Economic Optimization of an Integrated Regenerative Transcritical Cycle with a Small Modular Reactor

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1 Introduction

- High-level motivation
  - Energy demand is constantly increasing, especially from "green" sources
  - Nuclear energy has traditionally been expensive
  - SMRs are an emergent technology which may help reduce LCOE
- Literature for economic optimization of an integrated cycle design?
- Directly-relevant literature
  - Yili's paper for integrated cycle model, component models, etc.
  - ???
- Preview of the rest of the paper
  - New pump/regenerator solver
  - Structure of integrated cycle solver
  - Optimization results
  - Validity boundary and sensitivity analysis

2 Modeling of the Integrated Cycles

- Details of each of the components' models (pump, turbine, splitter/joiner valves, regenerator)
- Explanation of new pump/regenerator solver (FIG: flow chart of solver?)

2.1 Design Space

The design of the secondary cycle is defined by seven parameters: the maximum cycle pressure (P_{max}); the pressure ratios of the high-, mid-hi-, and mid-low-pressure turbines (R_1, R_2, R_3 respectively); and the splitter valve fractions (f_1, f_2, f_3). P_{max} is allowed to vary between 8.22 and 9.2 MPa. Note that the critical pressure of methanol is 8.21 MPa. The pressure ratios and splitter valve fractions can vary between 0 and 1. The minimum and maximum cycle temperatures are fixed at 35°C and 301°C, respectively.

2.1.1 Turbines

The turbines are modeled with the Baumann model,

$$\dot{W}_t = \eta_a \dot{m}_C (h_{in} - h_{isen,out}) \tag{1}$$

$$\eta_a = \eta_t (1 - a(1 - x_a)) \tag{2}$$

$$x_a = \frac{x_{in} + x_{isen,out}}{2}, \tag{3}$$

in order to allow for wet expansion, with Baumann factor $a = 0.72$. The turbine efficiency is assumed to be $\eta_t = 0.85$. This turbine model allows states 2-8 to be solved.

2.1.2 Pumps

The pumps operate with an assumed efficiency of $\eta_p = 0.75$. The pumps are modeled according to

$$\dot{W}_p = \frac{\dot{m}_C(h_{in} - hisen, out}{\eta_p}. \tag{4}$$

It is essential for pump operation for the fluid in the pump to be a liquid. For this reason, the fluid entering the pump is desired to be subcooled by at least 1°C, though any solution which had no vapor in the fluid at the pump inlet is accepted. Any design which would require the fluid at the pump inlet to have any vapor is not considered a valid design.

2.1.3 Regenerators

The regenerators are modeled as counterflow heat exchangers. By conservation of energy and assuming all heat lost from the hot fluid is transferred to the cold fluid,

$$\dot{m}_h(h_{h,in} - h_{h,out}) = \dot{m}_c(h_{c,out} - h_{c,in}).$$

2.1.4 Splitting & Mixing Valves

Splitting valves divert a portion of the flow exiting a turbine to the regenerator and the remaining fluid to the next turbine. The mass fractions, which are among the specified design parameters, are defined to be the portion of the mass flow that is directed to the regenerator, so

$$f = \frac{\dot{m}_H}{\dot{m}}.$$

The enthalpy in both exit streams is equal to that entering the splitting valve:

$$h_{in} = h_{out,1} = h_{out,2}.$$

Mixing valves combine the fluid exiting the hot side of a regenerator with that exiting the cold side of the upstream regenerator. By way of a simple energy balance,

$$h_{out} = \frac{\dot{m}_{in,1}h_{in,1} + \dot{m}_{in,2}h_{in,2}}{\dot{m}_{in,1} + \dot{m}_{in,2}}.$$

2.2 Pump/Regenerator Solver

When solving the states around a pump and regenerator (i.e. states 18-23 for the high pressure pump and regenerator), it is desirable to make the regenerator the smallest possible while still cooling the fluid on the hot side of the regenerator enough that the fluid at the pump inlet is subcooled. To this end, we attempt to specify the state at the pump inlet to be subcooled by 1°C. In other words,

$$T_{pump,des} = T_f - 1°\text{C}.$$

However, this desired state is not always possible. The maximum enthalpy that the fluid can have at the pump inlet is

$$h_{pump,max} = \frac{h_{H,i}\dot{m}_H + h_u\dot{m}_u}{\dot{m}_H + \dot{m}_u},$$

which corresponds to there being no regenerator. The minimum possible enthalpy at the pump inlet is more difficult to quantify. This is approximated by assuming the fluid on the hot side must condense and that the pinch point in the regenerator falls at neither the inlet nor the outlet, but where the hot side fluid enters the two-phase region. It then follows that the

$$h_{pump,min} = h_{s,out} + \eta_p\left[h_{C,pinch} - \left(1 - \frac{\dot{m}_H}{\dot{m}_C}\right)h_u - \frac{\dot{m}_H}{\dot{m}_C}\right],$$

where $h_{s,out}$ is the enthalpy at the outlet of the pump if the inlet state is the desired pump inlet state and if the pump were isentropic.

