text{INV}}\) is less than a required value) then the inlet valve opens; otherwise the outlet valve opens:

\[
\begin{align*}
  f_{\text{INV},i}^{\text{open}} &= f_{\text{INV}}, \quad \text{if } f_{\text{INV}} > 0, \\
  f_{\text{INV},o}^{\text{open}} &= -f_{\text{INV}}, \quad \text{if } f_{\text{INV}} < 0.
\end{align*} \quad (3.283)
\]

Rate and absolute value limits are applied to the valve action in Equation (3.283).

3.3.1.5 Turbine Inlet (Throttle) Valve Control

The turbine inlet (or throttling) valve reduces the turbine work by increasing the pressure drop prior to the turbine thus decreasing the pressure ratio available to the turbine. In addition, the same action increases the pressure ratio that the compressors need to deliver, increasing the compressor work. The efficiency of partial load operation under this control is somewhere in between the efficiency with the turbine bypass and inventory controls. Also note that turbine throttling is rarely applied at the full design conditions, since it will increase the pressure upstream of the valve, such that those parts of the cycle would need to be designed for higher-than-nominal pressure.
In the PDC, the action of the turbine throttle valve is based on the user-specified required pressure drop across the throttle valve as a function of the grid demand. The turbine throttle valve automatic control system calculates the difference between the actual pressure drop across the valve and the required value, and adjusts the valve opening.

\[
f'_{\text{TIN}} = k'_{o} E'_{\text{TIN}} + k'_{s} E'_{\text{TIN}} + k'_{z} \int_{0}^{t} E_{\text{TIN}}(t)dt\]  

(3.284)

where

\[f'_{\text{TIN}} = \text{rate of change of open area fraction, } f_{\text{open}}, \text{ or speed at which the valve is opening or closing,}\]

\[
E_{\text{TIN}} = \frac{\Delta p^{\text{spec}}_{\text{TIN}} - \Delta p_{\text{TIN}}(t)}{p_{\text{TIN}}} = \text{deviation of the pressure drop across the turbine inlet valve, } \Delta p_{\text{TIN}}, \text{ from its specified value.}
\]

The deviation derivative and integral are calculated as shown in Equations (3.275) and (3.276). The valve open area during the time step is calculated using Equation (3.277) subject to user-specified limits on the valve opening and closing rate.

In addition to the valve pressure drop table, the PDC provides two options for the turbine throttling valve control table. In the first option, the user specifies the target throttling valve open fraction, which is similar to manual control, but involves automatic action subject to control action response and rate limits. In the second of these options, the user specifies the target turbine bypass flow fraction, which is calculated by the code from the turbine bypass control. Both of these options are less common and are provided in the PDC for conditions where the main option with the valve pressure drop does not work or is not sufficient for any reason.

3.3.1.6 Compressor Outlet (Throttling) Valve

The compressor throttling valve action is similar to the turbine throttling, except the valve is usually located at the compressor outlet part. In addition to throttling the flow rate in the entire loop (which would be similar to the turbine throttling action), the compressor throttling valve can be used in flow-split cycle configurations, such as the recompression sCO\textsubscript{2} Brayton cycle shown in Figure 3-41, to control the flow split between two compressors.

Currently, the PDC only supports manual action of the compressor outlet valve.

3.3.1.7 Cooler Bypass Control

For supercritical cycles, it is important to actively control the minimum temperature in the cycle, for example, to avoid two-phase flow and liquid droplet formation at the compressor inlet. Even though compressor-inlet temperature control can be achieved by means of the cooling fluid (water or air) flow rate control (see Section 3.3.2), transient analysis of sCO\textsubscript{2} cycles with the PDC has
shown [28] that the flow rate control may not be fast and/or accurate enough for these cycles. This is because the cooling fluid flow rate change can only be communicated to the cycle conditions through the change of the cooler (tube) wall temperature change, which is a slow process with significant thermal inertia. To improve the accuracy and speed of the minimum temperature control, cooler bypass control (such as the one shown in Figure 3-41) can be used in addition to cooling fluid flow rate control.

The cooler bypass control adds hotter fluid from the cooler outlet to the flow at the compressor inlet, thus allowing fine tuning of the compressor-inlet temperature. There is little inertial in this control action since a change in the hotter fluid flow rate will affect the resulting compressor-inlet temperature almost immediately. Note that the control only works in one direction, meaning that it can only raise the compressor-inlet temperature. Therefore, the fluid coming from the cooler needs to be overcooled beyond the desired compressor-inlet temperature, if cooler bypass control is implemented. The results of transient control analysis of sCO₂ cycles have shown [28], however, that a small cooler bypass fraction of around 5% is sufficient to achieve fast and effective control of the compressor-inlet temperature.

Cooler bypass control is implemented in the PDC in the same way as turbine bypass control described in Section 3.3.1.3. The only difference is that the controlled variable is the compressor-inlet temperature, for which the user provides the target value in a table form.

As described in Section 2.3.3.2 of the User’s Guide portion of this document, it is important for supercritical cycles to distinguish the fluid conditions at various locations around the compressor inlet. Therefore, the PDC supports a choice of which temperature to use for the minimum temperature control (see Figure 2-24): impeller inlet, compressor inlet, or cooler outlet. The choice is made by the user in the “Minimum temperature control” section of the PDC dynamic input.

3.3.1.8 Recuperator Bypass Control

The recuperator bypass control in the PDC can be used similarly to the cooler bypass described in the previous section to actively control an outlet temperature for another heat exchanger. For example, in Figure 3-41, recuperator bypass control is used to control the high temperature recuperator (HTR) outlet temperature on the cold side, which is the same as control of the RHX-inlet temperature.

The control action is similar to cooler bypass control described in previous section, with one difference. To allow for high bypass flow fractions (up to 100%), the recuperator bypass control in the PDC uses, in addition to a bypass valve, a throttling valve located in the main line (see valve RTHv in Figure 3-41). When the control action is exhausted with the bypass valve alone (meaning the valve is fully open) but the target outlet temperature is not yet achieved, the PDC

---

1 The control of the cooler outlet temperature can only be used with cooling fluid flow rate control when the cooler bypass control is disabled (not used) as described in Section 3.3.1.7. Cooler bypass does not affect cooler-outlet temperature and therefore, the cooler-outlet temperature control option should not be used with cooler bypass.
control system will start to close that throttling valve. This action will further decrease the flow through the heat exchanger while increasing the flow through the bypass line.

The implementation of the automatic action for this control is similar to the turbine bypass control in Section 3.3.1.3 with the controlled parameter being the outlet temperature for the mixer of the main and bypass lines (temperature Node 33 at the outlet for the RBPmx mixer for the example in Figure 3-41). The control action is applied to the bypass valve first until it is fully open, then the same action is applied to the throttle valve. The throttle valve action is in reverse to the calculated action for the bypass valve, meaning that the throttle valve is closing when opening of the bypass valve is calculated by the control system. Figure 3-42 shows an example of such coordinated action when the throttle valve starts to close once the bypass valve reaches the fully open position. The control action to increase the outlet temperature is in reverse order to the decreasing temperature action: if the throttle valve is partially closed, it will be fully open first before the bypass valve starts to close. The user-specified valve opening closing rate limits are applied to both the bypass and the throttle valves.

![Figure 3-42. Example of Recuperator Bypass/Throttling Control Action.](image)

### 3.3.1.9 Compressor Surge Control

Unlike all other cycle controls in the PDC described in the chapter so far, the goal of compressor surge control is not to adjust conditions in the cycle, but rather to protect the cycle equipment, namely compressors, from surge. Since the compressors work opposite to the pressure gradient, there could be a condition when the pressure gradient is too high for the compressor to deliver a flow and flow reversal in the compressor could occur. This flow reversal would, in turn, decrease the pressure at the compressor outlet while increasing the pressure at the compressor inlet. The flow reversal conditions would exist until the pressure ratio across the compressor is reduced enough to re-establish the normal flow direction in the compressor. However, when the normal flow direction is established, the compressor pressure ratio will start to increase again, possibly leading to another occurrence of flow reversal. Since the compressors usually deliver a high pressure ratio, switching from normal to reversed flow conditions is usually a fast process that
can repeat itself several times until operator action is taken or the cycle conditions change. That oscillating flow pattern is called surge and can be damaging for a compressor since it rapidly changes the pressure loading on the blades, among other effects. In fact, a single surge cycle can be damaging. Therefore, the large industrial compressors almost always employ a compressor surge protection system, which detects the approach to surge conditions and takes action before a surge event can occur.

Usually [29], the surge control system consists of a compressor bypass (recirculation) line with an integrated cooler. Figure 3-43 shows the elements of a typical compressor surge control system. When an approach to surge is detected by the compressor control system, the bypass line valve is opened such that part of the flow is recirculated from the high-pressure compressor outlet to the low-pressure compressor inlet. This partial flow recirculation causes the compressor outlet pressure to decrease and the compressor inlet pressure to increase resulting in a lower pressure ratio across the compressor. Lowering the pressure ratio will result in increased flow rate through the compressor such that the compressor operating point moves away from low-flow high-pressure-ratio surge conditions. Since the flow recirculation brings hotter flow heated during compression from the compressor outlet to the colder compressor inlet, an additional cooler is installed in the recirculation line to avoid an otherwise uncontrolled temperature increase in the compressor.

![Figure 3-43. Compressor Surge Control.](image)

It is noted that initiation of the compressor surge protection system starts with a detection of approach to surge such that action can be taken before a surge condition is reached. Thus, a reliable surge prediction criterion is required. Several criteria have been proposed [14] for centrifugal compressors, such as conditions where the pressure ratio-versus-flow rate curve reaches its maximum point or some empirical blade stall criterion. However, there are no commonly accepted surge criteria mostly due to the lack of experiment data, since experiment verification of surge requires operation of a compressor under surge conditions which could damage a compressor. For these reasons, a combination of several surge conditions is used in the PDC. The surge flow is defined as a maximum of flow rates at which either the pressure curve reaches its maximum or a blade stall criterion is satisfied. That flow rate and, therefore, the
margin to surge are calculated in the PDC during the map generation phase and is recorded in the compressor maps.

Simulation of actual compressor surge control in Figure 3-43 would require adding a heat exchanger and also simulating startup of the cooling fluid flow in that heat exchanger. To avoid these complications, an idealized automatic surge control is implemented in the PDC where the surge loop cooler brings the recirculated flow temperature exactly to that of the compressor inlet temperature. Under this idealized approach, no effect on temperatures (enthalpies) is introduced by the surge control such that only flow (density) equations are affected by the surge flow. That is, when the surge recirculation flow exists, the time derivative of the density at the outlet of the compressor is decreased by the surge flow and the time derivative of the density at the compressor inlet is increased:

\[
\frac{\partial \rho_{\text{out}}}{\partial t} = \cdots - \frac{1}{V_{\text{out}}} \dot{m}_{\text{surge}} ;
\]

\[
\frac{\partial \rho_{\text{in}}}{\partial t} = \cdots + \frac{1}{V_{\text{in}}} \dot{m}_{\text{surge}} .
\]

(3.285)

(3.286)

Note that the equations above reflect only changes to the derivatives from surge control. There are other contributors to density equations, such as from the regular compressor flow in Equations (3.211) and (3.212), which are omitted from Equations (3.285) and (3.286) for simplicity.

A simple proportional control is modeled for compressor surge control in the PDC. It monitors the approach to stall and increases/decreases the recirculating flow as necessary. The stall margin is calculated during compressor map generation as a difference between the current flow rate and the surge flow rate, normalized to the compressor’s steady-state flow. When the stall margin falls below the controlled value (e.g., 0.2), surge control starts to increase the recirculating flow.

### 3.3.2 Cooler Cold-Side Flow Rate and Pump Head Control

As described in the heat exchanger Section 3.2.6.3, the cooling fluid (water or air) flow rate equation requires specification of the fluid’s pump pressure head, \( \Delta p_{\text{pump}} \), in Equation (3.248). The required pump pressure head is calculated from the control action. No realistic model of the water pump or air blower is incorporated in the code; it is assumed that the pump will deliver the required head all of the time. The user provides in the input files the upper and lower limits for the driving head (relative to the steady-state value) as well as the maximum rate of head change (in \%/s).

Two options for water/air flow rate control are introduced in the code. The water/air flow rate control is either used directly for the minimum cycle temperature control or assists cooler bypass control (Section 3.3.1.7). In the former mode, the pump driving head is adjusted though PID controls to maintain the temperature at the design value. In the latter mode, the water/air flow rate is adjusted to keep the cooler bypass flow fraction at the design level. Since cooler bypass control is selected as the main control for the cycle temperature in the PDC, the water/air flow rate is
used by default to maintain the cooler bypass fraction in order to prevent the bypass valve from being in either the fully open or fully closed position (i.e., to prevent bypass control from losing its maneuverability). The water/air flow rate is used for temperature control alone when the input file specifies that cooler bypass is turned off (when the cooler bypass valve opening and closing rates are set to zero).

