Progress Report on Dynamic Simulation of the Sandia Small-Scale Supercritical Carbon Dioxide Brayton Cycle Test Loop with the ANL Plant Dynamics Code

Nuclear Engineering Division
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Abstract

Validation of the Plant Dynamics Code (PDC) with available experiment data from the Sandia National Laboratories (SNL) small-scale S-CO₂ Brayton cycle demonstration has been continued. Previously, one of the earlier loop configurations from December 2010 was modeled with the steady-state portion of the PDC. In order to be able to simulate transient behavior of the loop with the PDC, several modifications specific to the SNL Loop needed to be implemented in the code. The modifications were mostly limited to simulating the particular controls implemented in the SNL S-CO₂ loop such as electrical heater control and the control of the cooling water flow rate by means of a bypass valve. Also, the steady-state and transient parts of the code were modified to allow calculation of heat losses in the pipes based on the input parameters specified by the user. The changes are specific to the SNL Loop and are not expected to be needed or significant for full-size commercial S-CO₂ cycles and, therefore, are not expected to affect the results of previous calculations with the code when it was applied to reactor systems with S-CO₂ Brayton cycle power converters. Following all of the modifications to the PDC, the transient simulation of the SNL S-CO₂ Loop experiments was carried out. When the code was applied to the December 2010 experiment, the calculations were automatically stopped by the code after about 270 s due to too small a time step. At this point, conditions very close to (and, at some instances, below) the CO₂ critical point were calculated by the code requiring very small time steps to resolve the properties variations. This finding was consistent with the December 2010 experimental data where the loop was operated below the critical temperature (and sometimes below the critical pressure) for the majority of the test. To avoid these problems, it was decided to seek experiment data with operation above the critical point. Such experiment data was found from July 2011 tests. However, some additional model development was needed to simulate this test, since some hardware modifications were implemented between December 2010 and July 2011. In particular, the high temperature recuperator (HTR) was installed in addition to the existing low temperature recuperator (LTR). Also, the main compressor wheel was replaced with the recompression compressor wheel. Consequently, models for these components had to be developed in the PDC. During the simulation of the July 2011 data with the steady-state portion of the PDC, it was realized that a satisfactory heat balance, needed for a starting point for the dynamic calculations, was not achieved in the transient run. Consequently, an introduction of a significant heat loss was needed and was implemented in the pipe connecting the HTR and the heaters, in order to simulate the conditions in the loop with the steady-state equations. In addition to that change, it was realized that in this test configuration, the LTR does very little heat transfer, since the larger HTR achieves almost 100 % effectiveness. Since the LTR was shown not to provide any significant temperature change of the high pressure and low pressure fluid, it was excluded from the current PDC modeling of the July 2011 configuration of the loop. The transient results obtained with the PDC were close to the actual experimental data. Almost all of the temperatures showed good agreement with the experimental readings. The noticeable exception was the heater inlet temperature which is consistently under predicted by the code. The analysis has shown that this is a result of incorporating the heat loss into the HTR-heater pipe. By comparing the PDC results with the experimental
data later in the transient, it was discovered that this heat loss wasn’t as large at later times as was needed for the steady-state simulation. The other findings from the temperature comparison suggest that the thermal inertia of the HTR may be underestimated by the code. This may be an effect of not knowing the exact internal configuration of the HTR. It may also be a consequence of not including the LTR mass into the PDC model. Comparing the pressure and density predictions, it was observed that the pressures on the low side of the cycle were predicted very accurately by the code. On the high side, there is a difference between the code predictions and actual data resulting from underestimating the pressure drops in the systems. This might also be an effect of not including the LTR into the model. It can also be a consequence of making some assumptions for the piping configuration and dimensions that are not known for the July 2011 tests. The compressor-inlet density (the only density measured in the tests) is predicted very accurately during the majority of the transient. Some differences in the density predictions later in the transient are most likely caused by a less than perfect match of the cooler-outlet temperature with the automatic water flow control. This result was expected since earlier work has demonstrated that the water flow control may not be sufficiently fast for this cycle and is better augmented by the cooler bypass control. Because some discrepancies were identified between the code predictions and the recorded experiment data, both in the steady state and in transients, the work on the SNL Loop simulation with the PDC should be continued in the future. Based on the results obtained in this report, it is recommended that future work be concentrated on areas including better simulation of the heat losses in the system; finding experiment data more suitable for the steady-state simulation for the starting point of transient simulation; refining the HTR model especially if information about the HTR internal configuration could be made available to ANL; carrying out more comparisons of turbine performance predictions with the experimental data, especially at higher rotational speeds; investigating ways to include into the PDC model the effect of the LTR on the pressure drops and the thermal inertia; considering modeling of heat transfer in the pipes; and continuing to apply the PDC to other experiment runs, including different loop configurations.
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1 Introduction

The ANL Plant Dynamics Code (PDC) [1] for the analysis of supercritical carbon dioxide (S-CO$_2$) Brayton cycle power converters has been under development at Argonne National Laboratory for several years. The PDC has been used previously for control and transient analysis of the S-CO$_2$ cycle coupled to Lead-Cooled Fast Reactors (LFRs), such as SSTAR and STAR-LM, as well as Sodium-Cooled Reactors (SFRs) such as various Advanced Burner Reactor (ABR) preconceptual designs.

The present report serves as a project update report on ongoing PDC code development and continuing application of the code to the Sandia National Laboratories (SNL) small-scale S-CO$_2$ Loop for the purposes of the code validation. The report covers activities and analyses carried out during Fiscal Year 2012 (FY2012).

The current year’s work is the continuation of the work started in FY2011 [2]. Last year, a steady-state simulation of one of the SNL S-CO$_2$ Loop’s configurations, involving a single turbo-alternator-compressor (TAC) unit and a single low-temperature recuperator, was completed. The results of that simulation showed that the PDC can predict the steady-state conditions pretty accurately such that the work could move on to analyzing transient behavior of the loop.

At the same time, several SNL Loop-specific issues were identified in FY11 report which precluded transient simulation of the SNL S-CO$_2$ loop with the PDC at that time. Those issues included:

- Insufficient information was available to simulate time-dependent control of the SNL Loop.

- The steady-state analysis revealed that a non-negligible heat loss occurs in the turbine volute which was not measured in the experiments. The magnitude for this heat loss was deducted in the steady-state analysis from the heat and mass flow balances around the loop. It was not clear how this heat loss mechanism could be determined under transient conditions.

- The heat supply to the S-CO$_2$ loop occurs by means of the electrical heaters which are not part of the components modeled in the PDC. For the steady-state analysis, the performance of the heaters was simulated with sodium-to-CO$_2$ shell-and-tube heat exchangers. Further code development was needed either to include the electrical heaters into the PDC or to simulate the electrical heaters with heat exchangers in transient conditions as well.

Resolving the issues listed above required further modifications of the Plant Dynamics Code. So, the FY12 work on the dynamic simulation of the SNL S-CO$_2$ Loop
data was started with modifications to the PDC in order to resolve these SNL Loop-specific issues and to be able to carry out transient simulation of the loop.

The above issues are specific to simulating the SNL S-CO\textsubscript{2} Loop and the resulting PDC modifications, which are described in the next section of this report, do not necessarily improve the code itself. Nor will they be necessarily applicable to other systems, including the reactor systems, for the analysis of which the PDC was originally developed. As discussed in the FY11 report, a separate version of the code was created for the SNL S-CO\textsubscript{2} Loop simulation purposes. The code modifications described below were applied only to that version of the code.
2 ANL Plant Dynamics Code Modifications for SNL S-CO₂ Loop Transient Simulation

To facilitate transient simulation of the SNL S-CO₂ Loop with the PDC, several modifications were introduced to the code. These modifications are described below.

2.1 Simulation of SNL S-CO₂ Loop Control

During a visit to SNL to examine the SNL S-CO₂ Loop and during related discussions with SNL personnel, it was learned that the following controls are implemented in the loop:

- Shaft rotational speed control,
- Heater control, and
- Water flow control.

These controls are discussed below in this report. Other control mechanisms which are simulated in the PDC, such as turbine bypass, turbine and compressor throttling, inventory, cooler bypass, and compressor surge, are either not implemented at all in the SNL S-CO₂ loop or cannot be used in experiment runs. Consequently, these control mechanisms were disabled in the PDC simulation by means of setting the control PID coefficients to zero. Since that was done through the input files, no further modifications to the PDC were needed to disable the controls not implemented in the SNL loop.