The pump inlet state has a valid solution if $h_{pump,des} \geq \min(h_{pump,min}, h_{pump,max})$, since it is not guaranteed that $h_{pump,max} > h_{pump,min}$. Then, if the desired state is valid,

$$h_{pump} = \min(h_{pump,des}, h_{pump,max}).$$

The remaining states in the pump/regenerator section can all be solved directly if h_{pump} is known. If the pump inlet state has no solutions in which the pump inlet state is not subcooled, the potential design point is rejected.

3 Simulation Results and Optimization

- View of all data generated; global convergence rate
- Optimization methods applied
- Results of random search and optimization routines: design points and corresponding outputs; mention runtimes?
- TODO: What exactly is the baseline in the code?
- Global and local (near optimum) sensitivity
  - Correlations between inputs and outputs (i.e. correlation coefficients)
  - Distribution of LCOE and ETA in optimal region (FIG: histograms)
- Analytical validity boundary, valid in small region near optimum (FIG: 3D scatter w/ dividing surface)

This optimization problem is treated as an optimization with hidden constraints because the validity of the cycle is not easily determined from the design parameters. Fortunately, by far the most common reason for a design point to be invalid is due to requiring vapor in a pump in the secondary cycle, and the secondary cycle solution is decoupled from the much more computationally-expensive iterative integrated cycle model solution, so checking the validity of a design point is inexpensive relative to determining the full solution.

This allows us to first perform a random search by uniform random sampling of the full design space. During this random search, it was seen that only a small portion of the design space contains valid designs, with 2.56% of over one million sampled points being valid designs. The Differential Evolution and Dual Annealing algorithms implemented in `scipy.optimize` were also applied to this problem [?]. These were chosen due being bounded, global optimization methods whose stochasticity can be tuned to ensure adequate exploration of the design space.

3.1 Comparison of Designs from Different Algorithms

The design points obtained from the random search, differential evolution, and dual annealing algorithms are summarized in Table 1. All of the optimal design points fall roughly in the same region of the design space, varying most significantly in the R_2 and R_3 parameters. However, analysis has shown that LCOE is least sensitive to the choice of these parameters. The similarity of the design points is reassuring and suggests that these points may lie near the true global minimum. Since the Differential Evolution point had the best LCOE, this point has been used for more detailed analysis.

3.2 Characteristics of the Optimal Region

- Sensitivity of LCOE and eta to each design variable in the region
- Sensitivity to combinations of parameters (i.e. actual pressures, mass flow rates, comparative mass flow rates, etc)?

Table 1: Output optimal design points from three global optimization algorithms.

	Random Search	Differential Evolution	Dual Annealing
P_{max} (MPa)	8.320	8.225	8.220
R_1	0.0616	0.1335	0.2052
R_2	0.4720	0.2955	0.1920
R_3	0.6441	0.3060	0.1685
f_1	3.023×10^{-3}	0.9791×10^{-3}	0.1787×10^{-3}
f_2	2.397×10^{-3}	1.462×10^{-3}	0.1380×10^{-3}
f_3	50.46×10^{-3}	59.81×10^{-3}	32.65×10^{-3}
η_I	0.2924	0.2931	0.2884
LCOE ($/MWh)	78.69	77.20	77.25

- Good performance of differential evolution even when zooming in.

To further characterize the near-optimal region, design points ($N = 116882$) were randomly sampled from a small region around the differential evolution point (+/- 0.05 for each design parameter). A scatterplot of the LCOE and first law efficiency of the valid design points is found in Figure **??**.

