The 4th International Symposium - Supercritical CO2 Power Cycles
September 9-10, 2014, Pittsburgh, Pennsylvania

DEVELOPMENT OF A FLEXIBLE MODELING TOOL FOR PREDICTING OPTIMAL OFF-DESIGN PERFORMANCE OF SIMPLE AND RECOMPRESSION BRAYTON CYCLES

John J. Dyreby
Ph.D. Candidate
University of Wisconsin-Madison
Madison, WI USA
jjdyreby@uwalumni.com

Gregory F. Nellis
Kaiser Chaired Professor
University of Wisconsin-Madison
Madison, WI USA
gfnellis@engr.wisc.edu

Sanford A. Klein
Ouweneel-Bascom Professor
University of Wisconsin-Madison
Madison, WI USA
klein@engr.wisc.edu

Douglas T. Reindl
Professor
University of Wisconsin-Madison
Madison, WI USA
dreindl@wisc.edu

ABSTRACT

This paper reports on the development of a cycle modeling tool capable of simulating both design-point and off-design performance of simple and recompression Brayton cycle configurations. The tool consists of a computationally efficient modeling framework written in Fortran, as well as optimization routines that enable various types of analyses. The framework is flexible with respect to its implementation of fluid property data and component models; the off-design performance predictions for the compressors, turbines, and heat exchangers in the cycle are provided from user-defined “black box” component models. This approach allows for design-specific analysis, which is advantageous given the range of applications being considered for supercritical carbon dioxide (SCO_2) power cycles. The optimal off-design performance of various recompression cycle designs is predicted using turbomachinery models based on the radial compressors and turbines currently being investigated by Sandia National Laboratory (SNL). The effect of the design point selection on the off-design performance of the cycle is investigated, as well as the effect of decoupling the shafts of the main compressor and turbine.

INTRODUCTION

Supercritical carbon dioxide (SCO_2) power cycles show promise for a wide range of applications, such as concentrating solar power (CSP), next-generation nuclear reactors, and waste-heat recovery. The optimal SCO_2 cycle design will depend on the application and, ultimately, the economic aspects of the power plant under consideration. For example, increasing the amount of recuperation in the cycle will result in a higher thermal efficiency but will require a larger and more expensive recuperative heat exchanger. The optimal recuperator size will depend on the application-specific relationship between the economic benefits of higher operating efficiency and the capital costs associated with a larger heat exchanger. If the power plant is expected to operate away from its design point for significant periods of time, the off-design performance of the cycle will also affect the selection of an optimal cycle design. Therefore, there is a need for models that are capable of predicting the design-point and off-design performance of SCO_2 power cycles for various applications. These models should be flexible in order to accommodate the range of designs under consideration and computationally efficient in order to enable timely optimization studies, possibly while considering cycle performance on an annual or life-cycle basis.

In order to accommodate these requirements, a modeling framework has been developed that is capable of predicting the performance of the simple recuperated cycle as well as the recompression cycle. The framework is flexible with respect to component-level specifics, such as the type of compressor used in the cycle or the method used to represent the off-design performance of the turbine. This flexibility is accomplished by providing well-documented interfaces to "black box" component models that allow a user to represent components with any degree of complexity that is desired. Optimization routines are integrated into the models, allowing exploration of optimal component and system designs or optimal operating/control strategies for a given system design. While the selection of the best-possible design for a given application will strongly depend on a number of economic variables, the developed framework provides the consistent performance predictions that are required for further economic analyses.

This paper describes the framework with respect to its off-design modeling capabilities, as the design-point capabilities have been previously documented (Dyreby et al, 2014). This paper also reports on the use of the framework to explore the relationship between design-point compressor inlet temperature and off-design performance of the recompression cycle, as well as the effects of various compressor / turbine shaft configurations. Specifically, the off-design performance of a variable-speed single-shaft design, a fixed-speed single-shaft design, and a split-shaft design (where the main compressor shaft speed may vary and the turbine shaft speed is fixed at 3,600 rpm) is considered. For these analyses, the turbomachinery models are based on the radial compressor and turbine being investigated at Sandia National Laboratory (SNL) for SCO_2 applications (Conboy, 2012).

MODELING FRAMEWORK

The modeling framework is written in Fortran and organized into the seven modules described in Table 1. A Fortran module is a self-contained unit of code, the use of which is considered best practice with modern Fortran because it simplifies the code structure and enforces compile-time argument checking (Brainerd, 2009). The major advantage of the module-based approach that is used in this work is the ability to easily implement various fluid property libraries and component models at compile time. Specifically, a user may replace any of the non-required modules with an alternative containing custom code. The files listed in Table 1 are available online[1] and the source code is well commented and intended to be the primary reference for the framework.

Table 1. Fortran modules used by the developed modeling framework.