2.1.1 Shaft Rotational Speed Control

Shaft rotational speed control (also known as RPM or revolutions-per-minute control) is implemented by means of the power supply to the alternator and load banks. The analysis of the experimental data showed that this control works very well: the turbine-alternator-compressor (TAC) speed follows very closely the target RPM value during a transient. The system response to the change in target RPM is relatively rapid with only a few seconds delay before the actual TAC speed reaches the new level.

Consequently, due to very good performance of the RPM control, no attempts were made to simulate the actual RPM control in the PDC calculations presented in this report. Instead, the target RPM value (rather than actual RPM) was used as an external input for the PDC transient calculations with an addition of a small delay at each RPM change to better reflect the system response to this change. As will be shown below, the method of using the target RPM with some delay for the actual RPM representation in transients produced satisfactory results for the TAC rotational speed.
2.1.2 Heater Control

In the SNL S-CO$_2$ Loop experimental setup, the operator has a choice of either automatic or manual control of the heaters. In the manual control mode, the operator provides the required electrical current input to each heater unit controller. The input varies from 4 mA for zero power to 20 mA for maximum power. Thus, the power supplied to the heater is calculated as:

\[ Q_{heater} = \frac{\text{Heater Control [mA]} - 4 \text{ mA}}{20 \text{ mA} - 4 \text{ mA}} Q_{\text{max}}, \]

where the maximum heater power, $Q_{\text{max}}$, is either the maximum design heater power per unit (130 kW) or a maximum dictated by the total available heat input (for the BNI location, the total heat input was limited by 390 kW for all units).

The heater control, in mA, is recorded in the experimental results and is available for each heater along with other experimental data. Although the control can be applied to each heater separately, usually the heater input is the same for all heater units.

In the automatic heater control mode, an operator can set the target CO$_2$ outlet temperature and the automatic heater control will adjust the power to match this temperature. In this case, both the target temperature and the actual values for the heater control input in mA are recorded in the experimental data.

Ideally, a transient model for incorporation into the PDC should be developed for an electric heater unit modeling an individual U-shaped heater with its presumed configuration of heating element, insulator (assuming that this actually is the configuration), and surrounding wall material as well as the shell from which heat losses to the atmosphere can occur. The electric heater units were fabricated by BNI and, unfortunately, detailed information about their design has not been made available to ANL. Thus, it is not possible at this time to develop a heater unit transient model with the desired fidelity for PDC analysis. Instead, simple models for approximating the heater behavior have been formulated.

Similar to the experimental setup, several options were implemented in the PDC for the heater control. It is noted, however, that the heaters are still simulated with shell-and-tube heat exchangers (S&T HX) in the PDC. The geometric parameters for such a heat exchanger are selected to match the heater design to the maximum possible extent. For example, the tube outer diameter, number of tubes, and CO$_2$ flow area are selected to match the corresponding design parameters for the heaters. The total tube length is selected to represent the total length of the heating elements. For other parameters, such as tube thickness, some assumptions had to be made. In the case of the tube thickness, for example, 1 mm was assumed for the PDC S&T HX model.
For the steady-state calculations, the total HX power is a PDC input and is calculated based on the CO$_2$ inlet and outlet conditions. The sodium inlet and outlet temperatures are selected to provide the correct CO$_2$ outlet temperature and also achieve a more or less uniform heat transfer rate along the HX tube length. The latter condition roughly represents multiple heater units with the usual uniform heat input per unit.

In the transient calculations, several options were developed for a S&T HX in the PDC to simulate the SNL S-CO$_2$ Loop heaters. In regular reactor heat exchanger (RHX) calculations in the PDC, the mass flow rate and the inlet temperature of the reactor-side fluid are either obtained from another code, such as SAS4A/SASSYS-1, or are provided as an input in a value-versus-time table. Unlike the steady-state calculations, heat balance requirements could not be used in dynamic calculations to obtain the inlet conditions on the reactor side fluid. Therefore, some modifications were needed to simulate heaters with a HX.

In the first option developed in the PDC for the SNL loop, the external heat input is provided in a time-versus-value table. In the transient, an assumption of instantaneous heat input to the reactor side fluid is used for this option. Under this assumption, the reactor side fluid flow rate is kept constant during entire transient. The inlet temperature on the reactor side is calculated at each time step using the required heat input, the outlet temperature and the flow rate on the reactor side:

\[ h(T_{in}) = h(T_{out}) + \frac{Q(t)}{m}, \]

where \( h(T) \) = enthalpy at temperature \( T \).

Since in this option the inlet temperature is a calculated value, a table input for this temperature is not needed. Therefore, that table is used to trigger this option by using “-1” input for the inlet temperature in the first table entry. Also, the flow rate table is not needed since the flow rate is kept constant in this option. Instead, the flow rate table is used to provide the required heat input as a function of time.

A disadvantage of this option is that with changing conditions in transient, the heat transfer to the CO$_2$ side may no longer be uniform along the HX tube length. This would be in contradiction with the experimental setup where the condition of uniform heat input is maintained during the entire transient (provided that the heat input is the same for each heater unit, which is the case for all data provided to ANL so far).

To maintain a uniform heat input along the length of a heater, another option was introduced into PDC transient calculations. In this option, no calculations on the reactor fluid side are done in the transients. Instead, the transient equations were modified to provide a direct heat input into the tube wall. Correspondingly, the tube wall’s rate of temperature change in each node is calculated based on the heat balance between the direct heat input and the heat transfer to CO$_2$ side:
\[ M_{w,i} C_p \frac{\partial T_{w,i}}{\partial t} = Q_i - \frac{T_{w,i} - T_{CO_2,i}}{r_{es,i}} \Delta x_i N_{tube}, \]

where \( M_{w,i} \) = tube wall mass in node \( i \),
\( C_p \) = wall heat capacity,
\( T_{w,i} \) = tube wall temperature in node \( i \),
\( Q_i \) = heat input in node \( i \),
\( T_{CO_2,i} \) = average CO\(_2\) temperature in node \( i \),
\( r_{es,i} \) = thermal resistance, per unit length, between the tube wall and CO\(_2\) in node \( i \),
\( \Delta x_i \) = length of node \( i \),
\( N_{tube} \) = number of HX tubes.

In the above equation, only the heat input, \( Q_i \), was newly introduced to replace the heat transfer term between the tube wall and the reactor side fluid. All other terms remain from the original PDC equations.

The heat input in each node, \( Q_i \), is calculated at the beginning of each time step using the current value for the heater input normalized to the steady-state value for this node:

\[ Q_i(t) = \frac{Q_{Heater}(t)}{Q_{Heater}(0)} \times Q_i(0) \]

Since the steady-state conditions (\( t=0 \)) are selected to provide a uniform heat transfer distribution, the above equation insures that the same uniform distribution is maintained throughout the entire transient.

The last option for the heater simulation in the transient calculations was developed to simulate automatic heater control. In this option, the desired CO\(_2\) outlet temperature versus time is specified in the input file. Along with this temperature, the following additional inputs were introduced to facilitate the automatic heater control:

- Maximum heater power, much like in the experimental setup,
- Maximum rate of heater power change to avoid too sharp changes in dynamic parameters. Currently, it is assumed that the power change is limited to 50% nominal (steady-state) power change per second, and
- Proportional, integral, and differential (PID) coefficients for the controller. These coefficients were selected to provide a response of the actual CO\(_2\) outlet temperature similar to what was recorded experimentally to a sharp change in target temperature (the values used in the experimental setup for control coefficients were not provided to ANL).

The automatic heater control was implemented in the PDC very similar to other existing controls. The control monitors the difference between the target and the actual
CO₂ outlet temperature and also calculates a derivative and an integral of this difference. Then, the PID coefficients are applied to calculate the rate of heater power change, subject to maximum power and maximum rate of power change limitations. The new heater power at the end of time step is calculated and supplied to the above equation as \( Q_{\text{Heater}}(t) \). The rest of the calculations for the tube wall and other temperatures are the same as described for the previous option.

2.1.3 Water Flow Control

Similar to the heater control described in the previous section, the operator of the SNL S-CO₂ Loop has an option of either automatic or manual water flow control. In both options, the water flow rate through the cooler is regulated by a bypass valve. For the automatic control, the controlled parameter is the CO₂ cooler outlet temperature. That option, though, was never used in the data provided to ANL so far.

For the manual control, the position of the cooler bypass valve on the water side is regulated with the similar 4 mA - 20 mA controller band as for the heater power. It is important to note, though, that the flow rate though the cooler is not measured in the SNL loop. Moreover, that flow rate could not be easily estimated based on the bypass valve position since, in addition to the lack of valve resistance-versus-valve position data, the flow distribution between the cooler and the bypass line is also a function of the pressure drop in the cooler which, in turn, is defined by the water temperature change in the cooler.