The required power input for the water/air circulation pump is calculated in the same manner as in the steady-state code:

\[
W_{pump} = \frac{1}{\varepsilon_{pump}} \Delta p_{pump} \frac{m_{H_2O}}{\rho_{H_2O}},
\]

where
\[
\varepsilon_{pump} = 
\text{pump efficiency (some assumed value)}, \quad 
\rho_{H_2O} = \text{water density at cooler inlet}.
\]

The automatic control for the water/air pump head is implemented in the same way as in Equation (3.274). Control Action in this case is the rate of pump head change. It is found beneficial for the stability of the water/air flow rate control to scale the Control Action with the flow rate. That is, in the PDC, the Control Action for this control from Equation (3.274) is multiplied by the ratio of the current water/air flow rate to that at the steady-state conditions. The deviation, \( E \), in Equation (3.274) is calculated based on the target cooler bypass flow fraction or the target minimum cycle temperature, depending on the user input, as described above.

3.3.3 Heat Addition Control

The control options available in the PDC for the heat addition to the cycle depend upon which options for heat addition are selected for the steady-state and transient, as described below.

3.3.3.1 Control with HAHX User Input Tables

With the HAHX option with user input tables, the user supplies the hot-side fluid conditions (pressure, temperature, and flow rate) at the HX inlet as a function of time. There is an option in the PDC to use automatic control for the cold side HAHX-outlet temperature. This option is used by setting the “Heat Addition calculation mode in dynamics” input to “Automatic control” on the Heat Addition form for the PDC dynamic input (Figure 2-25). On the same form, the target cold-side outlet temperature for this control is also provided.

The HAHX automatic control will adjust the HAHX hot side fluid inlet temperature to match the target outlet temperature on the cold side. The control implementation is similar to Equation (3.274), with the Control Action being the rate of hot-side inlet temperature change. This control

---

1 This equation (as well as those in the code) is written assuming water as the cooling fluid. However, the same equations are applied regardless of whether water or air are used.
can be viewed as a simulation of a perfect (no inertia or delays) external heater in the HAHX hot side fluid loop. The heater would control the fluid temperature at its outlet which would be the same as the HAHX inlet.

3.3.3.2 Control with Electrical Heater

If an electrical heater is used for the heat addition mode, then the user provides a table of the heater power versus time. That heater power will be applied to the heater rods, as described in Section 3.2.7.

Similar to the HAHX, there is an option to automatically control the cycle working fluid’s temperature at the heater outlet. This option is used by setting the “Heat Addition calculation mode in dynamics” input to “Automatic control” on the Heat Addition form for the PDC dynamic input (Figure 2-25). On the same form, the target outlet temperature for this control is also provided.

With automatic heater control, the code will calculate the required heater power to match the target outlet temperature. The control action is calculated using Equation (3.274), subject to the user-provided limit on the heater power change (and the thermal inertia of the heater rods). With automatic control, the user-defined table for the heater power is used to set the maximum heater power at each time during a transient.

3.3.3.3 Reactor Controls with SAS4A/SASSYS-1 Coupling

When PDC-SAS4A/SASSYS-1 code coupling is used (See Section 2.6), the PDC automatic control system can be used to control the power, flow rates, and temperatures on the reactor side. The reactor control in the PDC for SAS4A/SASSYS-1 coupling was developed for sodium-cooled reactors and assumes that there are primary and intermediate reactor loops, as shown in Figure 3-34. The flow rates in the primary and intermediate loops are controlled by the primary and intermediate sodium pumps, respectively. The reactor power is controlled by movement of the control rods. The heat is transferred from the reactor to the energy conversion cycle in the Reactor Heat Exchanger (RHX), which is modeled in the PDC as an HAHX.

The control mechanisms and approaches implemented with SAS4A/SASSYS-1 coupling are listed in Table 3-6. In general, flow rate control is used to match the target temperature at a heat exchanger outlet. For the primary loop, this would be the primary-side temperature at the IHX outlet. For the intermediate loop, the controlled temperature is the RHX-outlet temperature on the hot (reactor) side. The reactor power control is used to regulate the core-outlet temperature.
Table 3-6. Automatic Control with Coupled PDC-SAS4A/SASSYS-1 Codes

<table>
<thead>
<tr>
<th>Controllable Parameter</th>
<th>Measured Value</th>
<th>Controlled By</th>
<th>Control</th>
</tr>
</thead>
<tbody>
<tr>
<td>Intermediate loop cold-side</td>
<td>RHX-outlet temperature</td>
<td>Intermediate flow rate</td>
<td>Intermediate pump torque</td>
</tr>
<tr>
<td>temperatures</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Primary loop cold-side</td>
<td>IHX-outlet primary</td>
<td>Primary flow rate</td>
<td>Primary pump torque</td>
</tr>
<tr>
<td>temperatures</td>
<td>temperature</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Hot-side temperatures</td>
<td>Core-average outlet</td>
<td>Core power (reactivity)</td>
<td>External core reactivity</td>
</tr>
<tr>
<td></td>
<td>temperature</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Note that for all controls in Table 3-6 there would be a delay (sometimes significant) between the control action and the effect on the controlled parameter. For example, changing the intermediate flow rate would reflect on the RHX-outlet temperature only after a delay related to the change in the temperatures of the heat exchanger metal mass. Similarly, the change in core power would not immediately affect the core-outlet temperature. These effects should be expected and need to be taken into account for implementation and optimization of the controls.

The reactor-side control mechanisms from Table 3-6 are implemented in the PDC in the same way as other controls using Equation (3.274). In the case of the pump torques, the Control Action is the increase or decrease of the torque, subject to user-specified limits on the actual value of
torque and its rate of change. For the reactivity, the Control Action is the external reactivity itself. The controlled parameters are the temperatures defined in Table 3-6. For each temperature, the user specifies the target temperature, as a table-versus-time in the PDC input files.

For the reactor control system in the PDC to work, the information from the reactor-side calculations, such as flow rates, temperatures, etc., need to be provided to the PDC. This is done through specifying the required outputs in the SAS4A/SASSYS-1 output file as listed in Section 2.6.3.

Each reactor-side control mechanism in Table 3-6 can be turned on and off independently of each other such that various control combinations can be investigated with the coupled PDC-SAS4A/SASSYS-1 codes.
3.4 Materials, Properties, and Correlations

3.4.1 Heat Transfer and Pressure Drop Correlations

Table 3-7 lists the heat transfer and pressure drop correlations available in the PDC along with the sub-section number of this report where the correlations are presented.

<table>
<thead>
<tr>
<th>Code Name</th>
<th>Name</th>
<th>Applicable to</th>
<th>Section</th>
</tr>
</thead>
<tbody>
<tr>
<td>DB</td>
<td>Dittus-Boelter</td>
<td>Pipes, shell-and-tube HX</td>
<td>3.4.1.1</td>
</tr>
<tr>
<td>PG</td>
<td>Petukhov-Gneilinski</td>
<td></td>
<td></td>
</tr>
<tr>
<td>LM</td>
<td>Lockhart-Martinelli</td>
<td>Liquid metals for all geometries</td>
<td>3.4.1.1</td>
</tr>
<tr>
<td>PC</td>
<td>PCHE</td>
<td>PCHE</td>
<td>3.4.1.2</td>
</tr>
<tr>
<td>WF</td>
<td>Wavy fins</td>
<td></td>
<td></td>
</tr>
<tr>
<td>KL</td>
<td>Keys and London</td>
<td></td>
<td></td>
</tr>
<tr>
<td>BY</td>
<td>Briggs and Young</td>
<td>Cross-flow cooler</td>
<td>3.4.1.3</td>
</tr>
<tr>
<td>BK</td>
<td>BY for heat transfer</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>KL for pressure drop</td>
<td></td>
</tr>
</tbody>
</table>

In this section, as well as in the PDC, the following definitions are used.

Hydraulic diameter:

\[ D_h = \frac{4 \times \text{Flow Area}}{\text{Wetted Perimeter}} \]  \hspace{1cm} (3.288)

Reynolds, Prandtl, and Nusselt numbers:

\[ Re = \frac{\rho \cdot V \cdot D_h}{\mu} ; \]  \hspace{1cm} (3.289)

\[ Pr = \frac{\mu \cdot C_p}{k} ; \]  \hspace{1cm} (3.290)

\[ Nu = \frac{h \cdot D_h}{k} ; \]  \hspace{1cm} (3.291)

where

\( \rho \) = density,
\( V \) = fluid velocity,
\( \mu \) = viscosity,
\( C_p \) = specific heat,
\( k \) = thermal conductivity,
\( h \) = heat transfer coefficient.

For some geometries, the heat transfer correlations are defined through the Colburn factor:

\[
j = \frac{Nu}{Re \cdot Pr^{1/3}}; \tag{3.292}
\]

or,

\[
Nu = j \cdot Re \cdot Pr^{1/3}. \tag{3.293}
\]

The pressure drop correlations are formulated in terms of the friction factor, \( f \), which is related to the pressure drop per unit length as follows:

\[
\tau = \frac{\rho V^2}{2f}; \tag{3.294}
\]

\[
\frac{dp}{dl} = \frac{4\tau}{D_h}. \tag{3.295}
\]

3.4.1.1 Straight Channels

The following correlations are available in the PDC for straight channels, such as the shell and tube sides of shell-and-tube heat exchangers and pipes.

- Dittus-Boelter (DB in the PDC input) [30]

\[
Nu = 0.023Re^{0.8}Pr^n, \tag{3.296}
\]

where

\( n = 0.4 \) for heated flow and 0.3 for cooled flow.

- Petukhov-Gnielinski (PG in the PDC input) [31]

\[
Nu = \frac{f \left( Re-1000 \right) Pr}{1+12.7 \left( \frac{f}{2} \right)^{2/7} \left( Pr^{2/7}-1 \right)} \left[ 1+\left( \frac{D}{L} \right)^{2/7} \right], \tag{3.297}
\]

where

\( f \) = friction factor, found from \( \frac{1}{\sqrt{f}} = 4.0\log_{10} \left( \text{Re} \cdot \sqrt{f} \right) - 0.4 \),

\( D \) = hydraulic diameter,

\( L \) = channel length.
Both correlations above are applicable to turbulent flow (Re>2300) only. In laminar flow, the following correlation is used [32],

\[ Nu_{\text{lam}} = 4.364 \]  \hspace{1cm} (3.298)

For the flow of liquid metals (sodium, lead, etc..), the Lockhart-Martinelli (LM in the PDC input) correlation can be used for all geometries:

\[ Nu = 5 + 0.025(Re \cdot Pr)^{0.8} \] \hspace{1cm} (3.299)

For the friction factor, the following correlations are used:

- Turbulent Flow (Re>2300, Ref. 33)

\[ f = \frac{1}{4X^2} \] \hspace{1cm} (3.300)

where

\[ X = \text{hydraulic resistance found from } X = 1.74 - 2\log_{10}\left( \frac{2k_s}{D_h} + \frac{18.7X}{Re} \right) \],

\[ k_s = \text{wall roughness (10 } \mu \text{m is assumed),} \]
\[ D_h = \text{hydraulic diameter.} \]

- Laminar Flow (Re<2300, Ref. 34)

\[ f = \frac{16}{Re} \] \hspace{1cm} (3.301)

3.4.1.2 PCHE Channels

A special correlation for PCHE channels (PC in the PDC input) has been developed for the PDC [35]. The correlation is based on the enhancement of the friction factor and Colburn factor over those for straight channels to account for the effects of the zigzag channel angle.

The friction factor for the straight PCHE channels is calculated as

\[ f_0 = \begin{cases} 
\frac{16}{Re}, & \text{Re} < 1700 \\
0.0791 \left( \frac{Re}{0.25} \right)^0.25, & \text{Re} > 2300
\end{cases} \] \hspace{1cm} (3.302)

together with a simple linear function in the transition region (1700<Re<2300).
The zigzag channel enhancement is calculated in the following form:

\[
\frac{f}{f_0} = \begin{cases} 
1 + a_f (\text{Re} + 50), & \text{Re} < 1300 \\
1 + a_f (\text{Re} + 50), & \text{Re} \geq 1300 \\
k \text{Re}^c, & \text{Re} \geq 1300 
\end{cases}
\]  

(3.303)

where the coefficients, \(k, c, \) and \(a_f\), are found from curve fitting from the Argonne’s PCHE experiments [35]:

\[
c = \ln \left( \frac{1 + 223283 \cdot a_f^2}{1 + a_f (1300 + 50)} \right) ;
\]

\[
k = \frac{1 + a_f (1300 + 50)}{1300^c} ;
\]

\[
a_f = 4.5 \cdot 10^{-3} \tan(\alpha/2) ;
\]

where \(\alpha = \) zigzag channel angle (see Figure 3-8).