Module Name	Filename	Description
`core`	`core.f90` (required)	Defines a number of user-defined types and contains a number of subroutines and functions required by the `design_point` and `off_design_point` modules.
`design_point`	`design_point.f90` (required)	Contains the system-level subroutines used to model cycles at the design point.
`off_design_point`	`off_design_point.f90` (required)	Contains the system-level subroutines used to model cycles under off-design or part-load conditions.
`heat_exchangers`	`scaling_hxr.f90` (may be replaced)	Defines the functions responsible for scaling conductance and pressure drop under off-design mass flow rates.
`compressors`	`snl_compressor.f90` (may be replaced)	Contains compressor and recompressor sizing and performance subroutines based on the SNL compressor.
`turbines`	`snl_radial_turbine.f90` (may be replaced)	Contains the turbine sizing and performance subroutines based on a radial turbine similar to the SNL turbine.
`CO2_properties`	`module_CO2_properties.f90` (may be replaced)	Contains the required fluid property subroutines for carbon dioxide.

The user-replaceable modules provide the flexibility required to investigates various cycle designs, specifically with respect to the components in the cycle. For example, the `turbines` module, which

[1] Available at http://sel.me.wisc.edu/software.shtml

currently models a radial turbine with an efficiency curve based on the turbine being studied at SNL, can be replaced with a module that implements a model of a multi-stage axial turbine. Details of the heat exchanger and compressor models used for the analyses presented in this paper have been previously reported by Dyreby (Dyreby et al, 2011; 2012). The recompressor model currently assumes a two-stage compressor without intercooling where each stage is modeled using a dimensionless head-flow relationship based on the SNL compressor. Two stages are used for the recompressor in order to prevent the rotor tip speeds from becoming supersonic. The `CO2_properties` module currently assumes carbon dioxide for the working fluid, but any fluid or mixture can be implemented without requiring changes to the core cycle models. For these analyses the FIT library (Northland Numerics, 2014) is used to provide carbon dioxide properties, though an interface for REFPROP (Lemmon et al, 2014) is also provided online.

The `design_point` and `off_design_point` modules contain a number of subroutines that are capable of optimizing the model inputs with respect to thermal efficiency or power output. The subplex algorithm is used for these optimizations, as implemented by Rowan (1990). The system-level model implemented in the `design_point` module has been previously reported (Dyreby et al, 2014); this paper will focus on the off-design cycle model implemented in the `off_design_point` module. Additional information on the modeling framework is available in Dyreby (2014).

Off-Design Cycle Model

The off-design model inputs, shown in bold in Figure 1, are the main compressor inlet temperature ($T_{mc,in}$) and pressure ($P_{mc,in}$), the turbine inlet temperature ($T_{t,in}$), the recompression fraction (ϕ_{rc}), and the shaft speeds of the main compressor (N_{mc}) and turbine (N_t).

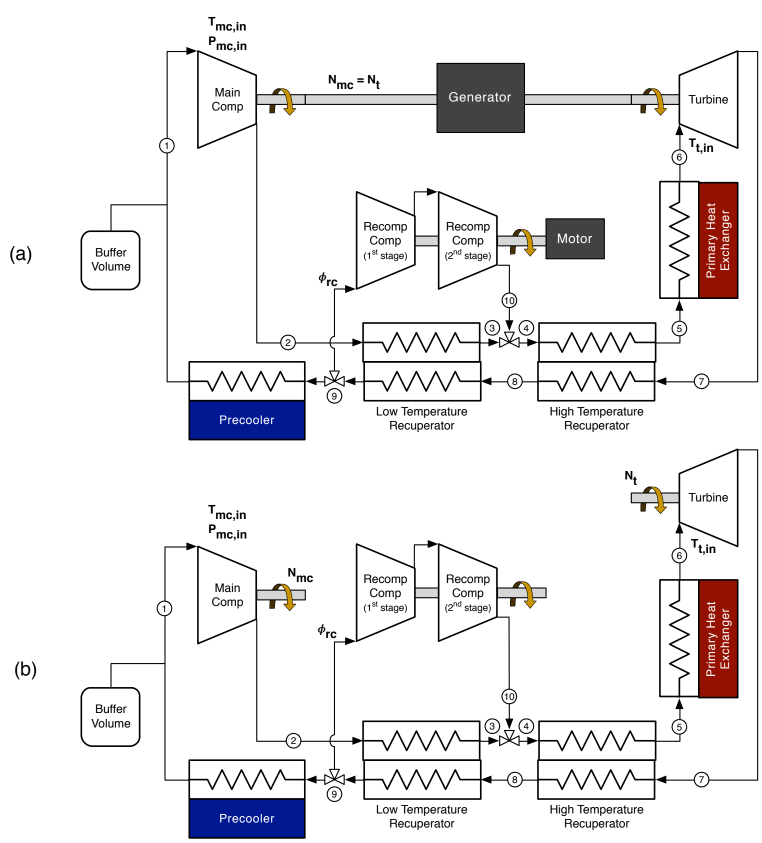

Figure 1. Diagram of a single-shaft recompression Brayton cycle (a) and a split-shaft recompression Brayton cycle (b); off-design model inputs are shown in bold.