In earlier experimental data, an estimation of the water flow rate was included. That value is calculated (rather than measured) based on the heat transfer rate on the CO₂ side and an assumption that the same heat transfer rate applies to the water side. That latter assumption, though, is applicable to steady-state conditions only and could not be reliably used in transients due to the thermal inertial of the cooler wall mass. Nevertheless, an option of direct water flow rate input through a value-versus-time table (much like for the reactor side fluid) was introduced to the PDC. The water flow rate estimation from the heat balance was used in the earlier calculations described in the next chapter of this report, at least as a first approximation of the actual water flow rate.

Later, an option of automatic water flow rate control was implemented for the PDC simulation. That water flow rate control already existed in the PDC. For the full-size cycle calculations, though, the water flow rate control was used to assist the cooler bypass in controlling the temperature at the main compressor first stage inlet, which is usually the minimum temperature in the cycle. Since that temperature was not measured in the SNL Loop, two other options for controlled minimum temperature were introduced, including the compressor inlet and the cooler outlet temperature. The selection of which temperature to control is now done through a special flag in the input.
file. In addition to this option, another input was created to specify the target value for the controlled temperature versus time.

For the most recent calculations presented in Chapter 4 at the end of this report, a cooler outlet temperature was selected as a controlled parameter. The target value for the automatic water flow rate control in the PDC was selected to be the measured cooler outlet temperature. An example of the input for this control is presented in Chapter 4 prior to the transient results (in Section 4.3.1).

In addition to the modifications described above, another input was introduced to the PDC to specify the time history of the water temperature at cooler inlet. This value was assumed to be constant in the previous calculations with the PDC but was actually changing in the SNL loop.

### 2.2 Simulation of Heat Loss in Transients

As described in the FY11 report [2], an account for the heat loss in the turbine volute was necessary to achieve heat and mass flow balances in the cycle during the steady-state calculations. In those calculations, a certain change to the CO₂ enthalpy in the pipe upstream of the turbine was introduced to the code. That value was changed manually to achieve the balance at steady state. This approach, although applicable to steady state, could not be used for the dynamic calculations for two reasons. First, the heat balance is not necessarily conserved in transient conditions. So, the amount of the heat loss could not be obtained from the heat balance assumption in transients. Second, manual adjustment of the heat loss magnitude is not practical for each time step in transient calculations.

Since the magnitude of the heat loss was not directly measured in the experiments, some approximation of this heat loss was needed in the transients. For this approximation, the following approach was implemented in the PDC. First, in steady-state calculations, the direct input of the enthalpy change in a pipe where the heat loss occurred was replaced with the enthalpy change due to heat loss, calculated as following:

\[ \dot{m}_{CO_2} \Delta h = Q_{HL} = (UA) [\bar{T}_{CO_2} - T_{HS}] , \]

where
- \( \dot{m}_{CO_2} \) = CO₂ flow rate in the pipe,
- \( \Delta h \) = enthalpy change in the pipe due to heat loss,
- \( Q_{HL} \) = heat loss,
- \( (UA) \) = heat transfer coefficient between the CO₂ and the ambient multiplied by the heat transfer area,
- \( \bar{T}_{CO_2} \) = average CO₂ temperature in the pipe,
- \( T_{HS} \) = temperature of the heat sink.
In the above equation, the heat transfer coefficient multiplied by the area, \((UA)\), and the heat sink temperature, \(T_{HS}\), are the inputs. The input file for the cycle in the PDC was modified to allow input of these two parameters for any pipe. However, only the input for the pipe upstream of the turbine was used to simulate the heat loss in the turbine volute.

For the heat sink temperature, 20 °C was assumed. This value is a good approximation of both the alternator water cooling temperature, which is stated to be 65 °F (18 °C) at the alternator inlet [3], and the ambient air temperature. The value for the \((UA)\) parameter was calculated to preserve the heat loss value calculated under the previous approach at the steady-state conditions.

In the dynamic calculations, the same equation is used to determine the heat loss in a pipe (or to simulate the heat loss in the volute). It is assumed that the values of \((UA)\) and \(T_{HS}\) are held constant during the entire transient. The amount of the heat loss is calculated at the beginning of each time step using the above equation with current CO\(_2\) temperatures. It is then assumed that the amount of the heat loss is constant during a time step and the CO\(_2\) enthalpy derivative equation was modified to include this heat transfer mechanism.
3 Dynamic Simulation of the December 2010 Experimental Data

3.1 Initial Conditions

In FY11, work on simulating the steady-state conditions of one of the experimental runs from December 2010 was completed. Figure 3-1, reproduced from the FY11 report [2], shows that good agreement on the main parameters, including the temperatures, pressures, and flow rates, was achieved. These steady-state conditions were used as a starting point for the dynamic simulation with the PDC.

3.2 External Input

As discussed in Section 2.1 above, the heater power input, the conditions on the water side, and the shaft rotational speed need to be supplied as external input tables for the PDC transient simulation. These parameters were obtained from the experimental data, fitted with piece-wise linear functions on a finite number of regions (40 points were selected), and converted into tables for PDC input. Figure 3-2 shows how these parameters were fitted for the PDC input. In most cases, the relative rather than absolute values were used to ensure consistency between the steady-state solution and transient simulation.

For the heater control, the first option described in Section 2.1.2, with a given heater power and calculated sodium inlet temperature, was used in the simulation. On the water side, the flow rate calculated by the loop operators based on the heat balance in the cooler was selected for the PDC input as a first approximation. For the shaft speed, the target RPM was selected for PDC input; no attempts were made so far to simulate the oscillations observed in the shaft speed as shown in Figure 3-2.

3.3 Pre-Transient Run

In the PDC, the transient calculations are always preceded by a time period during which the transient equations are solved for the steady-state conditions without any external input or variations. This period assures that the solutions of the transient (rather than steady-state) equations converge before the actual transient begins. This period is also used to confirm that the equations and the entire simulated system are stable. Figure 3-3 shows the results of such pre-transient simulation of the December 2010 SNL Loop data with the PDC. After the first initial adjustment, resulting from a finite convergence of the steady-state solution, the transient results return to values very close (within 0.5% at most) to the steady-state values.
Figure 3-1. PDC Results (Top) of the Simulated SNL S-CO₂ Loop Experimental Conditions (Bottom).
Figure 3-2. External Variables for December 2010 Simulation.
Figure 3-3. PDC Pre-Transient Results.
Figure 3-3. PDC Pre-Transient Results. (Continued)
3.4 Transient Simulation

With all the PDC modifications and the external input to simulate the SNL S-CO₂ Loop conditions described in the previous sections of this report, the transient simulations with the PDC could proceed. The turbomachinery maps, covering the range of the parameters for this particular experimental run, were generated. However, as the results below will show, this transient simulation did not progress far into transient. In this particular experimental run, the loop was operated at conditions below the CO₂ critical point at the compressor inlet. Figure 3-4 plots the conditions at the compressor inlet during the simulated run in comparison with the critical point. Note that for the pressure, the value measured at the cooler outlet is plotted in Figure 3-4 since this value was found to be more consistent with the compressor performance in FY11 [2]. It is easily seen from Figure 3-4 that most of the run was performed at temperatures below the critical value. The pressure also approached the critical pressure and, at some instances, dropped below the critical value.

The results of transient simulation of this data are shown in Figure 3-5. The calculations were stopped at about 270 seconds, shortly after the compressor impeller-inlet temperature dropped below the critical point. At this point, the pressure at the impeller-inlet was also very close to the critical value. Note that compared to the experimental data in Figure 3-4, the conditions in Figure 3-5 are plotted at the impeller-inlet, not the compressor inlet. The difference is the acceleration of the flow before the impeller which further reduces both the (static) pressure and temperature. For this reason, the minimum pressure and temperature are closer to the critical point in Figure 3-5 than they are in Figure 3-4. The PDC transient calculations were stopped automatically at about 270 seconds due to very small time steps which would be required to properly resolve the conditions that close to the critical point. Furthermore, even if it could be done, the data in Figure 3-4 showed that the conditions would be worse, from the convergence point of view later in the transient. In fact, even the experimental data shows some significant oscillations later in the transient, as apparent from the RPM plot in Figure 3-2, for example.

