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A comparative study between GDP and NLP formulations for conceptual design of distillation columns

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Abstract

In this work, a rigorous tray-by-tray distillation column model is presented based on a new open-source modeling framework built on Pyomo that is designed to specifically support optimization of steady state and dynamic processes. The modeling framework allows for process synthesis and design of conventional tray columns either as an NLP or as a GDP problem. The model was used to simulate a distillation column for a binary mixture using three different property packages (Ideal, NRTL and Peng-Robinson), and the results are compared to results from existing commercial tools. Furthermore, a comparative case study is presented for an optimal column design problem using both frameworks.

Keywords: conceptual design, optimization, modelling framework, distillation

1. Introduction

In the past two decades, the advent of inexpensive computing power and improved numerical algorithms has enabled the increased use of equation oriented (EO) process models in process systems engineering. Though the current commercial equation oriented simulators can be used to model complex unit operations, the platforms do not provide the flexibility required for solving large-scale conceptual design optimization problems. Typically, such design problems are either solved with simplifying assumptions that lead to sub-optimal solutions or with rigorous models that are developed from the ground up, which is both time and labor intensive. The optimal design of a distillation column is an open and extensively researched problem in conceptual design owing to its importance in the process industries. Optimization problems concerning distillation columns can be broadly classified into two categories: (i) minimizing the operating cost subject to purity constraints for a fixed column design and (ii) minimizing the capital and operating cost subject to purity constraints. The former is relatively easy to solve with existing commercial simulation tools, but the latter commonly requires workarounds to overcome challenges such as limited compatibility for deterministic optimization and the lack of initialization routines with existing tools. This is computationally difficult for two reasons: (1) the presence of discrete decision variables for the number of trays and the feed tray location and (2) the non-linearity of the problem when using rigorous models.

Both a Generalized Disjunctive Programming (GDP) and NLP formulations have been proposed to model the discrete decision variables in this problem. The GDP approach may be solved with a logic-based outer-approximation (LOA) algorithm, where the trays are activated/deactivated using Boolean variables (Yeomans and Grossmann, 2000). In the NLP approach, integer variables are avoided and trays are deactivated using bypass streams (Dowling and Biegler, 2015). The GDP approach simplifies the problem by eliminating the equations associated with deactivated trays. However, the solution to the GDP problem may require several major iterations (Barttfeld et al., 2004).

On the other hand, the NLP approach avoids the combinatorial problem associated with binary variables, but requires solving a larger NLP problem. In general, both approaches provide robust methods that can be solved with existing solvers; however, (i) a comparative study between the two methods is lacking (Dowling and Biegler, 2015) and (ii) distillation models available in existing commercial simulation tools are not compatible with either approach. The objective of the study is to present a comparison of the methodologies, which have been implemented within the IDAES conceptual design framework. A rigorous tray-by-tray unit model that has been developed to optimize the size, feed tray location and operating conditions of the distillation column is also be presented.

2. Unit Operations Modelling and Optimization – the IDAES approach

The goal of the Institute for the Design of Advanced Energy Systems (IDAES), a U.S. Department of Energy initiative, is to build an open-source, next generation process systems engineering framework that will help accelerate the development of advanced energy systems. The IDAES modeling framework is based on Pyomo (Hart et al. 2017) – a Python-based algebraic modeling language that leverages the capabilities of a high level programming language to support optimization. One of the major objectives of the IDAES framework is to simplify the formulation and solution of conceptual design problems encountered in process systems engineering, thus addressing limitations with existing commercial tools. To this end, the models that are developed within this framework will be specifically designed for optimization of steady state and dynamic processes.

3. Distillation Tray Column Model

The unit model for the conventional tray-by-tray column in IDAES consists of the standard MESH equations for a distillation column. The model can be used to simulate a tray column with or without a condenser (total or partial) and a reboiler. The trays are numbered from top to bottom where the condenser and reboiler are not included as trays i.e. a distillation column with ten trays has ten trays plus a condenser and reboiler. For every tray there is an option for a feed inlet, outlet side draws for the liquid and vapor streams and heat addition/removal. The IDAES PSE framework is modular such that the user has flexibility to add or remove objects. For example, the property methods are instantiated as separate objects at the flowsheet level keeping them independent of the unit models. This provides the flexibility to easily change property calculations without making any changes to the model equations. At every tray, there is a property block for the feed stream, a property block for the mixer outlet and a property block for the equilibrium separator. The property blocks contain the equations (or constraints) for a flash calculation and also to compute properties like the specific enthalpy, vapor pressure and equilibrium coefficient as a function of the local state variables.