The split-shaft configuration in Fig. 1(b) is characterized by the use of separate shafts for the main compressor and the turbine. A split-shaft configuration is advantageous in that it allows for a constant-speed, synchronous generator tied directly to the electrical grid, but it is more complex than a single-shaft configuration and the additional motor required to drive the main compressor will introduce an additional inefficiency in the system. In the interest of maximizing the flexibility of the model, the shaft speeds of the compressor and turbine are specified separately. The model allows the use of a single shaft by setting the turbine shaft speed to a negative value; this indicates to the model that the two speeds are linked. It should be noted that the shaft speed of the recompressor is not specified but is rather calculated according to the desired recompression fraction (ϕ_{rc}). Because the performance of the modeled recompression cycle is equivalent to the simple recuperated Brayton cycle when the recompression fraction goes to zero, this model is capable of simulating both cycle configurations under off-design and part-load conditions. A brief description and justification of the remaining model inputs follows.

The compressor inlet temperature is used as an input because the temperature to which the carbon dioxide can be cooled before entering the compressor is highly dependent on ambient conditions and the design of the precooler. For example, the lowest possible temperature for a dry, air-cooled cycle in the limit of a perfect precooler is the ambient dry bulb temperature. It is expected that the cycle heat rejection control strategy will target a known compressor inlet temperature (most likely as low as possible) in order to maximize efficiency. Directly specifying the compressor inlet temperature recognizes that there is a cooling system in place that is designed and operated appropriately to provide the desired temperature of carbon dioxide at the compressor inlet. Decoupling the operation of the cycle from the performance of the precooler heat exchanger reduces computational overhead of the core cycle model and allows any type of heat rejection system to be considered. While the thermal performance of the precooler is not considered when determining the operating point, once the system model has converged a precooler model may be used to determine the necessary cooling conditions required to achieve the target temperature. If those conditions are not possible (e.g., the compressor inlet temperature is specified as 33°C but the lowest possible temperature achievable with the precooler is 36°C), then the compressor inlet temperature can be adjusted and the model run again. In this way the precooler size and design can still be considered when evaluating cycle performance.

Specifying the compressor inlet pressure as an input to the model assumes a well-designed inventory control system. Using inventory control is advantageous in regards to maximizing cycle efficiency; specifically, increasing the compressor inlet pressure can reduce the efficiency degradation that would otherwise occur when operating a cycle under warmer off-design compressor inlet temperatures. While a disadvantage of inventory control is that it is slow (i.e., it has a relatively long time constant) compared to shaft speed or bypass control (Moisseytsev and Sienicki, 2009), this is not a concern for adjusting the operating point of the cycle based on slow changes in ambient conditions.

Increasing the carbon dioxide temperature at the turbine inlet of an SCO_2 Brayton cycle will always tend to increase the thermal efficiency. A desirable control strategy is to attempt to run the cycle at the highest possible temperature based on the available heat source (e.g., solar irradiance in a CSP application) but subject to one or more constraints such as the temperature limit for material properties. As is the case for the compressor, specifying the turbine inlet temperature assumes that the primary heat exchanger is adequately designed and controlled; this assumption reduces computational overhead.

The operating point of the cycle is determined by matching the head-flow curve of the compressor with the flow resistance of the turbine, as well as flow resistance associated with heat exchanger and piping pressure drops in the system. In order to determine this operating point, the model iteratively determines the corresponding mass flow rate through the turbomachinery using a combination of the bisection and secant root-finding methods (Chapra and Canale, 2009). A flowchart of the iteration logic used in the off-design cycle model is shown in Figure 2.