The PDC was originally developed to analyze conditions above the critical point since it is envisioned that a commercial-scale S-CO₂ cycle would be operated at such conditions and not the unprototypical conditions attained during the experiment. Even the SNL S-CO₂ Loop full design conditions showed operation above the critical point. Even though some provisions were made in the PDC to allow limited calculations below the critical point, for example for the critical two-phase flow and for the turbomachinery maps generation, the code was never thoroughly tested at such conditions. For these reasons, it was decided to seek more appropriate experimental transient data with operation above the critical point, rather than trying to extend the PDC range into the sub-critical region which is not relevant to the transient analysis of full-scale S-CO₂ power converters. Such experimental data was found from July 2011 experiments and simulation of that data with the PDC is described in the following chapter of this report.
Figure 3-4. Compressor-Inlet Conditions in December 2010 Run.
Figure 3-5. Results of Transient Simulation of December 2010 Data.
Figure 3-5. Results of Transient Simulation of December 2010 Data. (Continued)
4 Simulation of July 14, 2011 Experimental Data

The SNL S-CO₂ Loop experiment data from July 14, 2011 was selected for further simulation with the Plant Dynamics Code since for most of this experimental run the conditions at the compressor inlet were maintained above the critical point. The loop layout for this run is shown in Figure 4-1. This and several following figures related to the experimental data are reproduced from Reference 3 with permission from the authors.

![Figure 4-1. July 14, 2011 Layout of the SNL S-CO₂ Loop.](image)

The July 2011 configuration still includes a single TAC unit. At the same time, compared to the December 2010 configuration analyzed previously in this report, the July 2011 layout in Figure 4-1 includes several hardware changes. First, a high temperature recuperator (HT Recup or HTR) was installed in addition to the low temperature recuperator. Consequently, some piping layout had to be changed in order to accommodate an additional component. Second, two additional heater units were installed for this run. Lastly, the compressor wheel was replaced with a large wheel originally designed and built for the recompression compressor [4]. All of these changes affect the modeling of the loop and are discussed further in this document. In addition, these changes also required re-numbering of the measurement locations (the indexes shown in green in Figure 4-1), so these indexes may not be consistent with those used earlier in this report. The locations referenced in this chapter are consistent with those shown in Figure 4-1.
4.1 Experimental Data

The as-measured experimental data for the July 2011 run is show in Figure 4-2 for temperatures and in Figure 4-3 for pressures. Also, Figure 4-4 shows the heat balances in the loop during this run. The figures also plot the TAC speed which shows step-wise behavior during the experiment. In addition to the RPM changes, the other external input which can be observed from these figures is the periodical rump-ups of heater power, which are shown as increases in high temperatures. Between those changes, the loop was operated in more or less steady conditions, with some adjustment of water flow to maintain the compressor-inlet temperature.

Since the PDC calculations start from steady-state conditions, a point in the run had to be selected where the loop state can be modeled with steady-state equations. In addition to zero time, several candidate points for steady-state calculations were identified in Figures 4-2 through 4-4 at times 2290, 3356, and 4700 seconds. These points are preceded by a continuous operation for some time without either PRM or heater control changes. More detailed examination of the experimental data revealed that at time 2290 seconds and earlier, the conditions at the compressor inlet have not been brought to the supercritical state yet. Therefore, a data point at 3356 seconds was selected as a starting point for the transient calculations with the PDC. Although the conditions at 4700 s may be close to the steady-state, especially for the heater heat balance, this time is too late in the transient to provide a sufficient simulation interval after that time for the dynamic calculations with the PDC.

Since the PDC calculations start with time zero, the “PDC time” referred in this chapter will be 3356 s less the recorded experimental time. Unless clearly specified otherwise, all further plots in this chapter will be presented on the PDC time scale.

Figure 4-5 shows the instantaneous readings at the 3356 s point of the experimental time. For some parameters, such as water side pressures and flow, the experimental data was not available. The conditions in Figure 4-5 are used to simulate the starting point for the transient calculations with the PDC, as described in the following section.
Figure 4-2. Experimental Data for July 2011 Run – Temperatures.

Figure 4-3. Experimental Data for July 2011 Run – Pressures.
Figure 4-4. Heat Flows in July 2011 Run.

Figure 4-5. Experimental Data at 3356 s into July 2011 Run.
4.2 Steady-State Simulation

The steady-state simulation for the July 2011 data to a large extent is very similar to previous work reported in FY11 [2]. In this chapter, only the differences from the previous analysis are discussed in details.

4.2.1 High Temperature Recuperator

A high temperature recuperator (HT Recup in Figure 4-1 or HTR) was added to the experimental loop for the July 2011 run. At the time of this writing, very little information on the internal configuration of the HTR was provided to ANL (although some additional information may become available in future, subject to sensitive information handling procedures). Therefore, several assumptions on the HTR configuration had to be made in order to develop a model for the PDC. The conditions around the HTR in Figure 4-5 were selected for the model development. The inlet temperature and pressures on both sides along with the flow rates were used as the input data for the PCHE model in the PDC. The comparison of the model prediction with the experimental data is shown in Table 4-1.

Table 4-1. HTR Model Prediction

<table>
<thead>
<tr>
<th>Conditions</th>
<th>Parameter</th>
<th>Units</th>
<th>Experiment</th>
<th>Model</th>
</tr>
</thead>
<tbody>
<tr>
<td>Hot side inlet</td>
<td>Temperature</td>
<td>°C</td>
<td>207.2</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Pressure</td>
<td>MPa</td>
<td>7.464</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Flow rate</td>
<td>kg/s</td>
<td>1.779</td>
<td></td>
</tr>
<tr>
<td>Cold side inlet</td>
<td>Temperature</td>
<td>°C</td>
<td>45.4</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Pressure</td>
<td>MPa</td>
<td>9.784</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Flow rate</td>
<td>kg/s</td>
<td>1.779</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Conditions</th>
<th>Parameter</th>
<th>Units</th>
<th>Experiment</th>
<th>Model</th>
</tr>
</thead>
<tbody>
<tr>
<td>Hot side</td>
<td>Outlet temperature</td>
<td>°C</td>
<td>45.7</td>
<td>45.56</td>
</tr>
<tr>
<td></td>
<td>Pressure drop</td>
<td>kPa</td>
<td>-59.0</td>
<td>4.941</td>
</tr>
<tr>
<td></td>
<td>Heat balance</td>
<td>kW</td>
<td>381.6</td>
<td>380.0</td>
</tr>
<tr>
<td>Cold side</td>
<td>Outlet temperature</td>
<td>°C</td>
<td>145.1</td>
<td>150.3</td>
</tr>
<tr>
<td></td>
<td>Pressure drop</td>
<td>kPa</td>
<td>240.0</td>
<td>2.749</td>
</tr>
<tr>
<td></td>
<td>Heat balance</td>
<td>kW</td>
<td>370.7</td>
<td>380.0</td>
</tr>
</tbody>
</table>

As in the previous analysis, the prediction on the pressure drop does not agree with the experimental measurements. However, it can be seen from Figure 4-5 that the pressure measurements around the HTR were not accurate. The HTR-inlet pressure on the hot side (7.464 MPa) does not fall between the turbine-outlet pressure (7.742 MPa) and the HTR-outlet pressure (7.523 MPa). Similarly, the outlet pressure on the cold side...
is lower than both the HTR-inlet and the heater-inlet pressures. Therefore, the differences in the pressure drop prediction are not a concern at this point.

More importantly, there is a significant difference in predicting the outlet temperature on the cold side (although on the hot side the outlet temperature is predicted very accurately). As shown in Table 4-1, this difference comes from not achieving a perfect heat balance between the hot and cold flows in the recuperator at this time in the experimental run. There is about a 10 kW difference between the heat transfer rate on the hot and cold sides. This finding is consistent with the heat balance plot in Figure 4-4 where the “Q HTrcp LP” (hot side) line is almost always higher than the “Q HTrcp HP” (cold side) line. This difference in heat transfer could not be simulated with any change in the HTR model input since in steady state the model would always calculate a perfect balance as demonstrated in Table 4-1. Therefore, no further HTR model improvement could be carried out at this point and more data on the HTR performance would be required to further refine the HTR model.

It is noted here that the HTR is not insulated but its outer surfaces are exposed to the ambient air. It is conceivable that at least part of the lack of a heat balance between the hot and cold sides could be due to heat losses from the HTR outer surfaces as well as the piping segments in the manifolds.

To account for the difference in the heat balances in the HTR, it was decided to include in the PDC model a heat loss into the pipe connecting the HTR cold side outlet with the heater. The magnitude of the heat loss was selected to obtain a good agreement on the heater-inlet temperature given the performance prediction of the HTR. More discussion on the heat loss is provided in the entire loop simulation section below.