The heat transfer correlation is developed separately for the laminar and turbulent regions. Similar to the friction factor, the correlations incorporate an angle-dependent parameter, \(a_j\), which is defined from fitting of the available curves and data. In the turbulent region (\(\text{Re} > 2300\)), the Colburn factor is a function of the Reynolds number and the parameter \(a_f\):

\[
j_{turb} = a_f (0.1341) \text{Re}^{-0.3319} ;
\]

(3.304)

\[
a_f = 0.6 + 0.5 \tan(\alpha/2) .
\]

(3.305)

In the laminar region, the Colburn factor for a zigzag channel is defined as an enhancement over the straight channel:

\[
j_{0,\text{lam}} = \frac{4.1}{\text{Re}} , \quad \text{Re} < 2300 ;
\]

(3.306)

\[
\left( \frac{j}{j_{0,\text{lam}}} \right) = 1 + a_j (\text{Re} + 50), \quad \text{Re} < 2300 ;
\]

(3.307)

where the parameter \(a_{j,\text{lam}}\) is defined from the continuity of the heat transfer correlation as

\[
a_{j,\text{lam}} = \frac{a_f (0.1341) \cdot (1300)^{-0.3319} \cdot 1300 - 4.1}{1300 + 50} .
\]

It is found that the above correlations describe the heat transfer in zigzag channels pretty accurately such that no specific treatment in the transition region would be necessary. For the
straight channel, the heat transfer in the transition region was found to be approximated by the following law:

$$j_{0,\text{tran}}(\text{Re}) = 352 \text{ Re}^{-1.4562}.$$  \hfill (3.308)

The PDC also supports the modified wavy-fin correlation for PCHE channels. The “wavy fins” (WF) correlation is based on correlations available in the literature, but includes modifications to account for the varying zigzag angle. For the base correlations, the fits for the “11.44-3/8W” geometry from Reference [9] are used since they most closely represent the PCHE geometry:

$$j = 0.1635 \cdot \text{Re}^{-0.3465}$$  
$$f = 1.2039 \cdot \text{Re}^{-0.391}.$$  \hfill (3.309)

The friction factor correlation for wavy fins has been subsequently modified to introduce the effect of the zigzag channel angle to match the test data from the PCHE experiments [35]:

$$f = k(x) \cdot \text{Re}^{-m(x)}$$  
$$k(x) = 0.2074x^2 - 1.4587x + 2.4552$$  \hfill (3.310)  
$$m(x) = -0.1828x^2 + 0.3525x + 0.2213$$

where \(x = \frac{\alpha}{\alpha_{\text{ref}}}, \quad \alpha_{\text{ref}} = 44.9^\circ - \text{zigzag channel angle in the reference geometry.}\)

### 3.4.1.3 Cross-Flow Cooler

#### Heat Transfer

For the Kays and London (KL in the PDC input) correlation for cross-flow heat exchangers, one particular geometry from Reference [9] (CF-8.8-1.0J-A that is the closest to the cross-flow heat exchanger designs analyzed with the PDC) was selected and fitted with the power law:

$$j = 0.1408 \cdot \text{Re}^{-0.3705}.$$  \hfill (3.311)

In addition, the Briggs and Young correlation (BY in the PDC input) [36] is included in the PDC models of the cross-flow cooler:

$$\frac{h_{\alpha}d_{t,o}}{k_{\alpha}} = 0.134 \left(\frac{G_{\alpha}d_{t,o}}{\mu_{\alpha}}\right)^{0.681} \text{ Pr}_{\alpha}^{1/3} \left(\frac{H_f}{S_f}\right)^{-0.2} \left(\frac{t_f}{S_f}\right)^{-0.1134},$$  \hfill (3.312)

where

- \(h_{\alpha}\) = air-side heat transfer coefficient,
- \(d_{t,o}\) = tube outer diameter,
\( k_a \) = thermal conductivity of air, 
\( G_a \) = air mass flux based on \( A_{c,a} \) (see below), 
\( \mu_a \) = dynamic viscosity of air, 
\( \text{Pr}_a \) = Prandtl number of air, 
\( H_f \) = fin height, 
\( s_f \) = fin spacing, 
\( t_f \) = fin thickness.

The air-side flow area for Equation (3.312) is defined as the minimum free flow area when the air goes across the finned tube bank (and correspondingly the local air velocity will be the maximum). Specifically, it is defined as:

\[
A_{c,a} = \left((p_h - d_{t,o})L_t - (d_f - d_{t,o}) t_f N_f \right) N_c ,
\]

(3.313)

where

\( A_{c,a} \) = air-side flow area, 
\( p_h \) = horizontal tube pitch, 
\( L_t \) = tube length, 
\( d_f \) = fin diameter, 
\( N_f \) = number of fins per tube, 
\( L_t \) = tube length, 
\( N_c \) = number of tube columns (number of tubes per row).

**Pressure Drop**

Similar to the heat transfer correlation, the friction factor from the geometry CF-8.8-1.0J-A Reference [9] is fitted with a power law for the Kays and London (KL) correlation:

\[
f = 0.1484 \cdot Re^{-0.2436} .
\]

(3.314)

For the Briggs and Young (BY) correlation, a general pressure drop correlation that takes into account the finned tube geometry developed Robinson and Briggs [37] is used:

\[
f = 18.93 \left( \frac{G_a d_{t,o}}{\mu_a} \right)^{-0.316} \left( \frac{p_h}{d_{t,o}} \right)^{-0.927} \left( \frac{p_h}{p_v} \right)^{-0.515} .
\]

(3.315)

The total pressure drop for cross air flow over the finned tube bank is calculated based on \( f_r \) as:

\[
\Delta p_a = \frac{c_a^2}{p_a} f N_r ,
\]

(3.316)

where

\( N_r \) = number of tube rows.
In addition to the above correlations, the PDC also supports “BK” correlations which uses Briggs and Yong (BY) correlations for heat transfer and Kays and London (KL) correlation for pressure drop.

3.4.2 Fluid Properties

3.4.2.1 Cycle Working Fluid

Since the PDC is developed for analysis of supercritical cycles, accurate calculation of the working fluid’s properties, especially close to the critical point, are important for the PDC calculations. For this reason, the most accurate properties formulations available are used in the PDC where possible. The properties for the following fluids are incorporated in the PDC:

- Carbon dioxide (CO₂),
- Nitrogen (N₂),
- Water (H₂O),
- Air, and
- Helium (He).

However, so far, only CO₂ properties have been tested extensively for both the steady-state and dynamic models. The CO₂ properties in the PDC are modeled after Reference [38] for regular properties (density, pressure, enthalpy, etc.), Reference [39] for viscosity and Reference [40] for thermal conductivity.

References [41] through [47] list the sources for properties for other fluids used in the PDC.

Due to the complex equations for the fluid properties, these calculations may be the slowest part of the PDC, especially in dynamic calculations. Therefore, the code has been optimized extensively to speed up property calculations. Examples of such optimization include using array operations where possible, pre-calculating as many variables as possible before iterations, and using pre-calculated tables for the first guess for iterations. Also, to avoid iterations on properties, the dynamic equations in the PDC are formulated to be solved for in terms of the properties primary variables – temperature and density.

3.4.2.2 HAHX Hot-Side Fluids

The PDC supports the following fluids on the hot side of the Heat Addition Heat Exchanger:
• Sodium (Na),
• Lead (Pb),
• Helium (He),
• 80% Nitrogen - 20% Helium mixture (N2-He),
• Nitrogen (N₂),
• Air,
• LiF-BeF₂ salt (Salt1),
• NaBF₄-NaF salt (Salt2),
• LiF-NaF-KF salt (Salt3),
• NaF-ZrF₄ salt (Salt4).

3.4.2.3 Cooler Cold-Side Fluids

The following fluid are supported by the PDC for the cold side of the cooler:

• Water (H₂O),
• Air.

3.4.3 Structural Materials

Table 3-8 lists the materials for structures, such as heat exchanger walls and pipe walls, supported by the PDC. Note that although all the materials in Table 3-8 can be used for steady-state analysis, only some materials can be used in dynamic models since not all of the properties are incorporated in the code for all materials.
Table 3-8. Structural Materials Supported by PDC

<table>
<thead>
<tr>
<th>PDC Input</th>
<th>Material</th>
<th>Dynamic model</th>
</tr>
</thead>
<tbody>
<tr>
<td>SS316</td>
<td>316 Stainless Steel</td>
<td>Yes</td>
</tr>
<tr>
<td>SS304</td>
<td>304 Stainless Steel</td>
<td></td>
</tr>
<tr>
<td>HT9</td>
<td>HT9 ferritic steel</td>
<td>Yes</td>
</tr>
<tr>
<td>T91</td>
<td>9Cr-1Mo ferritic steel</td>
<td></td>
</tr>
<tr>
<td>Al617</td>
<td>Nickel-based Alloy 617</td>
<td></td>
</tr>
<tr>
<td>Al230</td>
<td>Nickel-based Alloy 230</td>
<td></td>
</tr>
<tr>
<td>800H</td>
<td>Alloy 800H</td>
<td></td>
</tr>
<tr>
<td>Al</td>
<td>Aluminum, Grade 1100</td>
<td>Yes</td>
</tr>
<tr>
<td>HastX</td>
<td>Hastelloy X</td>
<td></td>
</tr>
<tr>
<td>HastN</td>
<td>Hastelloy N</td>
<td></td>
</tr>
</tbody>
</table>
ACKNOWLEDGEMENTS

Argonne National Laboratory’s work was supported by the U. S. Department of Energy under Prime Contract No. DE-AC02-06CH11357 between the U.S. Department of Energy and UChicago Argonne, LLC.

The Plant Dynamics Code development was carried out under multiple DOE’s programs, including: the Nuclear Energy Research Initiative (NERI) Program, the Advanced Fuel Cycle Initiative (AFCI), the Advanced Reactor Concepts (ARC) Program, Advanced Small Modular Reactor (aSMR) Program, the Energy Conversion Technology area of the Advanced Reactor Technologies (ART) Program, and the Energy Conversion area of the Nuclear Technology Research and Development (NTRD) Program.

The authors are grateful to Gary Rochau (Sandia National Laboratories), the Technical Area Lead, Bob Hill (Argonne National Laboratory), the National Technical Director, as well as Brian Robinson (U.S. DOE), Headquarters Program Manager for the ART Energy Conversion Program. The authors are equally grateful to Paul S. Pickard (Sandia National Laboratories), the previous Technical Area Lead, and the previous DOE Program Managers who supported development of the Plant Dynamic Code in the past, including Carl Sink, Rob Versluis, Robert Price, Bhupinder Singh, Matt Hutmaker, Jason Tokey, Alice Caponiti and Thomas Sowinski (U.S. DOE).

The authors are also indebted to many individuals for their helpful advices and discussions during the course of this work including David C. Wade, James E. Cahalan, George Klopp, Dae H. Cho, Ike U. Therious, Ron Kulak, Bong Yu, Qiuping Ly, and Thomas H. Fanning (Argonne National Laboratory), Vaclav Dostal, Pavel Hejzlar and Michael Driscoll (Massachusetts Institute of Technology), Kenneth Nichols and Robert Fuller (Barber-Nichols, Inc.), Stephen Dewson, David Southall, Renauld Le Pierres, Colin Grady, and Xiuqing Li (Heatric Division of Meggitt (UK) Ltd.), and Jeremy Floyd and Nicholas Alpy (CEA Cadarache). The authors are also thankful to student interns at Argonne who contributed to the code development and analysis including Konrad Kulesza, John Edlebeck, Haomin Yuan, and Sandeep Pidaparti. The authors greatly appreciate help from Acacia Brunett (Argonne National Laboratory) in generating the PDC documentation in Appendix C of this report.

The authors also want to express their gratitude to the teams from Sandia National Laboratories (Jim Pasch, Steve Wright, Tom Conboy, and Blake Lance) and Bechtel Marine Propulsion Corporation (Patrick Fourspring, Eric Clementoni, Kevin Rahner, Kenneth Kimball, and Brian Morris) for sharing of test data for Plant Dynamics Code validation.
REFERENCES


45. The Engineering Tool Box, Air Properties, http://www.engineeringtoolbox.com/22_156.html


APPENDIX A: PDC VERIFICATION AND VALIDATION REFERENCES


APPENDIX B: EXAMPLE PROBLEM

The example problem here, and also supplied with the code, is the steady-state and transient analysis of a supercritical carbon dioxide (sCO₂) Brayton cycle energy converter for the Advanced Fast Reactor (AFR)-100 reactor. The AFR-100 is a 250 MWth (about 100 MWₑ) Sodium-Cooled Fast Reactor (SFR) Small Modular Reactor (SMR). It employs low pressure primary and intermediate sodium loops, both at about atmospheric pressure. The heat is supplied to the sCO₂ cycle in a number of modular intermediate sodium-to-CO₂ Reactor Heat Exchangers (RHX). The intermediate sodium RHX inlet and outlet temperatures are 528 °C and 373 °C, respectively.