3.3 Validity Boundary Near Optimum

The relevant constraints near this optimum are characterized near the optimal design point by sampling points from a small region around it (optimal design point +/- 0.05 for each parameter). For the design point identified by the differential evolution algorithm, the only model constraint causing potential design points to be invalid is the mid-low pressure pump state vapor constraint. An analytic expression for this validity boundary can be derived from the pump/regenerator solver model (see Section 2.2). Here, this expression is given as an inequality for values of mass fraction f_3 which will produce valid design points, given defined pressures:

$$f_3 \leq \frac{(h_{s,out} - h_{pump,des}) + \eta_p\,(h_u - h_{C,pinch})}{\eta_p\,(h_u - h_{H,sat.vap.})},$$

where $h_{s,out}$ is the isentropic pump exit enthalpy for $h_{pump,des}$ as the pump inlet enthalpy, h_u is the enthalpy of the fluid coming from the low-pressure pump/regenerator, $h_{g,H}$ is the saturated vapor enthalpy at the hot-side pressure, and $h_{C,pinch}$ is the enthalpy at $(P = P_C, T = T_{H,sat})$, The enthalpies in this inequality are uniquely defined for pressures $P_C = P_{max}R_1R_2$ and $P_H = P_{max}R_1R_2R_3$. It is important to note that this inequality only holds in a small region around the identified optimal design.

Plotting this inequality as a function of these pressures in Fig. 1, it can be observed that the resulting surface demarks the validity boundary in this near-optimal region. Also note that the surface is much more sensitive to P_H than P_C. Therefore, careful control of P_{max} and the three design pressure ratios is essential in this region of the design space to avoid vapor in the mid-low pressure pump in off-design operation, as variations in these values could result in a sufficiently large change to P_{low}, resulting in some vapor at the pump inlet.

4 Conclusion

- Big improvements to LCOE are possible when optimizing for this. Limited by accuracy of cost models.
- Reiterate amount LCOE is improved by
- Analysis of region near optimum showed sensitivity to the various design parameters
- Presented an analytical function defining where vapor will start to appear in the pump
- Next steps: experimental validation focusing on use of methanol as the working fluid (see correlations used for methanol, especially in primary heat exchanger code)

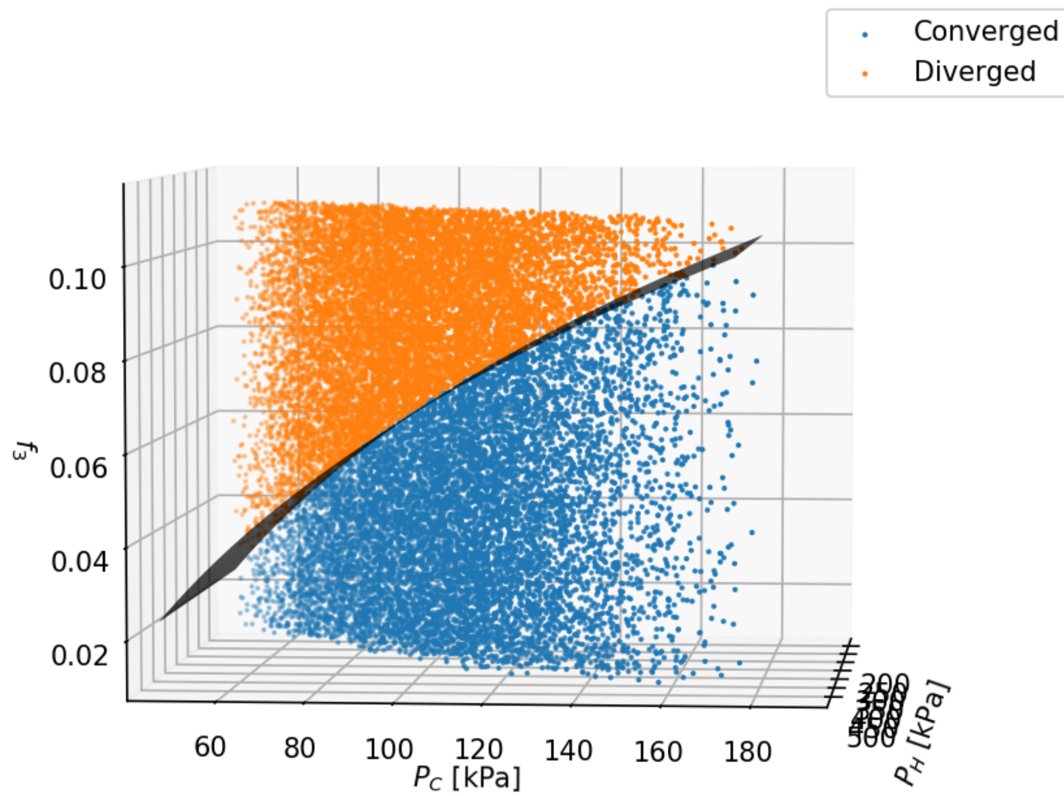

Figure 1: Validity surface in the region of the identified optimum design point.