4.2.2 Low Temperature Recuperator

Initially, an attempt was made to retain the low temperature recuperator (LT Recup in Figure 4-1 or LTR) in the PDC model. It was quickly realized, though, that the particular conditions of the July 2011 run present challenges in term of the LTR modeling. It can be seen from the temperature changes around the recuperators in Figure 4-5 that most, if not all, heat recuperation occurs in the larger HTR. As a result, the temperature change in the LTR is very small, well within the temperature measurement uncertainty of ±1.1 °C. Moreover, if the uncertainty is not included into the consideration, the results in Figure 4-5 show that the heat transfer occurs in the reverse direction in the LTR, i.e. the “hot” side flow is slightly heated while the “cold” side flow is further cooled in the LTR. These results agree with the heat transfer plot in Figure 4-4 where the LTR curves stay at or below zero level for the majority of the transient.

The reversed heat transfer presented challenges in finding the steady-state solution for the LTR, since the code was developed assuming the heat transfer from the hot side to the
cold side. Even if the heat transfer were in the right direction, the small temperature differences for the two flows would require much higher accuracy in resolving the heat transfer equations than currently implemented in the PDC. The results of the calculations showed that the steady-state solution for the LTR never achieved a proper convergence. Consequently, an attempt to apply transient equations to the LTR resulted in too large an initial variation of the parameters triggering the code to stop on too small a time step.

Because of this problem and since the LTR is not significantly changing the fluid temperatures in this particular run, it was decided to exclude this heat exchanger from the PDC modeling of the loop. The effects of the LTR on the pressure drop and the thermal inertia of the system would need to be evaluated based on the transient results. If needed, though, these factors could be included into the HTR model.

4.2.3 Recompression Compressor

For the experimental run in July 2011, the main compressor wheel was replaced with a larger recompression compressor wheel. This change allowed the loop operators to achieve better compressor performance at lower speed for this single-TAC configuration. Consequently, a recompression compressor model had to be developed for the PDC. This model is the same as for the main compressor, only the dimensions of the impeller and the diffuser were changed to be consistent with the recompression compressor design.

An initial attempt to apply the as-measured conditions in Figure 4-5 to the compressor model resulted in significant under prediction of the outlet temperature with simultaneous over prediction of the outlet pressure. A subsequent analysis revealed that with the direct input of the inlet pressure and temperature, there is a significant over prediction on the compressor-inlet density which was also measured in the experiments. The inlet density is considered to be a better indication of the CO$_2$ properties at the compressor inlet since the properties near the critical point are much less sensitive to the uncertainty in density than to that in pressure and temperature. When the inlet pressure and temperature were adjusted (within the measurement uncertainty) to match the measured inlet density, a much better agreement was obtained on both outlet pressure and temperature, as demonstrated in Table 4-2. Consequently, the compressor-inlet conditions defined in Table 4-2 were adopted for the steady-state conditions for the PDC model.
Table 4-2. Recompression Compressor Model Prediction

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Units</th>
<th>Experiment</th>
<th>Model</th>
</tr>
</thead>
<tbody>
<tr>
<td>Inlet temperature</td>
<td>°C</td>
<td>31.261</td>
<td>31.5</td>
</tr>
<tr>
<td>Inlet pressure</td>
<td>MPa</td>
<td>7.463</td>
<td>7.449</td>
</tr>
<tr>
<td>Inlet density</td>
<td>kg/m³</td>
<td>389.7</td>
<td>390.7</td>
</tr>
<tr>
<td>Flow rate</td>
<td>kg/s</td>
<td>1.779</td>
<td></td>
</tr>
<tr>
<td>Rotational speed</td>
<td>RPM</td>
<td>35,000</td>
<td></td>
</tr>
</tbody>
</table>

Results

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Units</th>
<th>Experiment</th>
<th>Model</th>
</tr>
</thead>
<tbody>
<tr>
<td>Outlet temperature</td>
<td>°C</td>
<td>46.296</td>
<td>46.146</td>
</tr>
<tr>
<td>Outlet pressure</td>
<td>MPa</td>
<td>9.867</td>
<td>9.884</td>
</tr>
</tbody>
</table>

4.2.4 Heaters

The heaters are still simulated with the shell-and-tube heat exchanger model in the PDC. The larger number of heater units is simulated with longer tubes of the heat exchanger. No other changes to the geometric input for the heater model were needed.

Similar to the HTR heat balance discussed above, there is a significant difference between the heat balances in the heaters at the experimental time of 3356 s, as shown by “Htr Pwr” for the heater input and “Q Heater” for the CO₂ side curves in Figure 4-4. In this case, though, the difference is much higher for the heater than for the HTR and is about 35 kW. To achieve proper conditions on the CO₂ side at the steady state, a power of 192.2 kW, representing the actual heat balance on the CO₂ side, was selected for the heater power (although the electrical heat input at this point is 226.4 kW).

4.2.5 Piping

Introduction of the additional recuperator for the July 2011 run necessarily required modifications to the piping layout. However, the exact piping dimensions were not provided to ANL. Instead, it was stated [4] that this cycle configuration was an intermediate state between the single-TAC layout in December 2010 and the most recent split-flow configuration. In fact, the piping configuration may not even have been recorded for this particular run. Therefore, due to the lack of real data, the same exact piping dimensions, used for the analysis of the December 2010 loop configuration, were retained for the PDC analysis of the July 2011 configuration. Since the LTR recuperator was excluded from the current model, no additional modifications to the piping and the cycle layout were needed.
4.2.6 Results for Entire Loop Simulation

With all the additional model development and assumptions described below, the steady-state calculation with the PDC to simulate the starting point for the dynamics calculations, at the 3356 s experimental time point, could be carried out. The comparison of the steady-state PDC prediction with the experimental data is shown in Figure 4-6. The compressor-inlet conditions (pressure and temperature) were intentionally modified to match the measured compressor-inlet density, as described in Section 4.2.3. With this modification, the compressor-outlet conditions are predicted very accurately. As discussed in Section 4.2.2, the LTR is not currently included into the PDC model, so it has no effect on the calculated temperatures and pressures (LTR is shown in Figure 4-6 only for comparison with the experimental configuration).

The performance of the HTR is not matched very well by the PDC on the hot side. This, however, is a result of not achieving a complete heat balance between the two flows in the HTR in the experimental run, as discussed in Section 4.2.1, and not a model deficiency. To compensate for this imbalance, a heat loss was added to the pipe connecting the HTR with the heater. Note that a significant heat loss adjustment (19 kW) was needed in order to achieve the temperature and pressure balance in the entire system. With this significant heat loss, it was not necessary to include an additional loss in the turbine volute (or in the turbine inlet pipe), as in the previous simulation. Thus, the heat loss in the HTR-heater pipe represents the heat loss in the entire system. It is just put in one place for the simplicity of the calculations; more detailed distribution of the heat loss throughout the system would be more prototypical of the actual conditions. However, modeling that would require more detailed knowledge on the system behavior at various steady-state conditions; i.e., more experimental data would be needed.

Even with the significant heat loss in the pipe upstream of the heater, the heater-inlet temperature is still about 3 °C higher in the model than the measured value. This difference resulted in prediction of slightly higher (by 4.5%) of the flow rate in the system in order to match the heater-outlet conditions. The turbine-outlet conditions are matched accurately by the code. To simulate the apparent significant pressure drop in the turbine-HTR pipe, an artificial valve was added to this pipe in the PDC model.

The conditions at the HTR hot side outlet, around the cooler, and back to compressor inlet are all matched closely by the code, within the experimental uncertainty.

It is also noted from comparing the modeled cycle layout in Figure 4-6 to that in Figure 4-1 that the TAC drain flow path driven by the Hydropac pump is not included into the PDC model. This flow rate is at least an order of magnitude less than the main loop flow rate.

Overall, the results in Figure 4-6 were judged satisfactory, given the fundamental differences arising from simulating not perfectly steady conditions with the steady-state equations. Therefore, the calculations of the transient part could proceed from this point.
Figure 4-6. PDC Results (Top) of the Simulated SNL S-CO$_2$ Loop Experimental Conditions (Bottom) for July 2011 Run.
4.3 Dynamic Simulation

Starting from the steady-state conditions described in the previous section, the transient simulation of the July 2011 experiment with the PDC was carried out. The pre-transient calculations of the steady-state conditions (without any transient initiator) with the dynamic equations showed that the system solution is stable and is very close to the solution found with the steady-state equations, much like in the previous simulation discussed in Section 3.3.

The transient itself was defined by the external input simulating the SNL loop control by the operators. That external input is described below.

4.3.1 External Input Data

As discussed in Section 2.1, the SNL S-CO$_2$ Loop experiments are defined by the operator input for the TAC rotational speed, heater power, and water flow rate controls. These controls were simulated for the PDC calculations as graphically shown in Figure 4-7 (the actual PDC input is done in text tables).

