Equation-Oriented Modeling of a Second-Generation Post-Combustion Carbon Capture Process in the IDAES Platform for Economic Optimization

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Abstract

A second-generation post-combustion capture process was modeled in the Institute for the Design of Advanced Energy Systems (IDAES) platform to be used for optimization, aiming to improve its economics and to aid its commercial deployment. This equation-oriented model enabled us to find the cost optimal design and operating conditions for varying plant capacities and capture rates. While transitioning this nonlinear model into the IDAES standard can cause some problems with model initialization and scaling, following these modeling principles ultimately led to an interpretable model, with unit models that are compatible with other models in the IDAES library.

**Keywords**: post-combustion carbon capture, equation-oriented modeling, nonlinear programming.

* 1. Introduction

Amine scrubbing is a well-established and efficient technology for post-combustion capture (PCC) that can be used to reduce the CO2 emissions at point sources in the industry. Despite, the research effort aiming to decrease the energy required for capture using new amine solvents and process modifications, one prominent example being the novel Piperazine/Advanced Flash Stripper (PZ/AFS) process (Rochelle et al., 2019), commercial deployment of PCC processes remain limited due to high costs. Therefore, these processes can benefit from process optimization to improve their economic viability, which requires a mathematical model of the process. The Institute for the Design of Advanced Energy Systems (IDAES) platform is a powerful tool to model these kinds of novel processes, which combines a model library with a framework that can handle a variety of optimization problems, such as but not limited to, large scale steady-state and dynamic optimization (Lee et al., 2021). Its core modeling framework leverages Pyomo, an open-source, algebraic modeling language, written in Python (Hart et al., 2011).

* 1. Modeling in IDAES

In Akkor et al. (2024), we have presented a validated, rigorous, equation-oriented model of the PZ/AFS process that was originally built in Pyomo. In this work, we discuss our experience with transitioning it to an IDAES model. The main units in the model are the absorber and stripper columns, which were modeled in a rate-based fashion, and then discretized using a finite difference method. The non-linear programming (NLP) flowsheet model also includes a heat exchanger network in split flow configuration with two bypasses and a recycle between the columns, resulting in over 8600 variables and constraints, for which we also developed a custom cascade initialization scheme. When transitioning the model for the IDAES platform, a custom packed column model was built to be used for the absorber and stripper columns. Custom property packages were built for the liquid and gas phases containing as components CO2, H2O and PZ, as well as N2 for the absorber side gas phase. These were contributed to the model library in IDAES.

Even though the modeling framework in IDAES leverages Pyomo’s capabilities, there are some important differences. The IDAES platform encourages better modeling practices for easier interpretability and reusability of unit models. Furthermore, using this platform has the advantage of gaining access to a comprehensive unit library, where each unit is implemented in a way that makes it compatible to be connected with other units, and to a variety of model diagnostic tools. However, this strict structure can cause problems when transitioning a model to this platform. Since a nonlinear model’s convergence is strongly dependent on its initialization, slight changes in the cascade structure while transitioning the model to the IDAES standard, can lead to different results. For instance, in the IDAES platform, the packed column was built as a custom unit model class, which should have its own initialization method. The AFS structure uses this column class and connects it to a flash tank model. The AFS model is therefore initialized on its own first for a chosen set of inlet conditions and only then is connected to the absorber. So, in our implementation, we had to ensure that the column initialization is robust enough on its own to work with other solvent amounts and concentrations after it is initialized. Moreover, in an IDAES model, there should be a complete separation between the unit model and the properties. This separation and the proposed unit model class structure is important so that the unit models are not system specific, however, it does cause some restrictions for the initialization of the model. To avoid introducing variables and constraints related to properties that are not needed in a specific step of the initialization scheme, we used the built-on-demand feature for the property models and disabled/activated the equations referencing said variables within the unit model. A second challenge is with the scaling of the model, which is another important factor for the convergence of an NLP model. The IDAES standard strongly encourages using a base set of units for the properties to ensure unit consistency between models. If the unit selected for a property in the original model was not from this set, then any constraint referencing this variable will have a different scaling in the new implementation. Therefore, manual effort is needed on the user’s end to ensure the scaling is the same.

After its transitioning to the IDAES standard was complete, our model was used for optimization to determine the cost optimal design and operating conditions. At the pilot scale, compared to the simulation with nominal design and conditions, it was seen that about 24% yearly savings can be achieved with process optimization. To test the robustness of the model and to investigate commercially-relevant PCC, optimization was performed also for a variety of different plant capacities, capture targets and with two different flue gas sources, namely coal-fired and natural gas combined cycle (NGCC) flue gases, which have different CO2 concentrations. Furthermore, whenever the column dimensions were too large to be constructed, two parallel trains—each processing half the flue gas—were evaluated as an alternative. Moreover, with the parallel train configuration, we were able to keep the absorber diameter below the practical limit of 20 meters, with only a slight increase in costs. Finally, it was confirmed that the cost increase between 95% and 99% capture targets was much more significant than the increase between 90% and 95%, as expected when targeting very high capture processes.

* 1. Conclusions

We built a validated, rate-based, equation-oriented model of a second-generation PCC process. This model was implemented following the IDAES standard to be made open-source, and the custom column model and the property models created were contributed to the IDAES unit library. The model’s simulation and optimization capabilities were used for finding the cost optimal design and operating conditions for different plant capacities and flue gas concentrations as well as to get insights on the process design. With the initialization scheme that we developed, we were able to demonstrate the robust convergence of our model under a wide range of different conditions, proving that rigorous modeling and optimization of PCC processes can indeed improve their economics and help their commercialization. This open-source model of the PZ/AFS process can now be used for simulation with different equipment dimensions and operating conditions, for other types of optimization problems or sensitivity analyses.

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