The sCO₂ cycle for the AFR-100 is designed to convert 250 MWth power from the reactor and RHX into electricity. The power conversion cycle is the recompression Brayton cycle with a single eight-stage axial turbine and two centrifugal compressors, located on a common shaft connected to a single generator. The first (main) compressor is a single-stage compressor which operates close to the CO₂ critical point and defines the minimum pressure and temperature for the cycle. Those are set at 8.2 MPa and 35.0 °C at the first compressor impeller inlet. The main compressor also sets the maximum cycle pressure at 25 MPa. The second compressor is a two-stage recompression compressor. The recompression cycle configuration is designed to improve the efficiency of the recuperative heat transfer by splitting the recuperative heat exchanger into two parts, a low-temperature recuperator (LTR) and separate high-temperature recuperator (HTR). The flow fraction in the recompression line, 33%, is calculated to maximize the cycle efficiency. Both recuperators, as well as RHX, are PCHE platelet heat exchangers. Heat is rejected from the cycle by air in a cross-flow finned tube cooler. The design air ambient temperature is 30 °C. Air pressure is 1 atm at the cooler outlet.

The sample transient is load following between 100% and 50% grid demand (details are discussed in Section B.3).

This appendix presents the input files and results for both the steady-state and transient analyses. The PDC input files presented here are those supplied with the code and also those used to obtain the PDC GUI forms presented in the User’s Guide part of this document.

The figure on the following page shows the AFR-100 sCO₂ cycle as modeled in this example problem, with all the components and connecting pipes. It also shows all flow and pressure/temperature nodes. The flow nodes correspond to the pipe indexes in the input files.
Cycle Configuration for Example Problem

<table>
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<tr>
<th>Index</th>
<th>From Component</th>
<th>Port</th>
<th>To Component</th>
<th>Port</th>
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<tr>
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<td>RHX</td>
<td>CO</td>
<td>Turb</td>
<td>I</td>
</tr>
<tr>
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<td>Turb</td>
<td>O</td>
<td>TBPmx</td>
<td>II</td>
</tr>
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<td>O</td>
<td>HTR</td>
<td>HI</td>
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<td>HI</td>
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<td>SP</td>
<td>I</td>
</tr>
<tr>
<td>6</td>
<td>SP</td>
<td>O1</td>
<td>INVmx</td>
<td>II</td>
</tr>
<tr>
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<td>CI</td>
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<tr>
<td>25</td>
<td>Tank</td>
<td>O</td>
<td>INVmx</td>
<td>I</td>
</tr>
</tbody>
</table>

Valve | Pipe#
--- | ---
TINv  | 1
C2Ov  | 20
CBPv  | 21
TBpv  | 22
RBpv  | 23
RTHv  | 15
INVlv | 24
INVov | 25
B.1. Steady-State Model Setup Input Files

The main goal of the steady-state model is to calculate the cycle performance as measured by the cycle efficiency. To do that, the PDC calculates the temperatures, pressures, and other fluid properties such as enthalpy, for all cycle nodes, as well as flow rates for all flow nodes (pipes).

This example problem was set up to use the turbomachinery design mode, meaning that the design and performance of the turbine and each compressor is calculated by the code. As part of the design calculations, the turbomachinery performance, as measured by the efficiency and outlet temperature is calculated.

For all of the heat exchanger calculations, the design is given and the code calculates their performance, in terms of the outlet temperatures on the two sides, pressure drops, and effectiveness. For the RHX (a HAHX), the code matches the required sodium-outlet temperature by adjusting the \( \text{CO}_2 \) flow rate. That flow rate also sets the main flow rate for the entire cycle. For the cooler calculations, iterations are carried out on the air flow rate to match the required \( \text{CO}_2 \) outlet temperature, which is set by the given main compressor impeller-inlet temperature, temperature drop in the main compressor inlet nozzle, temperature (and pressure) drop in the pipes between the cooler and the main compressor, and the cooler bypass flow fraction.

The fluid condition change in pipes is calculated from the pressure drop in the pipes themselves and corresponding valve pressure drops, where applicable. In this example problem, the pipes are assumed to be perfectly insulated so the heat losses from pipes is zero.

The following pages present the input files relevant to the steady-state calculation. In these files, irrelevant sections, such as input for HX types other than the selected type, are shaded in gray.
Input data file for CO₂ cycle efficiency calculations

Recalculate (1) or use output files (0) for the first iteration

0

Working fluid
CO₂

Heat addition mode (0-RHX, 1-Electrical heater)
0

Type of turbomachinery calculations (0-Design, 1-Performance)
0

Maximum pressure in cycle (MPa) (p_min and T_min are set in Comp input)
30

First guess for flow rate (if not read from output file), kg/s
1186.0

Piping material
SS316

Ambient temperature, °C
25

Heat transfer correlation in pipes
DB

Maximum number of iterations
60

Components

+ Types: HX T urb Comp Cool Rec Mixer Split Valve Tank
+ + Req. conn: CI, CO I, O I, O HI, HO HI, HO, CI, CO I1, I2, O I, O1, O2 - I, O
+ + (I=inlet, O=outlet, H=hot, C=cold, I1, I2, O1, O2=I/O with port number)
+ + Each component should have unique name
+ + Name should correspond to input file (Turb -> Turb_dat.txt)
+ +

HX(s) or El. Heater(s)
RHX

Turbine(s)
Turb

Compressor(s)
Comp1 Comp2

Cooler(s)
Cool

Recuperator(s)
HTR LTR

Mixer(s)
CBPmx MX TBPmx INVmx RBPmx

Splitter(s)
SP CBPsp TBPsp INVsp RBPsp

Valve(s)
TINv C2Ov CBpv TBPv INViv INVUV INVuv RBPv RTHv

Tank(s)
Tank
INVOv 25
INVIv 24
RTHv 15 0
RBPv 23
TBPv 22
CBPv 21
C2Ov 20 0
TINv 1
Valve Pipe# Resistance
-----------------------------------
+ Resistance includes closed valves
+ Resistance = 0 corresponds to pressure drop across the valve in MPa
+ (N bends), curvature (r_b/D), and heat loss factor (k_HL) should also be given
+ k_HL meaning: 0=perfectly insulated, 1=bare, >1=enhancement factor

<table>
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<th>No. Input</th>
<th>Output</th>
<th>Count</th>
<th>L,m</th>
<th>ID,m</th>
<th>t,mm</th>
<th>N_bends</th>
<th>r_b/D</th>
<th>k_HL</th>
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</tbody>
</table>

Flow splits
-------------------------------

Split Primary_fraction
SP 0.67
CBFsp 0.95
TBPsp 1
INVsp 1
RBPsp 1

Valves
-------------------------------

+++

+ For each valve (list by Name) specify the location (pipe #) and resistance
+ Resistance = 0 corresponds to pressure drop across the valve in MPa
+ (0 - no effect from valve)
+ Resistance = 1 corresponds that dP should be calculated in cycle
+ (includes closed valves)

 Valve Pipe# Resistance
 TINV 1 0
 C2OV 20 0
 CBPV 21 -1
 TBPV 22 -1
 RBPV 23 -1
 RTHV 15 0
 INVIV 24 -1
 INVUV 25 -1

PDC: Plant Dynamics Code for Design and Transient Analysis of Supercritical Brayton Cycles
September 27, 2018
************** Input data for RHX hot side ******************

RHX primary fluid (RPF)
Na
RPF inlet temperature, °C
528
RPF outlet temperature, °C
373
RPF inlet pressure, MPa
0.1
RHX total power, MW
250
RPF flow fractions for RHX #2,...
0.5

RHX_HS_dat.txt
--- Reactor Heat Exchanger parameters

| Type (0 - General, 1 - Shell-and-tube, 2 - Platelet PCHE, 3 - Z/I PCHE) | 2 |
| Given efficiency (for general only), % | 92.8 |
| Given pressure drops for hot and cold sides (for general only), Pa | 2200 150000 |
| Hot side inlet and outlet plena volumes, m³ | 0 0 |
| Cold side inlet and outlet plena volumes, m³ | 0 0 |

### Shell-and-tube HX data

- **HX outer diameter, m**: 3.8
- **HX length, m**: 6
- **Inner and outer tube diameters, m**: 0.01 0.014
- **HX pitch-to-diameter ratio**: 1.2
- **Tube material (5 characters)**: SS316
- **HT region pressure drop / total pressure drop ratio (hot and cold sides)**: 1.0 1.0
- **Number of points for temperature calculations**: 21
- **Required accuracy (in secondary outlet temperature), °C**: 0.001
- **Tube side (1 - Primary, 2 - Secondary)**: 2
- **Heat transfer correlations for hot and cold sides**: DB DB
- **Number of fins on inner surface per tube**: 12
- **Width of fins on inner surface, m**: 0.001
- **Length of fins on inner surface, m**: 0.0015
- **Number of fins on outer surface per tube**: 12
- **Width of fins on outer surface, m**: 0.001
- **Length of fins on outer surface, m**: 0.0025
- **Number of baffles on shell side**: 0
- **Baffle plate cut, % (0 = full plate)**: 45.14
- **Baffle hole diameter, cm**: 1.0
- **Baffle hole loss coefficient**: 1.5
- **Number of holes per HX tube**: 0

### PCHE data

- **Number of units**: 92
- **Unit length, m**: 1.5
- **Unit Width, m**: 0.6
- **Unit Height, m**: 0.6
- **Headers length (each side), cm**: 11
- **Pressure boundary thickness, mm**: 17
- **Zigzag channel angles (hot and cold sides), deg**: 0 60

---
<table>
<thead>
<tr>
<th>Description</th>
<th>Value</th>
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<tbody>
<tr>
<td>HT region pressure drop / total pressure drop ratio (hot and cold sides)</td>
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<tr>
<td>Channel diameter (or width) (hot and cold sides), mm</td>
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<td>Channel depth (hot and cold sides, input 0 for PCHE), mm</td>
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<td>Pitch-to-diameter ratio (hot and cold sides)</td>
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<td>Layer thickness (hot and cold sides), mm</td>
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</table>
PDC: Plant Dynamics Code for Design and Transient Analysis of Supercritical Brayton Cycles  
September 27, 2018

--------------- Recuperator parameters -------------------------------
Type (0 - General, 1 - Shell-and-tube, 2 - Platelet PCHE, 3 - Z/I PCHE)
2
Given efficiency (for general only), %
95.5
Given pressure drops for hot and cold sides (for general only), Pa
26100 9100
Hot side inlet and outlet plena volumes, m³
0 0
Cold side inlet and outlet plena volumes, m³
0 0

---------------------------- Shell-and-tube HX data -------------------------------
Recuperator outer diameter, m
3.8
Recuperator length, m
6
Inner and outer tube diameters, m
0.01 0.014
Recuperator pitch-to-diameter ratio
1.2
Tube material (5 characters)
SS316
HT region pressure drop / total pressure drop ratio (hot and cold sides)
1.0 1.0
Number of points for temperature calculations
21
Required accuracy (in secondary outlet temperature), C
0.001
Tube side(1 - Primary, 2 - Secondary)
2
Heat transfer correlations for hot and cold sides
DB
DB
Number of fins on inner surface per tube
12
Width of fins on inner surface, m
0.001
Length of fins on inner surface, m
0.0015
Number of fins on outer surface per tube
12
Width of fins on outer surface, m
0.001
Length of fins on outer surface, m
0.0025
Number of baffles on shell side
0
Baffle plate cut, % (0 = full plate)
45.14
Baffle hole diameter, cm
1.0
Baffle hole loss coefficient
1.5
Number of holes per HX tube
0

----------------------- PCHE data -----------------------
Number of units
48
Unit length, m
0.6
Unit Width, m
1.5
Unit Height, m
0.6
Headers length (each side), cm
11
Pressure boundary thickness, mm
17
Zigzag channel angles (hot and cold sides), deg
60 60
Fin efficiency
<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>HT region pressure drop / total pressure drop ratio (hot and cold sides)</td>
<td>0.85</td>
</tr>
<tr>
<td>Channel diameter (or width) (hot and cold sides), mm</td>
<td>1.3 1.3</td>
</tr>
<tr>
<td>Channel depth (hot and cold sides, input 0 for PCHE), mm</td>
<td>0.0</td>
</tr>
<tr>
<td>Pitch-to-diameter ratio (hot and cold sides)</td>
<td>1.4 1.4</td>
</tr>
<tr>
<td>Layer thickness (hot and cold sides), mm</td>
<td>1.065 1.065</td>
</tr>
<tr>
<td>Material</td>
<td>SS316</td>
</tr>
<tr>
<td>Number of points for temperature calculations</td>
<td>6</td>
</tr>
<tr>
<td>Required accuracy (in secondary outlet temperature), °C</td>
<td>1D-5</td>
</tr>
<tr>
<td>Heat transfer correlations for hot and cold sides</td>
<td>PC</td>
</tr>
<tr>
<td></td>
<td>PC</td>
</tr>
</tbody>
</table>
PDC: Plant Dynamics Code for Design and Transient Analysis of Supercritical Brayton Cycles  
September 27, 2018