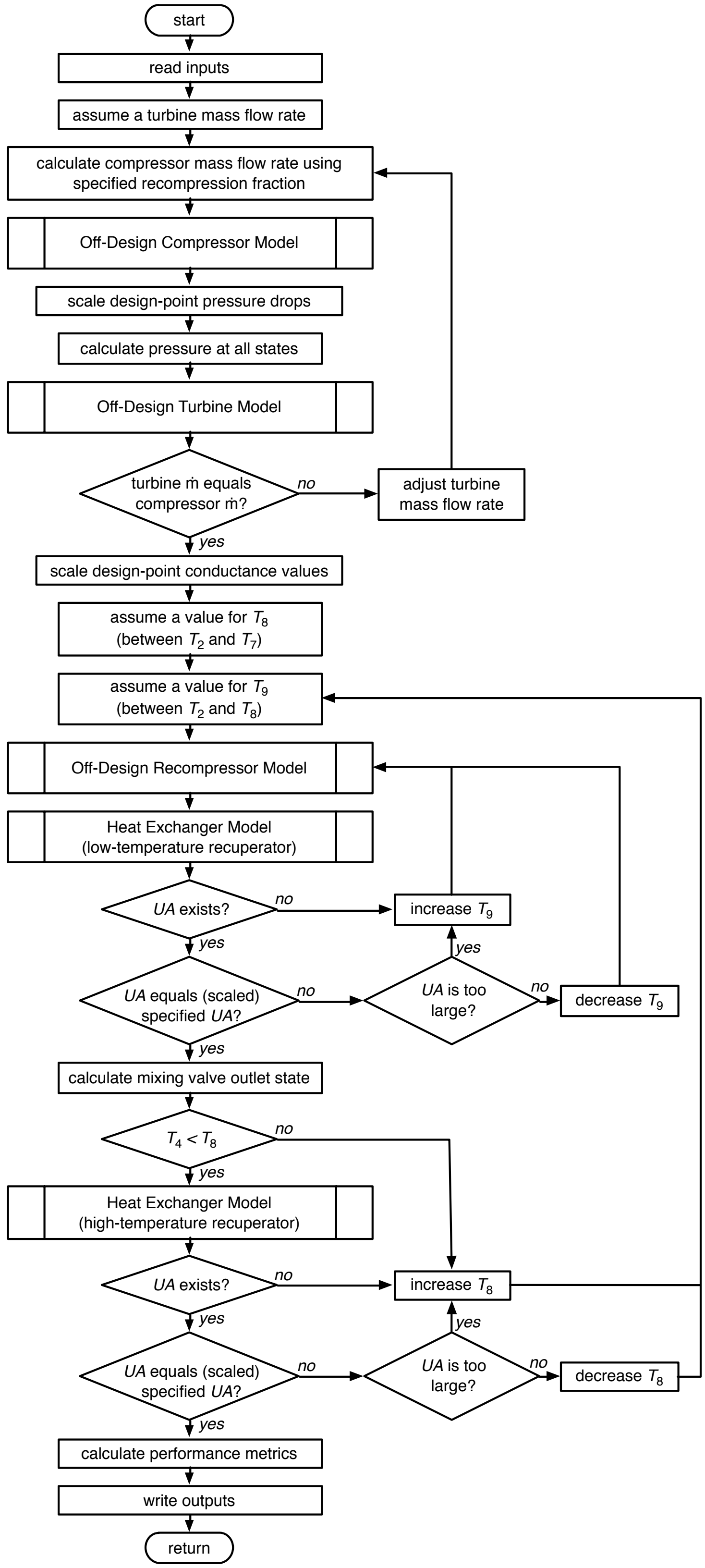

Figure 2. Iteration process for the off-design cycle model.

DESIGN POINT CONSIDERATIONS

It is expected based on simple Second Law considerations that the off-design thermal efficiency of the cycle will decrease as the temperature of the carbon dioxide at the main compressor inlet increases, and conversely the efficiency will increase as the compressor temperature decreases. What is not clear, however, is the relative magnitude of the efficiency degradation of a low-temperature design operating at above design-point temperatures versus the increase in efficiency experienced by a high-temperature design operating at below design-point temperatures. In order to explore this relationship, the off-design performance of three design options is considered. The three designs correspond to the single-shaft recompression configuration shown in Fig. 1(a) and are characterized by their compressor inlet temperatures of 32°C, 40°C, and 50°C, respectively. Each design is sized to generate 10 MW of mechanical power output at the design point, excluding generator losses and power associated with heat rejection and addition, with a high-side (turbine inlet) temperature of 550°C and a high-side pressure of 25 MPa. The total recuperator conductance at the design point is 3,000 kW/K, which provides a balance between cycle performance and heat exchanger size. Pressure drops through the heat exchangers, including the precooler and primary heat exchanger, are assumed to be 1 percent (relative to the inlet pressure to the heat exchanger). The design-point compressor, recompressor, and turbine isentropic efficiencies are 0.89, 0.89, and 0.93, respectively. Note that the recompressor isentropic efficiency is the overall efficiency of the two-stage compression process, which requires a stage efficiency of approximately 0.896. The parameters for the three designs are summarized in Table 2, as well as the resulting design-point thermal efficiencies. The thermal efficiency of the cycle does not take into account losses associated with the electric generator or any balance of plant required power (e.g., auxiliary pumping or fan power for heat addition or heat rejection from the cycle). The compressor inlet pressure, distribution of total conductance, and recompression fraction is optimized using the `optimal_design` subroutine contained in the `design_point` module. The approximate volume of the recuperators is determined by assuming a counter-flow configuration with flow channels that are 5 mm wide and 2.5 mm deep, which is representative of the printed circuit heat exchangers (PCHE) being considered for use with SCO_2 power cycles (Dostal, 2004).

Table 2. Three designs of interest, characterized by their compressor inlet temperatures.