For the heater control, the last option described in Section 2.1.2, namely the automatic heater control, was simulated for the July 2011 experiment. The heater-outlet set temperature in Figure 4-7 was directly imported from the recorded target temperature in the experiment. No other input for the heater was needed, except for the flags which define the automatic control option.

Similar to the heater control, an automatic water flow control was used in this simulation with the option of controlling the cooler-outlet temperature (see Section 2.1.3). The as-recorded cooler-outlet temperature was used as an input for the target temperature for the water flow control. In Figure 4-7 and in the PDC input this target temperature is defined in relative terms; i.e., normalized to the steady-state value in Figure 4-6. All other parameters of the water control, including the PID coefficients, were retained from those developed for analysis of the full-size systems; no attempts to optimize the control for this particular application were made.

The inlet water temperature in Figure 4-7 was supplied to the PDC from the as-measured data without any modifications. It was only fitted with piece-wise linear function to be suitable for table input form, as shown in Figure 4-7.

The TAC speed input was adopted from “Target RPM” input which is also recorded in the experimental data. A 5 second delay at each RPM change was introduced to better simulate the actual TAC speed, as shown in Figure 4-7. Note that the last change in RPM (around 2450 s) was not included into the PDC model.
Figure 4-7. PDC Input for External Control.
The external controls shown in Figure 4-7 were the only inputs to the PDC to define the transient. No other inputs were needed. Also, as discussed above, all other controls, previously incorporated into the PDC were disabled for this simulation.

The turbomachinery maps were re-calculated for this particular transient to cover the range of operating parameters recorded in the test. Also, re-calculation of the compressor map was necessary since the recompression compressor wheel was introduced for this test.

The simulation was carried out for 2500 seconds PDC time which is equivalent to the time interval from 3356 s through 5856 s of the recorded experimental time in Figures 4-2 through 4-4.

4.3.2 Transient Results

The results of the PDC transient simulation of the SNL S-CO₂ Loop experimental data from July 14, 2011 are presented in the following figures in comparison with the as-recorded data. In these figures, the PDC results are shown in thinner lines and are denoted with a symbol while the experimental data is shown with thicker lines without symbols. As a rule, the comparison is made between the results representing the same parameter; for example, the heater-outlet temperature is compared between the experimental data and the PDC prediction on the same plot. The individual plots are referenced in the text by the plot's title at the top of the plots with italic highlights in the report text. The results are plotted against the PDC time which, as discussed above, differs from the actual recorded time by 3356 seconds.

The comparison between the calculated and measured temperatures around the loop is shown in Figure 4-8. In general, the PDC predicted the temperatures very well despite all the uncertainties in the experimental data and the assumptions which had to be made for the simulation. Note that the vertical axis scales are not the same for all plots in Figure 4-8 as these scales are selected to better show results for each particular temperature. Therefore, the temperature scale in Figure 4-8 should be kept in consideration when comparing the accuracy of the code prediction between different temperatures.

The prediction of the heater outlet temperature is almost exact during the majority of the transient simulation. This is the result of the automatic control in both the experimental run and in the PDC simulation. This temperature was an external input as discussed in Section 4.3.1 above. The almost exact asymptotic prediction of this temperature confirms the appropriate simulation of the heater control. The biggest differences between the experimental data and the PDC prediction are calculated between 1400 and 1700 seconds and between 2000 and 2200 seconds. As will be discussed below (in the power and flow results), this is the result of not having enough reserved capacity in the heaters in the PDC simulation.
The turbine inlet temperature basically follows the heater outlet temperature. The only significant difference from the previous plot is a slight delay in turbine inlet temperature compared to the heater outlet temperature in the experimental data. For example, the heater outlet temperature reaches 280 °C at about 320 s while the turbine inlet plot crosses this mark at about 370 s. That delay is not captured in the PDC where both temperatures reach 280 °C at about the same time. This is due to the fact that pipe heat capacity and the heat transfer between the pipes and CO₂ is not currently simulated in the PDC. Note that these phenomena are expected to be much more significant for the small-scale loops with small piping diameters and small CO₂ flow rather than for commercial plants with much larger piping diameters and flow. For example, in the ABR-1000 design, the CO₂ flow rate of about 5600 kg/s is carried by four parallel pipes of 1 m diameter. Compared to the maximum flow rate of 2.6 kg/s in this experiment and 2 in pipes, and assuming that the pipe thickness-to-diameter ratio is about the same, the pipe mass-to-flow ratio for the SNL loop would be 27 times higher than for the ABR-1000.

The turbine outlet temperature shows good agreement with the experimental data earlier in the transient but later in the transient when flow rate and the turbine rotational speed increase, there is a noticeable difference between the calculated and measured temperature. Except for the time interval around 1500 s (when turbine inlet temperature is under predicted by the heater simulation as described above), the difference in turbine outlet temperature reaches about 10 °C. This difference indicates that turbine performance is over predicted by the PDC radial turbine model, especially at higher rotational speeds. Thus, these results indicate that the work on refining the radial turbine model in the PDC should be continued.

The HTR hot side inlet temperature shows the similar prediction as the turbine outlet temperature. However, the values calculated by the PDC are somewhat closer to the experimental results for this temperature compared to the turbine-outlet. This fact indicates that there is some heat loss in the turbine-HTR pipe, which is not currently modeled in the PDC and which somewhat compensates for over prediction of the turbine performance.

The results for the HTR hot side outlet temperature show that this temperature is consistently over predicted by the code in the transient, suggesting that the HTR transient performance is under predicted by the code. However, since the maximum difference in the temperature prediction reaches only about 1.5 °C at maximum (compared to the measurement uncertainty of 1.1 °C), that under prediction of the HTR performance is not a concern at this moment.

The agreement in the cooler inlet temperature is similar to that of the HTR-outlet. This temperature is also over predicted by the code; however, the difference is somewhat lower. At the initial stage of the transient, this temperature is predicted very accurately. Later in the transient, the maximum difference is about 1.2 °C which is very close to the measurement uncertainty of 1.1 °C. As discussed above, the simulated cycle layout for
the PDC does not include the low temperature recuperator which is located between the HTR and the cooler. So, the fact that the cooler inlet temperature prediction is not worse than the HTR-outlet confirms that in this experimental run the LTR does not change the fluid temperatures by any significant amount and not including the LTR in the current dynamic simulation does not affect the temperature results much.

The cooler outlet temperature is predicted very accurately by the code. The maximum difference is about 0.3 °C which is well within the measurement uncertainty. Note, however, that the as-measured cooler outlet temperature was specified for the PDC as an external variable for the water flow rate control. Therefore, a good prediction of this temperature by the code is only an indirect indicator of a correct cooler performance prediction. To a greater degree this agreement confirms the proper operation of the water control simulated in the PDC. However, since the water flow rate was not measured in the experiment, it is impossible to justify how the simulated control predicts the actual conditions on the water side. For the cycle performance, however, only cooler outlet temperature on the CO₂ side is important which is predicted accurately by the code. At the same time, not a perfect agreement between the specified control and the actual temperature, especially later in the transient, confirms the previous findings [5] that the cooling water flow control alone may not be sufficiently fast for the S-CO₂ cycle since its speed is limited by the thermal inertia of the cooler structure. This control should be augmented by faster acting cooler bypass control if more precise control of the compressor inlet temperature is required such as for commercial plants.

Similar results are obtained for the compressor inlet temperature. Note that this temperature is slightly lower than the cooler outlet temperature. In the PDC results, this is an indication of the pressure drop effect on the temperature since no heat transfer is simulated in these pipes. Therefore, similar agreement between the cooler outlet and compressor inlet temperatures indicate that the effect of the pressure drop on the temperature change is adequately represented in the PDC in the proximity of the critical point. Also notice that the consistently good agreement in the compressor inlet temperature during the entire transient confirms that the selection of this temperature for the steady-state simulation (to be consistent with the compressor-inlet density) was an appropriate approach.

The compressor outlet temperature is predicted very well by the code. Only during the second half of the transient is there some over prediction of this temperature. However, the difference is limited to 1 °C which is still within the measurement uncertainty.

The HTR cold side inlet temperature is shown to be consistently over predicted by the code by 1-2 °C. Since this prediction is somewhat worse than that for compressor-outlet, this difference is most likely is a result of not including the LTR into the dynamic model. Interestingly enough, the fact that the HTR inlet temperatures is measured to be lower than the compressor outlet temperature suggests that the LTR in this experimental setup is actually exchanging heat from the high pressure fluid to the low pressure fluid (i.e.,
transferring heat in the opposite direction), as discussed in the steady-state analysis section.