************** Recuperator parameters ****************************
Type (0 - General, 1 - Shell-and-tube, 2 - Platelet PCHE, 3 - Z/I PCHE)
2
Given efficiency (for general only), %
94.6 96.6
Given pressure drops for hot and cold sides (or general only), Pa
16D+3 8D+3
Hot side inlet and outlet plena volumes, m³
0 0
Cold side inlet and outlet plena volumes, m³
0 0

----------------------- Shell-and-tube HX data -----------------------
Recuperator outer diameter, m
3.8
Recuperator length, m
6
Inner and outer tube diameters, m
0.01 0.014
Recuperator pitch-to-diameter ratio
1.2
Tube material (5 characters)
SS316
HT region pressure drop / total pressure drop ratio (two sides)
1.0 1.0
Number of points for temperature calculations
21
Required accuracy (in secondary outlet/inlet temperature), °C
0.001
Tube side (1 - Primary, 2 - Secondary)
2
Heat transfer correlations for hot and cold sides
DB
DB
Number of fins on inner surface per tube
12
Width of fins on inner surface, m
0.001
Length of fins on inner surface, m
0.0015
Number of fins on outer surface per tube
12
Width of fins on outer surface, m
0.001
Length of fins on outer surface, m
0.0025
Number of baffles on shell side
0
Baffle plate cut, % (0 = full plate)
45.14
Baffle hole diameter, cm
1.0
Baffle hole loss coefficient
1.5
Number of holes per HX tube
0

------------- PCHE data --------------------------------------------
Number of units
56
Unit length, m
0.6
Unit width, m
1.5
Unit height, m
0.6
Headers length (each side), cm
11
Pressure boundary thickness, mm
17
Zigzag channel angles (hot and cold sides), deg
60 90
Fin efficiency
<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>HT region pressure drop / total pressure drop ratio (two sides)</td>
<td>0.85</td>
</tr>
<tr>
<td>Channel diameter (or width) (hot and cold sides), mm</td>
<td>1.3</td>
</tr>
<tr>
<td>Channel depth (hot and cold sides, input 0 for PCHE), mm</td>
<td>0</td>
</tr>
<tr>
<td>Pitch-to-diameter ratio (hot and cold sides)</td>
<td>1.35</td>
</tr>
<tr>
<td>Layer thickness (hot and cold sides), mm</td>
<td>1.04</td>
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<tr>
<td>Material</td>
<td>SS316</td>
</tr>
<tr>
<td>Number of points for temperature calculations</td>
<td>6 21</td>
</tr>
<tr>
<td>Required accuracy (in secondary outlet temperature), C</td>
<td>1D-5</td>
</tr>
<tr>
<td>Heat transfer correlations for hot and cold sides</td>
<td>PC</td>
</tr>
<tr>
<td></td>
<td>PC</td>
</tr>
</tbody>
</table>
************** Cooler parameters ****************************
Cooling fluid (3 characters)
Air
Inlet temperature of cooling fluid, C
30
Outlet pressure of cooling fluid, Pa
101325
Iterations option (0-No, 1-N_unit, 2-Length, 3-Cooling fluid flow rate)
3
Cooling fluid flow rate, kg/s (first guess, if iterated on)
14000
Cooling fluid inlet and outlet pipe diameters, m
1 1
CO2 side inlet and outlet plena volumes, m3
0 0
Cooling fluid pump efficiency, %
90
Accuracy on outlet temperature
1.0-6
Cooler type (1 - Shell-and-tube, 2 - PCHE, 5 - Cross-flow PCHE, 6 - Cross-flow finned tubes)
6

----------------------- Shell-and-tube HX data -----------------------
Number of units (first guess, if iterated on)
1
Cooler length, m (first guess, if iterated on)
10
Cooler outer diameter, m
30.6
Inner and outer tube diameters, m
0.01 0.014
Pitch-to-diameter ratio
1.3
Tube material (5 characters)
SS316
HT region pressure drop / total pressure drop ratio (hot and cold sides)
1.0 1.0
Number of points
21
Tube side (1 - Primary, 2 - Secondary)
1
Heat transfer correlations for hot and cold sides
DB DB
Number of fins on inner surface per tube
0
Width of fins on inner surface, m
0.001
Length of fins on inner surface, m
0.0015
Number of fins on outer surface per tube
6
Width of fins on outer surface, m
0.001
Length of fins on outer surface, m
0.0021
Number of baffles on shell side
0
Baffle plate cut, % (0 = full plate)
45.14
Baffle hole diameter, cm
1
Baffle hole loss coefficient
1.5
Number of holes per HX tube
0

----------------------- PCHE HX data -----------------------
Number of units (first guess, if iterated on)
4375
Cooler length, m (first guess, if iterated on)
1.5
Unit Width, m

Cool_dat.txt
0.6
Unit Height, m
0.6
Headers length (each side), cm
11
Pressure boundary thickness, mm
17
Zigzag channel angles (hot and cold sides), deg
90 50
Fin efficiency
0.85
HT region pressure drop / total pressure drop ratio (hot and cold sides)
0.01 0.8
Channel diameter (or width) (hot and cold sides), mm
1 6
Channel depth (hot and cold sides, input 0 for PCHE), mm
0 0
Pitch-to-diameter ratio (hot and cold sides)
1.2 1.05
Layer thickness (hot and cold sides), mm
0.75 3.3
Material
SS316
Number of points for temperature calculations
12
Heat transfer correlations for hot and cold sides
PC
PC
Number of passes (for cross-flow HX only)
3

----------------------- Crossflow Shell-and-tube HX data -----------------------
Number of units (first guess, if iterated on)
67
HX width, m
4.56
HX length, m (first guess, if iterated on)
18.29
Number of tube rows
4
Number of passes
3
Pass arrangement (0 - tubes / 1 - headers)
1
Inner and outer tube diameters, m
0.0221 0.0254
HX pitch-to-diameter ratio, horizontal and vertical
2.25 1.95
Tube material (5 characters)
SS316
HT region pressure drop / total pressure drop ratio (hot and cold sides)
1.0 1.0
Number of points for temperature calculations
4
Tube side (1 - Primary, 2 - Secondary)
1
Heat transfer correlations for hot and cold sides
PG
BK
Fouling factor, m2*K/W
1.76E-4
Number of fins on inner surface per tube
0
Width of fins on inner surface, m
0.001
Length of fins on inner surface, m
0.0012
Number of fins on outer surface per tube
7200
Thickness of fins on outer surface, m
0.000406
Outer diameter fins on outer surface, m
0.05715
Fin material
Al
Efficiency (for first guess, static-to-static), %
92.0
Desired pressure ratio
1.6
Minimum hub radius (cm)
1
Degree of reaction
0.5
Design incidence angle, deg
0
Design deviation angle, deg
0
Blade maximum thickness-to-chord ratio
0.2
Tip clearance-to-radius ratio
0.002
Number of tip seals for rotor (0 = unshrouded)
2
Number of tip seals for nozzle (0 = unshrouded)
2
Trailing edge thickness for rotor blades, mm
1.0
Trailing edge thickness for nozzle blades, mm
1.0
Rotor blades solidity (0 = optimum from Boyce)
1.5
Nozzle blades solidity (0 = optimum from Boyce)
1.5
Blade material density (kg/m3)
8300
Blade maximum total stress (MPa)
300
Vibrational stress factor
0.75
Number of stages
8 6
Inlet nozzle efficiency, %
90
Outlet diffuser efficiency, %
90
Pressure recovery coefficient
0.5
Volume at exit, m3
1.0 10.0
Accuracy on exit pressure
1.D-5
Blade profile coefficients
Coefficient for Ixx
1.165D-3
Coefficient for Iyy
1.0381D-2
Coefficient for x coordinate of center of gravity
7.434D-2
Coefficient for y coordinate of center of gravity
2.738D-2
Coefficient for x coordinate of trailing edge
4.372D-1
Coefficient for y coordinate of trailing edge
-4.656D-1
Average blade angle, degrees
60.33
Principal axes angle, degrees
67
<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Efficiency (for first guess, static-to-static)</td>
<td>89%</td>
</tr>
<tr>
<td>Desired pressure ratio</td>
<td>10</td>
</tr>
<tr>
<td>Minimum temperature control flag and value, C</td>
<td>35.0D0</td>
</tr>
<tr>
<td>Minimum pressure control flag and value, MPa</td>
<td>8.2D0</td>
</tr>
<tr>
<td>Outlet pressure control flag and value, MPa</td>
<td>25.0D0</td>
</tr>
<tr>
<td>Accuracy on exit pressure</td>
<td>1.D-8</td>
</tr>
<tr>
<td>Inlet nozzle efficiency, %</td>
<td>90%</td>
</tr>
<tr>
<td>Volume at exit, m³</td>
<td>1.0</td>
</tr>
<tr>
<td>Compressor type (1=axial, 2=centrigugal)</td>
<td>2</td>
</tr>
<tr>
<td>Minimum hub radius (cm)</td>
<td>1</td>
</tr>
<tr>
<td>Degree of reaction</td>
<td>0.85</td>
</tr>
<tr>
<td>Blade profile coefficient</td>
<td>1.0</td>
</tr>
<tr>
<td>Design incidence angle thickness correction factor</td>
<td>1.0</td>
</tr>
<tr>
<td>Blade maximum thickness-to-chord ratio</td>
<td>0.1</td>
</tr>
<tr>
<td>Tip clearance-to-radius ratio</td>
<td>0.002</td>
</tr>
<tr>
<td>Rotor blades solidity (0= optimum from Boyce)</td>
<td>1.0</td>
</tr>
<tr>
<td>Nozzle blades solidity (0= optimum from Boyce)</td>
<td>0.5</td>
</tr>
<tr>
<td>Blade material density (kg/m³)</td>
<td>8300</td>
</tr>
<tr>
<td>Blade maximum total stress (MPa)</td>
<td>300</td>
</tr>
<tr>
<td>Vibrational stress factor</td>
<td>0.75</td>
</tr>
<tr>
<td>Number of stages</td>
<td>10</td>
</tr>
<tr>
<td>Outlet diffuser efficiency, %</td>
<td>90%</td>
</tr>
<tr>
<td>Pressure recovery coefficient</td>
<td>0.5</td>
</tr>
<tr>
<td>Coefficient for Ixx</td>
<td>1.165D-3</td>
</tr>
<tr>
<td>Coefficient for Iyy</td>
<td>1.0381D-2</td>
</tr>
<tr>
<td>Coefficient for x coordinate of center of gravity</td>
<td>7.434D-2</td>
</tr>
<tr>
<td>Coefficient for y coordinate of center of gravity</td>
<td>2.738D-2</td>
</tr>
<tr>
<td>Coefficient for x coordinate of trailing edge</td>
<td>4.372D-1</td>
</tr>
<tr>
<td>Coefficient for y coordinate of trailing edge</td>
<td>4.656D-1</td>
</tr>
<tr>
<td>Principal axes angle, degrees</td>
<td>60.33</td>
</tr>
<tr>
<td>de Haller coefficient (W2/W1)</td>
<td>0.75</td>
</tr>
<tr>
<td>Inlet GV angle, degrees</td>
<td></td>
</tr>
<tr>
<td>Number of stages</td>
<td>10</td>
</tr>
<tr>
<td>Impeller inlet angle, deg</td>
<td></td>
</tr>
</tbody>
</table>
0
Impeller tip medium radii by stage, cm
15
Number of splitter blades per one full blade
1
Splitter blade length (ratio to full blade length)
0.5
Blade thickness, mm
1
Number of diffuser blades (0-vaneless diffuser)
29
Diffuser incidence angle, deg
1
Diffuser discharge target angle, deg
70
Diffuser blade thickness at inlet, mm
1
Diffuser blade thickness at discharge, mm
1
Return channel loss coefficient
0.4
Blade surface roughness, um
4
Tip (shroud) clearance-to-radius ratio
0.002
Number of labyrinth seal on impeller tip (0-unshrouded)
0
Compressor #2

Efficiency (for first guess, static-to-static), %
89
Desired pressure ratio
1.63
Min. temperature control flag and value, C (used only if flag=1)
0 31.25D0
Min. pressure control flag and value, MPa (used only if flag=1)
0 7.4D0
Outlet pressure control flag and value, MPa (used only if flag=1)
0 20D0
Accuracy on exit pressure
1.D-8
Inlet nozzle efficiency, %
90
Volume at exit, m³
1.0
Compressor type (1-axial, 2-centrigual)
2