Power Output	10 MW		
Turbine Inlet Temperature	550°C		
Compressor Outlet Pressure	25 MPa		
Compressor Isentropic Efficiency	0.89		
Turbine Isentropic Efficiency	0.93		
Heat Exchanger Pressure Drops	1%		
Compressor Inlet Temperature	32°C	40°C	50°C
Compressor Inlet Pressure	7.7 MPa	9 MPa	10 MPa
LT Recuperator Conductance	1.74 MW/K	1.59 MW/K	1.52 MW/K
LT Recuperator Minimum ΔT	5.3°C	7.2°C	7.2°C
LT Recuperator Approx. Volume	80 m^3	50 m^3	40 m^3
HT Recuperator Conductance	1.26 MW/K	1.41 MW/K	1.48 MW/K
HT Recuperator Minimum ΔT	5.1°C	7.7°C	11.4°C
HT Recuperator Approx. Volume	40 m^3	35 m^3	35 m^3
Compressor Rotor Diameter	0.120 m	0.148 m	0.183 m
RC First Stage Rotor Diameter	0.162 m	0.162 m	0.157 m
RC Second Stage Rotor Diameter	0.137 m	0.141 m	0.139 m
Turbine Rotor Diameter	0.218 m	0.241 m	0.265 m
Turbine Effective Nozzle Area	1,140 mm^2	1,450 mm^2	1,790 mm^2
Main Shaft Speed	37,080 rpm	31,410 rpm	27,030 rpm
Recompressor Shaft Speed	34,620 rpm	32,570 rpm	32,790 rpm
Recompression Fraction	0.3752	0.3266	0.2578
Turbine Mass Flow Rate	96.8 kg/s	114.5 kg/s	134.2 kg/s
Thermal Efficiency	47.7%	45.0%	41.8%

The primary difference between the three designs is the size of the turbomachinery, specifically the main compressor and turbine; designing for warmer compressor inlet temperatures results in slightly larger turbomachinery operating at lower shaft speeds. The recompressor design does not follow this trend as its size is driven by the optimal recompression fraction, which decreases as the low-side temperature increases. The warmer designs require less recompression because the properties of carbon dioxide do not vary as rapidly at conditions away from the critical point, decreasing the amount of flow that must be diverted in order to balance the hot and cold stream capacitance rates of the recuperator.

The off-design thermal efficiency at the rated power output is plotted in Figure 3 for the three designs, and the corresponding control parameters are plotted in Figure 4. In order to achieve the rated power output at temperatures above the design point, an increase in compressor inlet (and hence outlet) pressure is required. However, the maximum allowable pressure in the system must be considered, as it is likely that the equipment in the cycle is not designed to operate significantly above its design pressure. In the present analysis this operational constraint is accounted for by limiting the maximum pressure in the system to 30 MPa. Consequently, the 32°C design and, to a lesser extent, the 40°C design are limited with respect to the range of off-design compressor inlet temperatures over which the rated power can be delivered. Increasing the maximum operating pressure in the cycle will increase the off-design operational range, but at the cost of larger and more expensive equipment. This tradeoff highlights the usefulness of the developed modeling tool for application-specific investigations, as the optimal maximum allowable pressure in the cycle will be determined based on the balance between operating and efficiency characteristics and mechanical design considerations.

In general, designing for a lower compressor inlet temperature will result in a higher thermal efficiency but at the cost of a limited off-design operating envelope. This is not a concern if the power plant is expected to primarily operate at or very near its design point, but for other applications (e.g., a dry-cooled CSP plant) it requires consideration. It is worth noting that reducing the power output of the cycle extends the range over which it can operate. Whether this is a favorable operating strategy will depend on the specific application (and its economic factors) being considered.

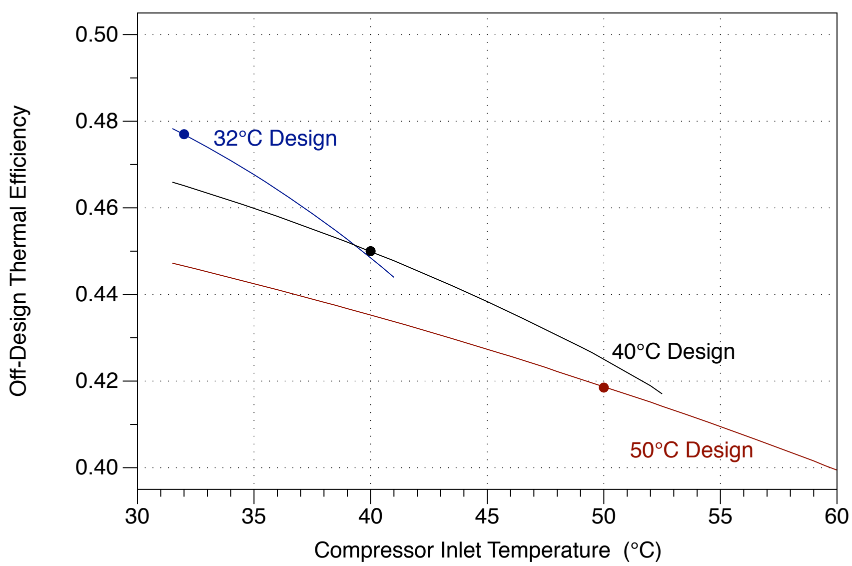

Figure 3. Thermal efficiency of the three designs at the rated 10 MW power output as a function of off-design compressor inlet temperature. The design points are indicated with a circle and only achievable values (with a high-pressure limit of 30 MPa) are plotted.