The *HTR cold side outlet temperature* shows good agreement for the majority of the transient. The biggest differences are observed during the system heat ups around 400, 1600, and 2100 seconds. In most of these cases, the PDC predicts higher rates of temperature increase than measured experimentally (the apparent slower rate around 1400 s is attributed to a lower temperature on the hot side as discussed above). This higher rate suggests that the thermal inertia of the HTR structure is underestimated by the HTR model in the PDC, meaning that the assumptions made for the internal configuration of this heat exchanger (which was not available to the authors of this report) were not completely accurate. These results suggest that more metal mass should be present in the HTR than currently simulated. Such a mass increase can be achieved by increasing the metal volume fraction inside the plates either by increasing pitch-to-channel diameter ratios or by decreasing the channel diameter. Also notice that the measured temperature in this location shows significant oscillations which are not present in any other temperature. In the middle of the transient, these oscillations can reach a magnitude of 10 °C which is an order of magnitude higher that the measurement uncertainty. Unless this is a result of a faulty thermocouple, these oscillations may indicate a not-so-perfect mixing of flow in the HTR outlet plenum. However, this explanation is unlikely since the temperature measurements are usually done about 1 foot away from the heat exchangers.

The *heater inlet temperature* is under predicted by the code for most of the transient. Except for the time period around 400 s, where the HTR outlet temperature itself is over predicted, the under prediction of the heater inlet temperature is about 10 °C. This is perhaps the most significant difference between the code results and the measured data. As discussed in the steady-state simulation section above, a significant heat loss in the pipe connecting the HTR and the heater had to be simulated in order to obtain a good heat balance at the steady-state conditions. This heat loss was naturally present throughout the entire simulation. Although it was effective in achieving good agreement in temperatures earlier in the transient, the results of the heater inlet temperature suggest that this heat loss may be overestimated by the code for the majority of the transient run. This heat loss correction is further discussed in the power and flow results section below.
Figure 4-8. PDC Transient Results – Temperatures.
Figure 4-8. PDC Transient Results – Temperatures. (Continued)
Figure 4-8. PDC Transient Results – Temperatures. (Continued)
The comparison between the measured and calculated by the PDC pressures and densities is shown in Figure 4-9 that compares the high and low pressures in the cycle in terms of compressor and turbine inlet/outlet pressures. Unlike the temperatures, all intermediate pressures will be between those values. For this reason, it is only necessary to analyze the agreement between these limiting pressures. For the density plots, only the value at the compressor inlet was measured in the experiment and can be compared with the density calculated by the PDC.

Similar to the temperature in previous figures, the general trend in both pressures and density is captured very well with the PDC simulation. At the same time, some differences exist between the code prediction and the experimental data. Those differences are discussed below in more detail.

The compressor outlet pressure show good agreement earlier in the transient and towards the end of the transient but in the middle of the transient, at higher rotational speeds, the code over predicts this pressure. More analysis is needed to investigate the cause for this difference. However, given the fact that both the inlet pressure and density (as discussed below) show much better agreement, it seems that the code over predicts compressor performance at higher rotational speeds.

The turbine inlet pressure is a derivative of the compressor outlet pressure and the pressure drops on the cycle’s high-pressure side. Similar to the compressor outlet pressure, the code over predicts the turbine inlet pressure. However, the difference between the calculated and measured value is even higher for the turbine inlet case. This is most likely a result of not including the low temperature recuperator into the PDC model and, consequently, not catching the effect of the pressure drops in the LTR.

The pressures on the low side of the cycle show much better agreement between the PDC prediction and the measured data. The compressor-inlet pressure is matched by the PDC almost exactly. There is some difference in the turbine-outlet pressures in the first half of the transient but that difference is much smaller than on the high-pressure side. Later in the transient, the turbine outlet pressure is also predicted almost exactly. Comparing the turbine inlet and outlet pressure predictions, it seems that the code overestimates the pressure ratio in the turbine. As discussed above, the temperature change in the turbine is also over predicted by the code meaning that the overall turbine performance is somewhat higher in the code compared to the experimental performance. This, however, might be a result of over predicting the flow rate, as discussed below, since both the pressure ratio and temperature change in the turbine are proportional to the flow rate. In any case, the performance prediction of the radial turbine is not as important as for the other components since this radial design is not expected to be used for medium- and large-scale S-CO₂ cycles for which the PDC is being developed.

The compressor inlet density is predicted sufficiently well by the code, especially in the middle of the transient. Note that the density change itself is not great; during the entire transient, the density variation is limited to about ±10%. Some difference in the
density prediction is most likely due to the difference in predicting the compressor inlet (or cooler outlet) temperature. As discussed above, this temperature is set to be controlled by the cooler water flow rate variation and there is always some difference between the measured (set) and calculated (controlled) temperatures.
Figure 4-9. PDC Transient Results – Pressures and Densities.
The comparison of the PDC results with the experimental data in terms of power and flow is shown in Figure 4-10. For the flow rate, the PDC results show the values calculated for turbine and compressor since the code accounts for CO₂ compressibility in the cycle. However, these two values are almost the same in the simulated transient. The measurement of the flow rate was done at the compressor inlet location. For most of the transient, the mass flow rate is overestimated by the code by about 5%. This is consistent with the steady-state results (see Figure 4-6) where the CO₂ flow rate was overestimated by the same 5% due to incomplete heat balance. Also notice that the change in flow rate in the experiment is more gradual than in the PDC simulation. This is probably due to the heat capacity of the structures around the turbine and compressor such as the casing which are not modeled in the PDC. Also, this is a result of an instantaneous turbomachinery response assumption used in the PDC to be able to use the turbomachinery maps in the dynamic calculations.

Figure 4-10 also compares the heat balance in the heater as calculated by the code on the heater and CO₂ sides with that calculated from the heater control input recorded in the experiment. The calculated heater input is a function of the automatic heater control setup which was used to maintain the required CO₂ temperature at the heater outlet. This calculated input is close in shape to the actual heater control power. However, the code consistently overestimates the required heater input after 600 seconds. The largest difference between the calculated and recorded heat input is calculated prior to the second heater power increase, at about 1350 s into the PDC run. This discrepancy is most likely a result of not achieving a complete balance at the conditions which were used for the steady-state calculations for the starting point of dynamic run. As discussed in Section 4.2.6 above, not achieving a heat balance in the HTR required an introduction of a heat loss in the HTR-heater pipe. That heat loss mechanism was retained in the dynamic calculations with the PDC and the amount of heat transfer to the environment was calculated to increase as the system heats up. Figure 4-11 compares the instantaneous results at 1350 s obtained with the PDC code with the corresponding experimental data at 4700 s of the experimental time. As confirmed by the plots shown above, most of the calculated values agree well with the experimental measurements. However, as the PDC plot shows, a heat loss of 23.6 kW is calculated at this point in the HTR-heater pipe. At the same time, the measured temperatures at the ends of this pipe are almost the same at 186.3 and 186.9 °C. This means that the heat loss mechanism, which was needed to achieve convergence at steady-state, is no longer there (or, at least, is not that significant). This heat loss in the PDC results in lower temperature at the heater inlet leading to higher requirements for the heat input. Currently, there is no provision in the PDC to vary the heat loss in pipes with time but it is clear from Figure 4-11 that maintaining the heat loss, needed at steady state, throughout the transient is not consistent with the measured data. That issue, though, could not be easily resolved with the input data or a simple modeling modification to the PDC, since it would require different approaches to the heat loss treatment in steady-state and in transients.
Figure 4-10. PDC Transient Results – Flow and Power.
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Figure 4-11. Instantaneous PDC Transient Results at 1350 s (Top) and Corresponding Experimental Data at 4700 s (Bottom).
Figure 4-12 shows additional PDC results which have no equivalent in the experimentally measured data. The minimum cycle pressure and temperature are the static values calculated at the compressor impeller inlet. At two instances at the beginning of the transient, the conditions at this location are calculated to approach the critical point; for the rest of the transient, some margin to the critical values exists.

The water flow rate is calculated by the code in an attempt to match the specified cooler outlet temperature on the CO$_2$ side. The water flow rate was not measured in the SNL S-CO$_2$ loop.

The last plot in Figure 4-12 shows the stall/choke margins in the turbomachinery. Although the compressor margins stay about the same in the course of the transient, the turbine is calculated to approach choke conditions with time as the rotational speed increases. The margins are calculated in the PDC using the turbomachinery maps and are normalized to the steady-state flow rate. For example, the choke margin in the turbine is calculated as a difference between the choke flow and the current flow divided by the steady-state flow rate through the turbine:

\[
Choke\ margin = \frac{Choke\ flow\ at\ current\ conditions - Current\ flow}{Steady\ state\ flow}
\]

Since the conditions at 3356 s into the experimental run are selected as the steady-state for the PDC simulation, the steady-state flow in the definitions of stall and choke margin refer to the flow rate at that time.
Figure 4-12. PDC Transient Results – Not Measured Values.
5 Summary and Future Work

Validation of the Plant Dynamics Code (PDC) with experimental data from the Sandia National Laboratories (SNL) small-scale S-CO\textsubscript{2} Brayton cycle demonstration has been continued as data is made available to ANL. Previously, one of the earlier loop configurations from December 2010 was modeled with the steady-state portion of the PDC.