Axial compressor data

Minimum hub radius (cm)
1
Degree of reaction
0.85
Blade profile coefficient
1.0
Design incidence angle thickness correction factor
1.0
Blade maximum thickness-to-chord ratio
0.1
Tip clearance-to-radius ratio
0.002
Rotor blades solidity (0 - optimum from Boyce)
1.0
Nozzle blades solidity (0 - optimum from Boyce)
0.5
Blade material density (kg/m³)
8300
Blade maximum total stress (MPa)
300
Vibrational stress factor
0.75
Number of stages
9
Outlet diffuser efficiency, %
90
Pressure recovery coefficient
0.5

Blade profile coefficients

Coefficient for Ixx
1.165D-3
Coefficient for Iyy
1.0381D-2
Coefficient for x coordinate of center of gravity
7.434D-2
Coefficient for y coordinate of center of gravity
2.738D-2
Coefficient for x coordinate of trailing edge
4.372D-1
Coefficient for y coordinate of trailing edge
4.656D-1
Principal axes angle, degrees
60.33
de Haller coefficient (W2/W1)
0.75
Inlet GV angle, degrees

Centrifugal compressor data

Number of stages
2
Impeller inlet angle, deg
Impeller tip medium radii by stage, cm
15 15
Number of splitter blades per one full blade
1
Splitter blade length (ratio to full blade length)
0.5
Blade thickness, mm
1
Number of diffuser blades (0-vaneless diffuser)
28
Diffuser incidence angle, deg
1
Diffuser discharge target angle, deg
70
Diffuser blade thickness at inlet, mm
1
Diffuser blade thickness at discharge, mm
1
Return channel loss coefficient
0.4
Blade surface roughness, um
4
Tip (shroud) clearance-to-radius ratio
0.002
Number of labyrinth seal on impeller tip (0-unshrouded)
0
***************  Input data file for CO\textsubscript{2} cycle turbomachinery shaft ***************
Components on this shaft (exact names from "Cycle_dat.txt" file; one per line)
Gen
Turb
Comp1
Comp2
------------------------------------ (this line ends the list)
Shaft revolution speed (rev/s)
60
Generator's moment of inertia, kg-m\textsuperscript{2}
2500
Generator efficiency, %
98.5
Mechanical losses, %
1.0
Grid connection mode (0-not connected, 1-synchronous, 2-asynchronous)
1

Shaft_dat.txt
*********** Inventory Tank Data *******************************

Tank volume, m³
140

CO₂ initial temperature in tank, °C
40

CO₂ initial pressure in tank, MPa
9

Tank_dat.txt
B.2. Steady-State Results

The figure below shows the main results of the PDC steady-state calculations for the example problem. It shows the cycle efficiency (42.44 %) and the net generator output (104.7 MW_e), the temperature and pressure distributions around the cycle, CO₂ flow rate and split fractions, performance of each heat exchanger in terms of heat transfer rate and effectiveness, and performance of turbomachinery components, such as power and total-to-static efficiencies.

Steady-State Results for Example Problem

On the following pages, some of the PDC steady-state output files are shown.
PDC: Plant Dynamics Code for Design and Transient Analysis of Supercritical Brayton Cycles
September 27, 2018

[Repeat of input file is omitted from this report]
-------- Cycle nodes ---------Point#
Component
Conn.
p
T
MPa
C
1
RHX
CO
24.842
521.782
2
Turb
I
24.818
521.768
3
Turb
O
8.619
394.216
4
TBPmx
I1
8.609
394.203
5
TBPmx
O
8.609
394.203
6
HTR
HI
8.598
394.188
7
HTR
HO
8.576
194.510
8
LTR
HI
8.566
194.475
9
LTR
HO
8.556
86.520
10
SP
I
8.542
86.432
11
SP
O1
8.542
86.432
12
INVmx
I1
8.541
86.425
13
INVmx
O
8.541
86.425
14
CBPsp
I
8.540
86.418
15
CBPsp
O1
8.540
86.418
16
Cool
HI
8.535
86.387
17
Cool
HO
8.528
35.680
18
CBPmx
I1
8.526
35.674
19
CBPmx
O
8.526
36.423
20
Comp1
I
8.524
36.414
21
Comp1
O
25.000
76.277
22
INVsp
I
24.998
76.275
23
INVsp
O1
24.998
76.275
24
LTR
CI
24.997
76.273
25
LTR
CO
24.992
180.004
26
MX
I1
24.989
179.997
27
MX
O
24.989
183.004
28
RBPsp
I
24.988
183.002
29
RBPsp
O1
24.988
183.002
30
HTR
CI
24.982
182.990
31
HTR
CO
24.975
353.097
32
RBPmx
I1
24.972
353.094
33
RBPmx
O
24.972
353.094
34
TBPsp
I
24.969
353.090
35
TBPsp
O1
24.969
353.090
36
RHX
CI
24.954
353.075
37
SP
O2
8.542
86.432
38
Comp2
I
8.540
86.419
39
Comp2
O
24.990
189.199
40
MX
I2
24.989
189.196
41
CBPsp
O2
8.540
86.418
42
CBPmx
I2
8.526
86.335
43
TBPsp
O2
24.969
353.090
44
TBPmx
I2
8.609
394.203
45
RBPsp
O2
24.988
183.002
46
RBPmx
I2
24.972
353.094

ANL-ART-154

248

Cycle_res.txt
s
kJ/kg-K
-8.812E-02
-8.794E-02
-7.290E-02
-7.268E-02
-7.268E-02
-7.244E-02
-4.786E-01
-4.784E-01
-8.083E-01
-8.080E-01
-8.080E-01
-8.080E-01
-8.080E-01
-8.080E-01
-8.080E-01
-8.079E-01
-1.370E+00
-1.370E+00
-1.341E+00
-1.341E+00
-1.335E+00
-1.335E+00
-1.335E+00
-1.335E+00
-8.254E-01
-8.253E-01
-8.151E-01
-8.151E-01
-8.151E-01
-8.151E-01
-3.872E-01
-3.872E-01
-3.872E-01
-3.871E-01
-3.871E-01
-3.870E-01
-8.080E-01
-8.080E-01
-7.945E-01
-7.945E-01
-8.080E-01
-8.078E-01
-3.871E-01
-7.268E-02
-8.151E-01
-3.872E-01

h
kJ/kg
4.898E+02
4.898E+02
3.529E+02
3.529E+02
3.529E+02
3.529E+02
1.245E+02
1.245E+02
-1.056E+01
-1.056E+01
-1.056E+01
-1.056E+01
-1.056E+01
-1.056E+01
-1.056E+01
-1.056E+01
-1.923E+02
-1.923E+02
-1.832E+02
-1.832E+02
-1.556E+02
-1.556E+02
-1.556E+02
-1.556E+02
4.592E+01
4.592E+01
5.058E+01
5.058E+01
5.058E+01
5.058E+01
2.790E+02
2.790E+02
2.790E+02
2.790E+02
2.790E+02
2.790E+02
-1.056E+01
-1.056E+01
6.002E+01
6.002E+01
-1.056E+01
-1.056E+01
2.790E+02
3.529E+02
5.058E+01
2.790E+02

rho
kg/m3
1.588E+02
1.587E+02
6.861E+01
6.854E+01
6.854E+01
6.845E+01
1.052E+02
1.051E+02
1.678E+02
1.675E+02
1.675E+02
1.675E+02
1.675E+02
1.674E+02
1.674E+02
1.673E+02
5.890E+02
5.890E+02
5.509E+02
5.508E+02
7.051E+02
7.051E+02
7.051E+02
7.051E+02
3.556E+02
3.556E+02
3.507E+02
3.507E+02
3.507E+02
3.507E+02
2.120E+02
2.120E+02
2.120E+02
2.120E+02
2.120E+02
2.119E+02
1.675E+02
1.674E+02
3.413E+02
3.413E+02
1.674E+02
1.672E+02
2.120E+02
6.854E+01
3.507E+02
2.120E+02

w
m/s
4.574E+02
4.573E+02
3.960E+02
3.959E+02
3.959E+02
3.959E+02
3.231E+02
3.231E+02
2.605E+02
2.605E+02
2.605E+02
2.605E+02
2.605E+02
2.605E+02
2.605E+02
2.605E+02
2.210E+02
2.209E+02
2.074E+02
2.073E+02
4.278E+02
4.277E+02
4.277E+02
4.277E+02
3.490E+02
3.490E+02
3.498E+02
3.498E+02
3.498E+02
3.497E+02
4.074E+02
4.074E+02
4.074E+02
4.074E+02
4.074E+02
4.073E+02
2.605E+02
2.605E+02
3.515E+02
3.515E+02
2.605E+02
2.604E+02
4.074E+02
3.959E+02
3.498E+02
4.074E+02

cp
kJ/kg-K
1.251E+00
1.251E+00
1.161E+00
1.161E+00
1.161E+00
1.161E+00
1.152E+00
1.152E+00
1.504E+00
1.503E+00
1.503E+00
1.503E+00
1.503E+00
1.503E+00
1.503E+00
1.503E+00
1.028E+01
1.029E+01
1.375E+01
1.377E+01
2.251E+00
2.251E+00
2.251E+00
2.251E+00
1.555E+00
1.555E+00
1.540E+00
1.540E+00
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1.540E+00
1.258E+00
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1.503E+00
1.503E+00
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1.512E+00
1.503E+00
1.502E+00
1.258E+00
1.161E+00
1.540E+00
1.258E+00


HTR  : LP     0.2480 %
Comp2   64.6526 m/s
Comp1   58.2848 m/s
Comp1   92.6698 %
m = 1186.1818 kg/s

--- Pipe# Start End m A u M# dp_f/dL dp_f dp_b dp_v dp_tot
   Node Node kg/s m\^2 m/s   - kPa/m m kPa kPa kPa
---\
   1  1  2  1.186E+03 3.664E-01 2.039E+01 0.045 5.377E+01 1.075E+01 1.309E+01 0.000E+00 2.384E+01
   3  4  0  1.186E+03 3.664E-01 4.721E+01 0.119 1.244E+00 2.488E+00 7.342E+00 0.000E+00 9.829E+00
   5  6  1  1.186E+03 3.664E-01 4.726E+01 0.119 1.245E+00 3.736E+00 7.350E+00 0.000E+00 1.109E+01
   7  8  0  1.186E+03 3.664E-01 3.078E+01 0.095 8.103E+01 1.621E+01 9.152E+00 0.000E+00 1.077E+01
   9 10  2  1.186E+03 1.963E-01 3.604E+01 0.138 2.559E+00 5.118E+00 9.243E+00 0.000E+00 1.436E+01
   11 12  3  7.947E+02 1.963E-01 2.417E+01 0.093 1.151E+00 1.151E+00 0.000E+00 0.000E+00 1.151E+00
   13 14  2  7.947E+02 1.963E-01 2.417E+01 0.093 1.151E+00 1.151E+00 0.000E+00 0.000E+00 1.151E+00
   15 16  4  7.550E+02 1.963E-01 2.297E+01 0.088 1.059E+00 1.039E+00 4.049E+00 0.000E+00 5.088E+00
   17 18  7  7.550E+02 1.963E-01 6.528E+00 0.030 2.959E+01 5.918E+01 1.308E+00 0.000E+00 1.899E+00
   19 20  1  7.947E+02 1.963E-01 7.348E+00 0.035 3.504E+01 7.008E+01 1.514E+00 0.000E+00 2.215E+00
   21 22  5  7.947E+02 1.963E-01 5.740E+00 0.013 2.742E+01 5.483E+01 1.260E+00 0.000E+00 1.809E+00
   23 24  6  7.947E+02 1.963E-01 5.740E+00 0.013 2.742E+01 2.742E-01 1.260E+00 0.000E+00 1.535E+00
   25 26  7  7.947E+02 1.963E-01 1.138E+01 0.033 5.424E-01 1.085E+01 2.264E+00 0.000E+00 3.349E+00
   27 28  8  1.186E+03 1.963E-01 1.722E+01 0.049 1.224E+00 1.224E+00 0.000E+00 0.000E+00 1.224E+00
   29 30  9  1.186E+03 1.963E-01 1.723E+01 0.049 1.224E+00 1.224E+00 4.775E+00 0.000E+00 5.999E+00
   31 32 10  1.186E+03 3.664E-01 1.527E+01 0.037 4.024E-01 4.024E-01 2.400E+00 0.000E+00 2.802E+00
   33 34 11  1.186E+03 3.664E-01 1.527E+01 0.037 4.025E-01 8.050E-01 2.400E+00 0.000E+00 3.205E+00
   35 36 12  1.186E+03 3.664E-01 1.527E+01 0.037 4.026E-01 6.844E+00 7.202E+00 0.000E+00 1.405E+01
   37 38 13  3.914E+02 1.963E-01 1.130E+01 0.046 2.736E-01 8.399E-01 1.216E+00 0.000E+00 2.055E+00
   39 40 14  3.914E+02 1.963E-01 7.211E+00 0.021 2.373E-01 7.118E-01 9.646E-01 0.000E+00 1.676E+00
   41 42 15  3.974E+01 4.909E-02 4.839E+00 0.019 1.062E+01 4.248E-01 5.265E-01 1.253E+01 1.348E+00
   43 44 16  4.000E+00 4.909E-02 0.000E+00 0.000 0.000E+00 0.000E+00 0.000E+00 1.636E+04 1.636E+04
   45 46 17  4.000E+00 1.963E-01 0.000E+00 0.000 0.000E+00 0.000E+00 0.000E+00 1.587E+01 1.587E+00
   47 48 18  7.854E-03 0.000E+00 0.000E+00 0.000 0.000E+00 0.000E+00 0.000E+00 1.600E+04 1.600E+04
   49 50 19  7.854E-03 0.000E+00 0.000E+00 0.000 0.000E+00 0.000E+00 0.000E+00 4.592E+02 4.592E+02