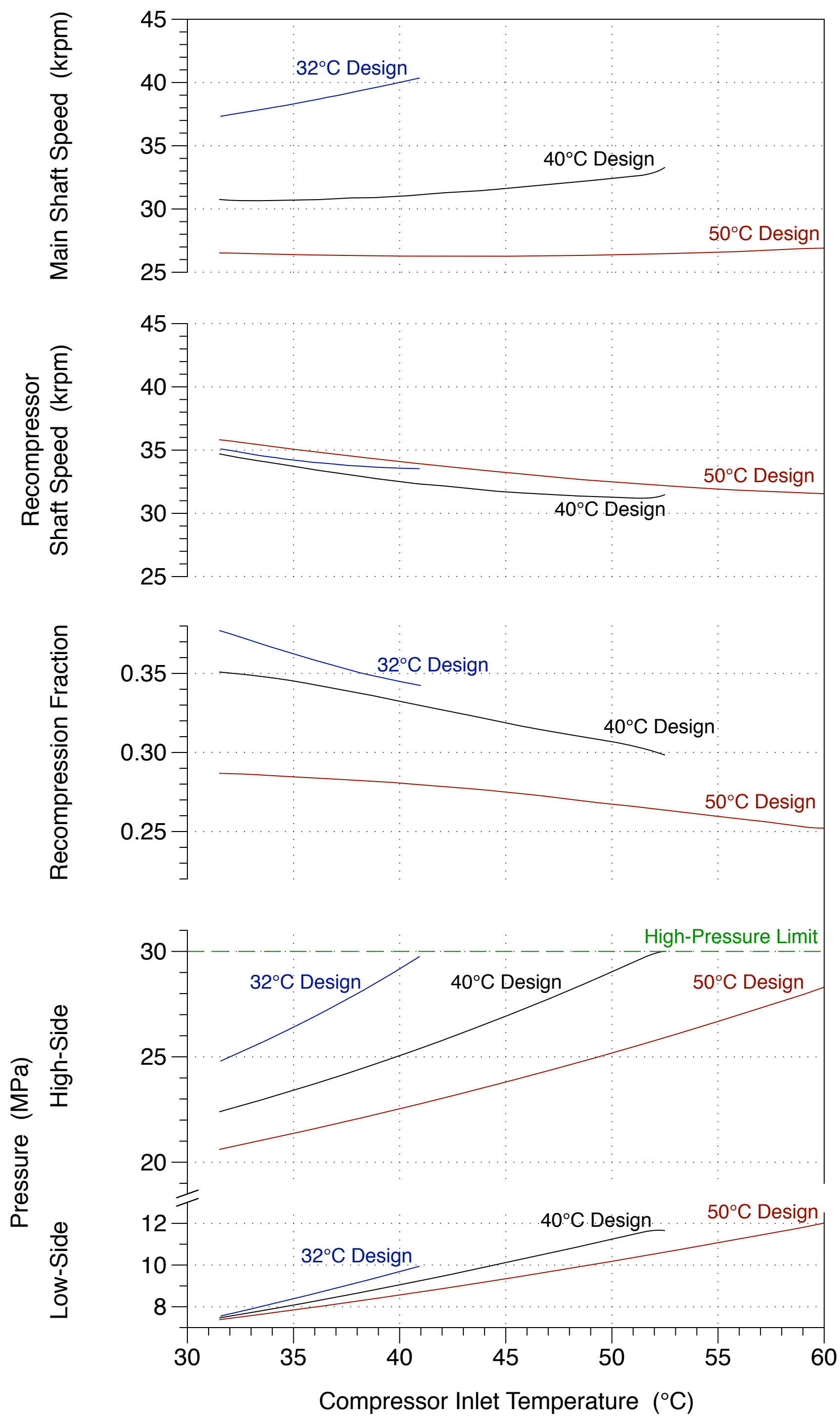

Figure 4. Control parameters associated with the efficiencies predicted in Fig. 3.

SHAFT CONFIGURATION CONSIDERATIONS

Three shaft configurations are considered for the 32°C design and 50°C design described in Table 2. In the “Normal” configuration, a single shaft connects the main compressor and turbine and shaft speed is allowed to vary. The “Fixed-Shaft” configuration is identical to the “Normal” configuration, with the exception that the shaft speed is fixed at its design-point value. In the “Split-Shaft” design, the main compressor and turbine use separate shafts, with the compressor shaft speed allowed to vary and the turbine shaft speed fixed at 3,600 rpm to facilitate the use of a grid-tied, synchronous generator. Note that this configuration does change the geometry of the turbine, while the “Normal” and “Fixed-Shaft” turbine geometries for the two designs remain as listed in Table 2. For the “Split-Shaft” configuration, the turbine rotor diameter is 2.25 m for the 32°C design and 2.0 m for the 50°C design. An independent motor with variable speed control drives the recompressor for all three configurations.