In order to be able to simulate transient behavior of the loop with the PDC, several modifications were introduced to the code. These modifications were limited to simulating the particular controls implemented in the SNL S-CO\textsubscript{2} loop such as the electrical heater control and the control of the cooling water flow rate by means of a bypass valve. Most of the implemented code changes are related to the control logic and did not concern the transient equations modeled in the PDC. Only for the heaters, which are currently represented using the existing PDC shell-and-tube heat exchanger model, some modification to the code equations were introduced in order to simulate the direct heat input into the heat exchanger “tubes”. Since the electrical heaters, as well as the loop-specific controls, are not expected to be used for the full-size commercial S-CO\textsubscript{2} cycles, the changes implemented in this work to the PDC are not expected to affect the results of previous calculations with the code when it was applied to reactor systems. Also, the steady-state and transient parts of the code were modified to allow calculation of heat losses in the pipes based on input parameters specified by the user. These modifications are specific to the small-scale SNL loop where piping is not always thermally insulated and where the specific design features of the turbine result in a non-negligible heat loss in the turbine volute.

With all of the implemented modifications to the PDC for the SNL Loop, the transient simulation of the SNL S-CO\textsubscript{2} Loop experiments was carried out. The pre-transient calculations, where the PDC time-dependent equations are applied to the steady-state conditions, showed that the transient solution of the entire system is stable and is very close to that found using the steady-state equations.

When the code was applied to the December 2010 experiment, the calculations were automatically stopped by the code after about 270 s due to too small a time step. At this point, the conditions very close to and, at some instances, below, the CO\textsubscript{2} critical point were calculated by the code requiring very small time steps to resolve the properties variation. This finding was consistent with the December 2010 experimental data where the loop was operated below the critical temperature (and, sometimes, below the critical pressure) for the majority of the test. Rather than trying to extend the applicability range of the PDC to these particular conditions (which are not envisioned to occur in commercial plants), it was instead decided to seek other experimental data for operation above the critical point.

Such experimental data was found from the July 2011 test. However, some additional model development was needed to simulate this test, since some hardware modifications were implemented between December 2010 and July 2011. In particular, the high temperature...
recuperator (HTR) was installed in addition to the low temperature recuperator (LTR). Also, the main compressor wheel was replaced with the recompression compressor wheel. Consequently, new models for these components had to be developed in the PDC. Note, though, that model development in these cases refers to obtaining the input data, since both the heat exchanger and compressor models were already implemented in the code and no code modifications were needed. It was found, however, that not all of the necessary data can be obtained for these components such that some assumptions had to be made. (It is expected that some of these assumptions may be removed in future, if more detailed information on the compressor and HTR becomes available to ANL.)

In addition to these changes, two extra heater units were installed for the July 2011 experiments. That modification, however, required minimal change in the PDC model; only the tube length of the shell-and-tube heat exchangers representing the heaters was doubled compared to the previous analysis.

During the simulation of the July 2011 data with the steady-state portion of the PDC, it was realized that a satisfactory heat balance, needed for a starting point for the dynamic calculations, was not achieved in the transient run. Consequently, an introduction of significant heat loss was needed in the PDC model and was implemented in the pipe connecting the HTR and the heaters, in order to simulate the conditions in the loop with the steady-state equations. In addition to that change, it was realized that in this test configuration, the LTR does very little heat transfer work, since the larger HTR achieves almost 100% effectiveness. Moreover, in most of the case, the LTR actually transferred some small amount of heat from what is supposed to be cold flow to the “hot” flow. Modeling the LTR this way resulted in convergence problems in both the steady-state and transient conditions. Since this heat exchanger was shown not to provide any significant work, it was excluded from the current PDC modeling of the July 2011 configuration of the loop.

Based on the discussion above and other analysis presented in this report, the major assumptions for the transient simulation with the PDC of the July 2011 configuration of the SNL S-CO$_2$ Loop were the following:

- The low temperature recuperator was excluded from the PDC model.
- The electrical heaters are simulated with shell-and-tube heat exchangers with sodium flow on the hot side for the steady-state model. In transient calculations, a direct heat input into the HX “tubes” was simulated for the automatic control of the CO$_2$ outlet temperature.
- All of the heat losses in the system (including that in the turbomachinery) were simulated to occur in the HTR-heater pipe. The amount of the heat loss was determined to achieve a heat balance throughout the system at steady-state conditions. In a transient, the heat loss is scaled with the changing CO$_2$ temperatures in the pipe.
- The water flow rate control is used in transients in order to try to match the recorded temperature at the cooler outlet. The same control setup, developed for reactor systems, was used in this simulation without an optimization of the control for this particular application.

- Other than the heat loss, no heat transfer is simulated in the pipes in the PDC. This also includes the absence of heat exchange between the CO\(_2\) and the pipe walls.

- The piping layout and dimensions were assumed to be identical to those in the earlier loop configuration.

- The TAC drain flow is not included into the PDC steady-state and transient models.

Despite all of these assumptions, the transient results obtained with the PDC were close to the actual experimental data. Almost all temperatures showed good agreement with the experimental readings. The noticeable exception was the heater inlet temperature which is consistently under predicted by the code. The analysis has shown that this is the result of incorporating the heat loss into the HTR-heater pipe. By comparing the PDC results with the experimental data later in the transient, it was discovered that this heat loss wasn’t as large as was needed for the steady-state simulation. So, the discrepancy in the heater-inlet temperature prediction is believed to be a result of the adjustment needed to simulate a not-perfectly-balanced system with the steady-state equations.

The other findings from the temperature comparison suggest that the thermal inertia of the HTR may be underestimated by the code. This may be an effect of not knowing the exact internal configuration of the HTR. It may also be a consequence of not including the LTR mass into the PDC model.

Also, the results show that the effect of the heat transfer between the CO\(_2\) and the pipe walls not currently modeled in the PDC has a somewhat noticeable effect on the temperatures during the rapid temperature changes, especially at the turbine inlet. This effect, though, is expected to be smaller (in relative terms) for larger systems with larger piping diameters.

Comparing the pressure and density predictions, it was observed that the pressures on the low side of the cycle were predicted very accurately by the code. On the high side, there is a difference between the code predictions and the actual data resulting from underestimating the pressure drops in the systems. This might also be an effect of not including the LTR into the model. It can also be a consequence of making some assumptions for the piping configuration and dimensions.

There are also indications that the turbine performance may be overestimated by the code, especially at higher PRM. This result, however, may have originated from overestimating the flow rate in transients. The over prediction of the flow rate in transients is consistent, though, with the magnitude at the steady-state conditions where it results from not achieving a perfect heat balance around the heaters in the experiments.
The compressor-inlet density (the only density measured in the tests) is predicted very accurately during most of the transient. Some differences in the density prediction later in the transient are most likely caused by a not-so-perfect match of the cooler-outlet temperature with the automatic water flow control. This result was expected since earlier work has demonstrated that the water flow control may not be sufficiently fast for this cycle and is better augmented by cooler bypass control.

Because some discrepancies were identified between the code predictions and the recorded experimental data, both in the steady state and in transients, the work on the SNL loop simulation with the PDC should be continued in the future. Based on the results obtained in this report, it is recommended that future work be concentrated in the following areas:

- Better simulation of the heat losses in the system possibly with a distributed loss model.

- Finding experiment data more suitable for the steady-state simulation for the starting point of transient simulation. This may be achieved by simulation of the cold conditions very earlier in the transient but it may require simulating the sub-critical region. Alternatively, ways could be investigated to better simulate a less than complete heat balance at the beginning of the transients.

- Refining the HTR model, if more design data is made available to ANL.

- Carrying out more comparisons of the turbine performance prediction with the experimental data, especially at higher rotational speeds. Refine the turbine model, if necessary. It is important to note, though, that the SNL loop configuration includes a radial turbine in each of the two TACs which is not envisioned to be used for reactor systems with S-CO$_2$ power converters.

- Investigate the ways to include in PDC model the effect of the LTR on the pressure drops and the thermal inertia.

- Consider the possibility to model the heat transfer in the pipes.

- Continue to apply the PDC to other experiment runs including different loop configurations to investigate whether the effects identified in this report are specific to the particular tests simulated in this study.
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References