--- Mass flow rate -------
m = 1186.1818 kg/s
--- Turbine/compressor efficiencies ---
Turb 93.2094 %
Comp1 92.6698 %
Comp2 91.2151 %
--- Turbine/compressor axial speeds ---
Turb 55.3833 m/s
Comp1 58.2848 m/s
Comp2 64.6526 m/s
--- Turbine/compressor exit speeds ---
Turb 36.8843 m/s
Comp1 58.2848 m/s
Comp2 64.6526 m/s
--- Recuperator efficiencies ---
HTR 94.5455 %
LTR 91.3314 %
--- Recuperators pressure drops ---
HTR 0.2480 %
HTR : HP  0.0283 %
LTR : LP  0.1081 %
LTR : HP  0.0180 %

---------- Cooler(s) required length ---------------
---Cool---
L_cooler = 18.2900 m
PD_cooler = 0.0761 %
PDL2_cooler = 0.0001 MPa
Tw_out = 39.2840°C
pw_in = 0.1014 MPa
Effectiveness = 89.9260 %

--------- Works ----------------
W_Turb = 161.5458 MW
W_Comp1 = 23.2562 MW
W_Comp2 = 28.4457 MW
W_Cool_pump = 1.3755 MW
Q_RHX_HS = 250.0000 MW
Q_RHX = 250.0002 MW
Q_HTR = 270.9815 MW
Q_LTR = 160.1629 MW
Q_Cool = 137.1814 MW
W_gen (gross) = 106.0906 MW

----------- Inside components -------------
M_Turb = 93.56 kg
M_Comp1 = 749.39 kg
M_Comp2 = 389.43 kg
M_RHX = 559.37 kg
M_HTR = 964.42 kg
M_LTR = 2095.99 kg
M_Cool = 58901.04 kg

------- Inside pipes ------------------
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<th>98.6 kg</th>
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<td>Pipe</td>
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<tr>
<td>Pipe</td>
<td>24</td>
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<td>Pipe</td>
<td>25</td>
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Brayton cycle efficiency

\[ E = \frac{\text{Brayton cycle efficiency}}{42.4362\%} \]
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<td>MPa</td>
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<tr>
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<td>Hot side flow rate</td>
<td>0.1</td>
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**ANL-ART-154**

**BC_des.txt**

**PDC: Plant Dynamics Code for Design and Transient Analysis of Supercritical Brayton Cycles**

**September 27, 2018**
### HTR Properties

<table>
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<tr>
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### Parameters

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<tr>
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### Unit Properties

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<tr>
<td>Plate length</td>
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### Analysis

- **PDC:** Plant Dynamics Code for Design and Transient Analysis of Supercritical Brayton Cycles
- **September 27, 2018**
- **27, 201**

---

**Note:** All parameters below are per unit.
| Cold side channel length | 0.439 | m | Heat transfer region |
| Cold side channel angle | 1.500 | m | From channels |
| Void fraction | 33.5 | % | |
| Metal mass | 2.863 | tonnes | Dry |
| Cost | 171.8 | K$ |
| CO₂ mass | 20.1 | kg | Operating conditions |
| Properties | |
| Hot side - inlet | |
| Density | 68.5 | kg/m³ |
| Spec. heat | 1161.4 | J/kg-K |
| Viscosity | 31.1 | mKPa*s |
| Thermal cond. | 48.9 | mW/m-K |
| Hot side - outlet | |
| Density | 105.2 | kg/m³ |
| Spec. heat | 1152.0 | J/kg-K |
| Viscosity | 23.9 | mKPa*s |
| Thermal cond. | 34.3 | mW/m-K |
| Cold side - inlet | |
| Density | 350.7 | kg/m³ |
| Spec. heat | 1539.9 | J/kg-K |
| Viscosity | 32.5 | mKPa*s |
| Thermal cond. | 47.5 | mW/m-K |
| Cold side - outlet | |
| Density | 212.0 | kg/m³ |
| Spec. heat | 1258.1 | J/kg-K |
| Viscosity | 33.1 | mKPa*s |
| Thermal cond. | 52.2 | mW/m-K |

LTR | Type | PCHE |
--- | --- | ---
Quantity | 56 |
Heat transfer capacity | 2.86 | MW |
Hot side temperature inlet | 194.5 | °C |
Hot side temperature outlet | 86.5 | °C |
Hot side pressure inlet | 8.566 | MPa |
Hot side pressure outlet | 8.556 | MPa |
Hot side flow rate | 21.2 | kg/s |
Hot side pressure drop | 9.3 | kPa |
Cold side temperature inlet | 76.3 | °C |
Cold side temperature outlet | 180.0 | °C |
Cold side pressure inlet | 24.997 | MPa |
Cold side pressure outlet | 24.992 | MPa |
Cold side flow rate | 14.2 | kg/s |
Cold side pressure drop | 4.5 | kPa |
Efficiency | 91.3 | % |
Heat transfer area | 288.4 | m² |
Unit width | 1.500 | m |
Unit height | 0.600 | m |
Unit length | 0.600 | m |
Heat transfer length | 0.380 | m |
Plate material | SS316 |
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<td>Max diameter</td>
<td>0.81 m</td>
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<tr>
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<td>Hub radius min</td>
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### Comp1

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Total-to-static Operating conditions
| Working fluid  | CO₂ |  |
| Turbine inlet pressure | 24.818 MPa | |
| Turbine inlet temperature | 521.768 °C | |
| Turbine outlet pressure | 8.619 MPa | |
| Mass flow rate | 1186.182 kg/s | |
| Shaft revolution speed | 60.000 rev/s | |
| Number of stages | 8 | |
| Minimum hub radius | 1.000 cm | |
| Degree of reaction | 0.500 | |
| Design incidence angle | 0.000 deg | |
| Design deviation angle | 0.000 deg | |
| Trailing edge thick. for rotor | 1.000 mm | |
| Trailing edge thick. for nozzle | 1.000 mm | |
| Rotor blades solidity | 1.500 | |
| Nozzle blades solidity | 1.500 | |
| Blade maximum thickness-to-chord ratio | 0.200 | |
| Tip clearance-to-radius ratio | 0.002 | |
| Number of tip seals for rotor | 2 | |
| Number of tip seals for nozzle | 2 | |
| Blade material density | 8300.000 kg/m³ | |
| Blade maximum stress | 300.000 MPa | |
| Vibrational stress factor | 0.750 | |
| Coefficient for Ixx | 1.165E-03 | |
| Coefficient for f_y | 1.038E-02 | |
|---------------------|------------|
| Coefficient for f_x | 7.434E-02 | |
| Coefficient for f_y | 2.738E-02 | |
| Coefficient for f_x (trailing edge) | 4.372E-01 | |
| Coefficient for f_y (trailing edge) | 4.656E-01 | |
| Principal axes angle | 60.330 | deg |
| Avarage blade angle | 67.000 | deg |

Loss components

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Axial flow speed = 55.383 m/s

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Turbine length (stages) = 1.164 m
Diffuser length = 1.637 m
Total turbine length = 2.801 m

Turbine isentropic static-to-static efficiency = 93.209 %
Turbine isentropic total-to-total efficiency = 93.637 %
Turbine isentropic total-to-static efficiency = 92.746 %
B.3. Transient Definition and Input

The transient for the example problem is load following from 100% to 50% in 600 seconds (at a 5%/min rate) followed by steady operation at 50% load. The total transient time is 1000 seconds. The transient is defined by setting the electrical grid demand decreasing from 100% at 0 seconds to 50% at 600 seconds. The transient starts at time =0 and is preceded by 50 seconds of steady-state stabilization time.

The HAHX hot-side fluid conditions (intermediate sodium at the RHX inlet) are set using the table mode. The sodium temperature is fixed at the design value of 528 °C, the pressure is fixed at the 100% steady-state level (1 atm). The sodium flow rate is set to change from 100% to 60% between 120 and 600 seconds.

The air temperature at the cooler inlet is set to the design value of 30 °C for the entire transient.

The turbomachinery shaft is in synchronous mode so its speed is fixed by the grid frequency at the 100% design value.

Turbine bypass control is used to regulate the net generator power to match the requested grid demand. The inventory control is set to operate between 90% and 50% load by specifying the amount of CO₂ that needs to be removed from the cycle, as a function of load. The cooler bypass and air flow rate controls are set to maintain the main compressor impeller-inlet temperature at the design value of 35 °C. The turbine throttling, compressor outlet, recuperator bypass, and compressor surge controls are inactive in this simulation.

The turbomachinery performance is calculated based on the maps, without any verification from the performance subroutines.

On the following pages, the PDC input files for the dynamic calculations are presented.
*************** Input data for dynamic calculations *******************
Use (=1) restart file? and restart file names (PDC \ SAS), if used
0 Restart_r1_t120.bin \ Restart_r1_t5_SAS.bin
Simulation time, s
1000
Time to obtain SS (not included into simulation time), s
50
Time step (initial), s
0.001
Report every N calculations
10
Minimum time change between reported points
1
Times to save restart file (up to 20) (end time is always saved)
0 5 10 25 50 60 85 100 110 120 200 400 600 1000 1600
Print out (=1) the detailed results for components?
1
Convergence option (0 = halving time step, 1 = based on derivatives)
1
Required convergence
1.0-5
Order (max=9) [recommended pairs for Conv_opt are {0,5} and {1,2}]
2
Compressibility value to switch to incompressible flow
-1
Compressibility value to switch to compressible flow
0
Number of points in grid load table (1 = no action)
2
Grid load table (Time,s; % nominal) (For LOL put <=100)
0 600
100 50
Equivalent pipe break diameter, cm
0
Location of the break (dynamic-code T-node)
1
Run mode: 0 = calculation, 1 = test (allow files access)
1
Heat capacity reduction factor in Get_SS (>=1)
100
******** Input parameters for the Heat Addition (HA) control ***************

### Automatic control (used only if HA Mode=2) 
- **Number of points in the heater control table** (1 = no control)
  - 2
- **Heater control table** (Time, s; $T_{out_{CO_2}}$, C)
  - (Not used for user input [HA DY Mode=0] - $Q_{lim}$ table is used for heater power)
  - 0 100
  - 522 502

**Coefficients for heater control (P D I)**
- 10 50 0

**Maximum heater power, W**
- 250000000

### Number of points in the heater power limit table (1 = no control)
- 1
- **Heater power limit table** (Time, s; $Q_{lim}$, % max power)
  - 0 100

**Maximum rate of power change, %_full_power/s**
- 50

---

**Number of table points**
- 2
- **Time**  T_in[K]/T_in_SS[K]
  - 0.00000E+00  528
  - 1.00000E+03  528

---

**Number of table points**
- 2
- **Time**  Pressure/Pressure_SS
  - 0 1
  - 1000 1

---

**Number of table points**
- 3
- **Time**  Relative flow rate
  - 0.00000E+00  1.00000E+00
  - 120  1.00000E+00
  - 600  0.6

---

**Number of table points**
- 2
- **Time**  T_in[C]
  - 0.0  30.00
  - 1000.0  30.00
**Input parameters for the Brayton cycle control**

### Rotational speed control

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Rotational speed control table (Time; Nr, % nominal)

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### Minimum temperature control

Controlled temperature (1=Imp.In, 2=Comp.In, 3=Cool.Out)

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### Turbine Bypass

Valve name (from SS CycleDat.txt file)

TBPv

Flow splitter name (from SS CycleDat.txt file)

TBPsp

Controlled shaft name (from SS CycleDat.txt file)

Shaft

Coefficients for turbine bypass control (P I D - synchronous / P I D - asynchronous)