The predicted off-design thermal efficiencies at the rated 10 MW power output for the six designs are shown in Figure 5. The more complicated “Split-Shaft” configuration performs better under off-design conditions, but for the 50°C design its advantage is minimal. However, these results do not take into account the additional losses associated with the efficiency of the motor used to drive the main compressor. The efficiencies plotted in Fig. 5 also do not consider the advantages associated with using a fixed-speed synchronous generator compared to the power electronics that are necessary to condition the power generated using a variable shaft speed in the “Normal” configuration. The operating envelope of the “Fixed-Shaft” configuration for the 32°C design is reduced because that configuration has one less control parameter than the other configurations. The performance of the “Fixed-Shaft” configuration for the 50°C design is not noticeably different than the “Normal” configuration. This result is expected based on the relatively constant optimal off-design shaft speed for that design shown in Fig. 4.

The modeling tool developed here is also capable of predicting part-load performance of the cycle. The thermal efficiency from 10% to 100% of rated power output for the six designs is shown in Figure 6, with the compressor and turbine inlet temperatures held constant at their design-point values. Interestingly, the part-load thermal efficiency of the “Normal” configuration is consistently higher than the “Split-Shaft” configuration.

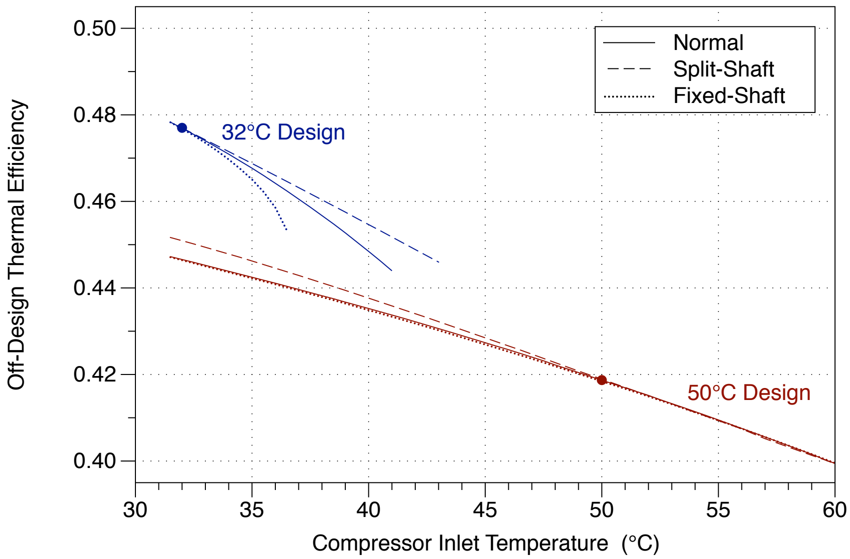

Figure 5. Off-design thermal efficiency of the three shaft configurations for the 32°C and 50°C designs at the rated 10 MW power output. The design points are indicated with a circle and only achievable values (with a high-pressure limit of 30 MPa) are plotted.

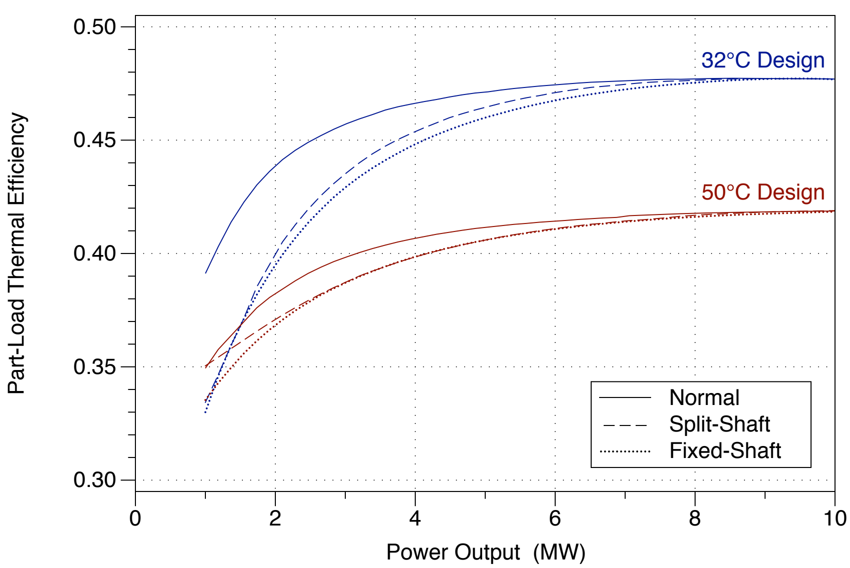

Figure 6. Part-load thermal efficiency of the three configurations for the 32°C and 50°C designs.