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Opening and closing rate limits, %/s

10 10

Average signal over N points

1

### Manual control

Number of points in the manual control table (1 - no action)

1

Turbine bypass valve control table (Time; f_open, %)

<table>
<thead>
<tr>
<th>Time</th>
<th>f_open, %</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>

### Inventory

Inlet valve name (from SS CycleDat.txt file)

INVIv

Outlet valve name (from SS CycleDat.txt file)

INVOv

Number of points in the inventory control table

7

Inventory control table (Load, %; dM_tank, kg)

<table>
<thead>
<tr>
<th>Load %</th>
<th>dM_tank, kg</th>
</tr>
</thead>
<tbody>
<tr>
<td>100</td>
<td>90</td>
</tr>
<tr>
<td>80</td>
<td>70</td>
</tr>
<tr>
<td>60</td>
<td>50</td>
</tr>
<tr>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>

Coefficients for inventory control (P I D - synchronous / P I D - asynchronous)

<table>
<thead>
<tr>
<th>Power exponents for coefficients (C in k=k0*(Nr/Nr_nom)**C)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Power exponents for coefficients (C in k=k0*(Nr/Nr_nom)**C)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
</tr>
</tbody>
</table>

Opening and closing rate limits, %/s

Inlet valve opening and closing rate limits, %/s

1 1

Outlet valve opening and closing rate limits, %/s

1 1

### Manual control - Inlet valve

Number of points in the manual table - inlet (1 - no action)

1

Inventory inlet valve control table (Time, s; f_open, %)

<table>
<thead>
<tr>
<th>Time, s</th>
<th>f_open, %</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>

### Manual control - Outlet valve

Number of points in the manual control table - outlet (1 - no action)

1

Inventory outlet valve control table (Time; f_open, %)

<table>
<thead>
<tr>
<th>Time</th>
<th>f_open, %</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>

### Turbine Inlet

BCcontrol_dat.txt
Valve name (from SS Cycle_dat.txt file)  
TINv  
Controlled parameter in table (0=Open fr., 1=Valve dP, 2=Turb BP flow fraction)  
1  
Number of points in the valve control table  
1  
Valve control table (Load,%; dp_valve,MPa or TBP flow fraction, %)  
100  
0  
Coefficients for valve control (P I D - synchronous / P I D - asynchronous)  
5 0 0.1  
2.5 0 0.1  
Power exponents for coefficients (C in k=k0*(Nr/Nr_nom)**C)  
0 0 0  
Valve opening and closing rate limits, %/s  
5 5  
Average signal over N points  
1  
---------- Manual control ----------  
Number of points in the manual control table (1 - no action)  
1  
Turbine inlet valve control table (Time; f_open,%)  
0 100  

#################################### Compressor2 outlet ####################################
Valve name (from SS Cycle_dat.txt file)  
C2Ov  
Valve opening and closing rate limits, %/s  
0.5 0.5  
---------- Manual control ----------  
Number of points in the manual control table (1 - no action)  
1  
Compressor outlet valve control table (Time; f_open,%)  
0 100  

#################################### Compressors Surge ####################################
Minimum stall margin to maintain (for each compressor)  
0.1 0.1  
Control coefficient (for each compressor)  
0 0  
Average signal over N points  
10  

#################################### Cooler Bypass ####################################
Valve name (from SS Cycle_dat.txt file)  
CBPv  
Flow splitter name (from SS Cycle_dat.txt file; for fraction printout only)  
CBPsp  
Coefficients for valve control (P I D - synchronous / P I D - asynchronous)  
200 10 1  
6.5 0.0145 3  
Power exponents for coefficients (C in k=k0*(Nr/Nr_nom)**C)  
1.161 1.661 -1  
Valve opening and closing rate limits, %/s  
10 10  
Average signal over N points  
1  
---------- Manual control ----------  
Number of points in the manual control table (1 - no action)  
1  
Cooler bypass valve control table (Time; f_open,%)  
0 0  

---------- Water flow rate ----------  
Coefficients for water flow rate control (P I D - synchronous / P I D - asynchronous)  
0.1 0 10  
0.145 0 7.243  
Power exponents for coefficients (C in k=k0*(Nr/Nr_nom)**C)  
1.661 0 1.661  
Water flow rate change limit, %nom/s  
10  
Water pump head limits, min and max, %nom
- **Recuperator Bypass**
- Valve name: RBPv
- Throttling valve: RTHv
- Flow splitter name: RBSp
- Flow mixer name: RBMx
- Number of points in the HTR-outlet temperature control table: 1
- Temperature control table: 
  - Load: 100%
  - Temperature: 365°C
- Coefficients for RBP control:
  - P: 10
  - I: 0.1
  - D: 0.25
- Power exponents for coefficients: 0
- Valve opening and closing rate limits: 0%/s
- Manual control table:
  - Number of points: 1
  - HX Bypass valve control table:
    - Time: 0
    - f_open: 0
******** Input data for turbomachinery maps generation ***************
Generate (1) or use existing (0) map?
0
Verify (1=Always, 2=Active Nr control) maps with performance subroutines (slow)
0
Min and max values for relative shaft speed
1 1
Number of points for relative shaft speed (0 = use pre-def)
1
Min and max values for relative inlet temperature
0.985 1.05
Number of points for relative inlet temperature
61
Min and max values for relative inlet pressure
0.8 1.15
Number of points for relative inlet pressure (density)
121
Lower limit for surge factor
0.95
Number of points for relative outlet pressure
120
Min (start) value for relative flow rate
0.0001
Initial and minimum steps for relative flow rate
0.0001 1D=6

******** Input data for turbomachinery maps generation ***************
Generate (1) or use existing (0) map?
0
Verify (1=Always, 2=Active Nr control) maps with performance subroutines (slow)
0
Min and max values for relative shaft speed
1 1
Number of points for relative shaft speed (0 = use pre-def)
1
Min and max values for relative inlet temperature
0.985 1.05
Number of points for relative inlet temperature
61
Min and max values for relative inlet pressure
0.8 1.15
Number of points for relative inlet pressure (density)
121
Lower limit for surge factor
0.95
Number of points for relative outlet pressure
120
Min (start) value for relative flow rate
0.0001
Initial and minimum steps for relative flow rate
0.0001 1D=6
******** Input data for turbomachinery maps generation **************

Generate (1) or use existing (0) map?
0
Verify (1=Always, 2=Active Nr control) maps with performance subroutines (slow)
0
Min and max values for relative shaft speed
 1 1
Number of points for relative shaft speed (0 - use pre-def)
 1
Min and max values for relative inlet temperature
 0.7 1.1
Number of points for relative inlet temperature
 91
Min and max values for relative inlet pressure
 0.5 1.25
Number of points for relative inlet pressure (density)
 121
Minimum pressure ratio
 0.5
Number of points for relative outlet pressure
 120
Min (start) value for relative flow rate
 0.001
Initial and minimum steps for relative flow rate
 0.001 1D=6

Map_Turb.dat.txt
B.4. Transient Results

The transient results for the example problem are shown in plots on the following pages.

The cycle control system responds to the requested grid demand by opening the turbine bypass valve. This control action proves to be accurate such that in the plots the grid demand \( W_{\text{grid}} \) and net generator output \( W_{\text{2_grid}} \) lines lie on top of each other. The inventory control responds by opening the inventory control tank’s inlet valve, its action starts at 120 seconds when the grid demand reaches the 90% level. The cycle pressures reduce from this action, while the tank pressure increases. The inventory control action reduces the CO\(_2\) flow rate everywhere in the cycle, while the turbine bypass control reduces the flow rate through the turbine but increases the flow through the compressors. The combined action of the cooler bypass and air flow rate controls maintain the compressor-inlet temperature at the 35 °C design value.

The heat transfer rates in the RHX are calculated from temperature and flow rate changes on the two sides. The cycle efficiency decreases linearly with turbine bypass control (first 120 seconds). It also decreases with inventory control, but at a lower rate.

The temperatures in the cycle and heat exchangers are defined by the control actions and the thermal inertia of the heat exchanger wall.

The time step is maintained between \( 10^{-3} \) and \( 10^{-2} \) seconds.

The actual PDC output files from dynamic calculations are too large to be included in this report. As an example, a partial listing of one of these files, “T_RHX_res.txt”, for the transient results of the RHX component, is provided in this document after the plots. The entire files for the example problem are supplied with the code, in the “\Data\DY\Output\” folder.
Transient Results for Example Problem

HEAT BALANCE IN RHX

- \( Q_{\text{RHX,Rx}} \)
- \( Q_{\text{RHX,CO2}} \)

REACTOR COOLANT FLOW RATE IN RHX

- \( m_{\text{RPF}} \)

TURBINE AND COMPRESSORS WORK AND GENERATOR OUTPUT

- \( W_{\text{Turb}} \)
- \( W_{\text{Comp1}} \)
- \( W_{\text{Comp2}} \)
- \( W_{\text{2_grid}} \)
- \( W_{\text{grid}} \)

VALVES CONTROL ACTION

- \( f_{\text{op_TBPv}} \)
- \( f_{\text{op_INViv}} \)
- \( f_{\text{op_INVOv}} \)
- \( f_{\text{op_TINv}} \)
- \( f_{\text{op_C2Ov}} \)
Transient Results for Example Problem

COMPRESSORS STALL MARGIN

TURBINE AND COMPRESSORS CHOKE MARGIN

FLOW SPLIT

COOLER BYPASS FLOW FRACTION
Transient Results for Example Problem

- **Shaft Speed**
  - 0 to 120% nominal speed over time from 0 to 1000 seconds.

- **Cooling Fluid Flow Rate**
  - Flow rate in kg/s over time from 0 to 1000 seconds.

- **Compressor Inlet Temperature**
  - Temperature in °C from 30.5°C to 35°C over time.

- **Compressor Inlet Pressure**
  - Pressure in MPa from 7.3 MPa to 8.3 MPa over time.
Transient Results for Example Problem

INSTANTANEOUS EFFICIENCIES

COOLER BYPASS VALVE ACTION

VALVE OPEN AREA FRACTION

MAIN TIME STEP SIZE

TURBINE BYPASS FLOW FRACTION

BYPASS FLOW FRACTION
Transient Results for Example Problem

FLOW RATES: TURBOMACHINERY

FLOW RATES: CONTROL

TEMPERATURES: TURBOMACHINERY

PRESSURES: TURBOMACHINERY
Transient Results for Example Problem

TEMPERATURES: RHX

TEMPERATURES: HTR

TEMPERATURES: LTR

TEMPERATURES: COOLER
Transient Results for Example Problem

FLOW RATES: SURGE CONTROL

FLOW RATES: INVENTORY CONTROL

PRESSURES: INVENTORY CONTROL

TEMPERATURES: PIPE WALLS

PIPE HEAT LOSS
### Example of a PDC Dynamic output file: partial content of “T_RHX_res.txt” file

<table>
<thead>
<tr>
<th>Time (s)</th>
<th>mRPF</th>
<th>RPF</th>
</tr>
</thead>
<tbody>
<tr>
<td>4.10000E+01</td>
<td>&gt; 1.26703E+03</td>
<td>&gt; 5.28000E+02</td>
</tr>
<tr>
<td>5.40000E+01</td>
<td>&gt; 1.26703E+03</td>
<td>&gt; 5.28000E+02</td>
</tr>
<tr>
<td>7.40000E+01</td>
<td>&gt; 1.26703E+03</td>
<td>&gt; 5.28000E+02</td>
</tr>
<tr>
<td>7.60000E+01</td>
<td>&gt; 1.26703E+03</td>
<td>&gt; 5.28000E+02</td>
</tr>
<tr>
<td>7.90000E+01</td>
<td>&gt; 1.26703E+03</td>
<td>&gt; 5.28000E+02</td>
</tr>
<tr>
<td>8.40000E+01</td>
<td>&gt; 1.26703E+03</td>
<td>&gt; 5.28000E+02</td>
</tr>
<tr>
<td>8.70000E+01</td>
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<td>&gt; 5.28000E+02</td>
</tr>
<tr>
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<td>&gt; 1.26703E+03</td>
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<td>&gt; 1.26703E+03</td>
<td>&gt; 5.28000E+02</td>
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<tr>
<td>9.90000E+01</td>
<td>&gt; 1.26703E+03</td>
<td>&gt; 5.28000E+02</td>
</tr>
<tr>
<td>1.04000E+02</td>
<td>&gt; 1.26703E+03</td>
<td>&gt; 5.28000E+02</td>
</tr>
</tbody>
</table>

### Additional Data

- **PDC:** Plant Dynamics Code for Design and Transient Analysis of Supercritical Brayton Cycles
- **September 27, 2018**

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**ANL-ART-154**

278
APPENDIX C: PDC MODULES, FUNCTIONS, SUBROUTINES, AND CALL DIAGRAMS
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