CONCLUSIONS

A flexible and computationally efficient modeling framework is presented that is appropriate for investigating the off-design performance of the recompression and simple SCO_2 power cycles. The framework enables multiple types of analysis and optimization and its module-based approach allows application-specific design constraints to be considered. The source code for the framework is available online, and the included core cycle models are envisioned as building blocks for more complex and specific simulations. For example, the models can easily be integrated into the TRNSYS simulation environment and combined with models developed for a specific power plant. Likewise, the cycle models can be coupled with models of various heat rejection mechanisms in order to investigate the effects of cooling-related parasitic losses on cycle design.

Turbomachinery models based on the radial compressor and turbine being studied by SNL for SCO_2 applications are used to investigate the off-design performance of three recompression cycle designs, characterized by their respective compressor inlet temperatures. The lowest-temperature design (32°C) is the most efficient, but high-pressure constraints limit its operating envelope. The highest-temperature design (50°C) is less efficient but is able to operate over the entire range of off-design low-side temperatures considered in this analysis. Various shaft configurations are considered for the 32°C and 50°C designs. Namely, the off-design and part-load efficiency of single-shaft (both fixed-speed and varying-speed) and split-shaft configurations are considered. Under off-design operation the split-shaft configuration is predicted to be more efficient than the single-shaft (variable speed) configuration. However, when operating at part-load the single-shaft (variable speed) configuration is predicted to be more efficient than the split-shaft configuration. These results are consistent for the two design-point low-side temperatures investigated, though the difference in performance among the shaft configurations is less significant for the higher-temperature, 50°C design.

NOMENCLATURE

ϕ_{rc}	=	recompression fraction
CSP	=	concentrating solar power
HT	=	high-temperature, referring to the high-temperature recuperator
LT	=	low-temperature, referring to the low-temperature recuperator
N_{mc}	=	main compressor shaft speed
N_t	=	turbine shaft speed
$P_{mc,in}$	=	main compressor inlet pressure, also referred to as the “low-side” pressure
RC	=	recompressing compressor, also referred to as the “recompressor”
SCO_2	=	supercritical carbon dioxide
SNL	=	Sandia National Laboratory
$T_{mc,in}$	=	main compressor inlet temperature, also referred to as the “low-side” temperature
$T_{t,in}$	=	turbine inlet temperature, also referred to as the “high-side” temperature
UA	=	heat exchanger conductance value

REFERENCES

Brainerd, W. S., 2009, *Guide to Fortran 2003 Programming*, Springer.

Chapra, S. and Canale, R., 2009, *Numerical Methods for Engineers*, Sixth Edition, 6th ed., McGraw-Hill Science / Engineering / Math.

Conboy, T., Wright, S., Pasch, J., Fleming, D., Rochau, G., and Fuller, R., 2012, “Performance Characteristics of an Operating Supercritical CO2 Brayton Cycle,” *Journal of Engineering for Gas Turbines and Power*, Vol. 134, No. 11, pp. 111703.

Dostal, V., 2004, “A Supercritical Carbon Dioxide Cycle for Next Generation Nuclear Reactors,” Ph.D. Thesis, Massachusetts Institute of Technology, Cambridge, MA.

Dyreby, J. J., 2014, “Modeling the Supercritical Carbon Dioxide Brayton Cycle with Recompression,” Ph.D. Thesis, University of Wisconsin-Madison, Madison, WI.

Dyreby, J. J., Klein, S. A., Nellis, G. F., and Reindl, D. T., 2011, “Modeling Off-Design Operation of a Supercritical Carbon Dioxide Brayton Cycle,” Proceedings of the Supercritical CO2 Power Cycle Symposium, Boulder, CO.

Dyreby, J. J., Klein, S. A., Nellis, G. F., and Reindl, D. T., 2012, “Development of Advanced Off-Design Models for Supercritical Carbon Dioxide Power Cycles,” Proceedings of ICAPP 2012, No. 12335, Chicago, IL.

Dyreby, J. J., Klein, S. A., Nellis, G. F., and Reindl, D. T., 2014, “Design Considerations for Supercritical Carbon Dioxide Brayton Cycles with Recompression,” *Journal of Engineering for Gas Turbines and Power*, Vol. 136, No. 10, pp. 101701.

Lemmon, E. W., Huber, M.L., & McLinden, M.O., 2014, NIST Standard Reference Database 23: Reference Fluid Thermodynamic and Transport Properties-REFPROP, http://www.nist.gov/srd/nist23.cfm.

Moisseytsev, A. and Sienicki, J. J., 2009, “Investigation of alternative layouts for the supercritical carbon dioxide Brayton cycle for a sodium-cooled fast reactor,” *Nuclear Engineering and Design*, Vol. 239, No. 7, pp. 1362-1371.

Northland Numerics, 2014, access online: http://www.northlandnumerics.com.

Rowan, T., 1990, "Functional Stability Analysis of Numerical Algorithms", Ph.D. Thesis, Department of Computer Sciences, University of Texas at Austin, Austin, TX.

ACKNOWLEDGEMENTS

Initial development of the modeling framework presented in this work was supported by the National Renewable Energy Laboratory under contract number AXL-0-40301-1.