A major limitation for distillation column models that employ the MESH equations is the lack of consistent and robust initialization schemes. The IDAES framework ensures that sufficient flexibility is available to simplify the initialization procedure. For the column model in IDAES, the following three methods have been built to initialize the column:

- **Method 1:** The trays are initialized one by one starting from the top tray.
- **Method 2:** All trays are initialized together by sequentially activating and solving the mass, pressure, and energy balances.
- **Method 3:** Similar to method 1 but the feed stage is solved first followed by the rectification section and then the stripping section.

4. Optimization Framework for Distillation Columns in IDAES

4.1 NLP framework

Figure 1: NLP framework with bypass streams

The NLP framework that has been implemented for solving conceptual design problems concerning distillation columns in IDAES is based on Dowling and Biegler (2015). The formulation allows trays to be bypassed using bypass variables ($x_{i,bypass}$) as shown in Figure 1. Typically, these variables should be binary where 1 denotes active and 0 denotes inactive trays. However, in the NLP formulation these variables are continuous variables bounded between 0 and 1, i.e., a relaxed MINLP problem. The general consensus while using bypass variables in distillation columns is to split the tray outlet streams (liquid/vapor) to two streams: a bypassed stream and a stream input to the tray above or below. While this formulation allows trays to be bypassed, using a conventional splitter results in a zero flow if the tray is bypassed, which will affect convergence of the flash calculations on the tray. Instead, this framework duplicates the bypass stream and employs a mixer for the vapor and liquid outlets such that zero flows are avoided through bypassed trays. The mass/energy balances for these mixers are shown in Figure 1. When a tray is bypassed, the bypass variable $x_{i,bypass}$ should be 0. Then from the mass and energy balances for the mixer, it can be observed that the inputs to next tray (above/below) are appropriately accounted for depending on whether the tray is active or inactive. Furthermore, engineering knowledge tells us that partial bypass will be avoided as it is inefficient to mix an impure stream with a pure stream. Another feature with this framework is that it indirectly, concurrently optimizes for the optimal feed tray location. Although the feed tray is fixed, the bypass variables are restricted to trays in the stripping and rectification sections. Thus, the feed tray location is determined depending upon the number of trays eliminated in each section.

4.2 GDP framework

The GDP framework for conceptual design of distillation columns is based upon the formulation given in Barttfeld et al. (2003). Disjunctions at each candidate tray describe the presence or absence of the tray. The general form of the disjunctions is given in Equation 1.

$$\begin{bmatrix} Y_t \\ g_1(x) \leq 0 \end{bmatrix} \vee \begin{bmatrix} \neg Y_t \\ Ax \leq b \end{bmatrix} \quad (1)$$

Y_t is the Boolean variable associated with tray existence. Constraints denoted by g_1 contain the MESH equations for each stage. When the tray does not exist, linear bypass constraints $Ax \leq b$ ensure that flowrates and enthalpies are transmitted unchanged to the next stage. An analogous disjunction governs selection of the feed tray: a tray either is the feed stage and has the relevant inlet material and energy flows OR it is not and the flows are set to zero. A logical proposition enforces that if a tray is selected as the feed, then it implies that the tray is also active. The first and final stages correspond to the condenser and reboiler; the Boolean existence variables associated with these trays are fixed to True. The GDP model was initialized using the column profile results from a 10-stage square problem; to accommodate additional conditional trays, a linear interpolation of the profile was used.

5. Results and Discussion

The IDAES tray-by-tray column model was used to simulate a distillation column with ten trays (+ condenser + reboiler) to separate an equimolar mixture of benzene and toluene using three different property methods: Ideal, Ideal-NRTL and the Peng-Robinson cubic equation of state. The feed specifications are as follows: Feed = 100 mol/s, T_{feed} = 368 K, P_{feed} = 101 kPa, feed tray = 5. The molar reflux and reboil ratio were set to 1.4 and 1.3 respectively. The results were compared to a “RadFrac” model in Aspen Plus and are presented in Table 1. The results using the EO IDAES model show an excellent match with Aspen Plus models solved sequentially. The model was successfully initialized using “Method 2” for all the three simulations and demonstrates robustness even when using a rigorous property method like the cubic equation of state.

Table 1: Comparison of model predictions using IDAES and Aspen Plus models

Variable	Ideal		Ideal – NRTL		Peng-Robinson	
	IDAES	Aspen	IDAES	Aspen	IDAES	Aspen
Distillate (mols/)	47.76	47.71	47.94	47.82	45.31	45.33
$x_{D,benzene}$	0.886	0.887	0.885	0.887	0.900	0.900
$x_{D,toluene}$	0.114	0.113	0.115	0.113	0.100	0.100
Bottoms (mol/s)	52.24	52.29	52.06	52.18	54.69	54.67
$x_{B,benzene}$	0.147	0.147	0.145	0.145	0.168	0.168
$x_{B,toluene}$	0.853	0.853	0.855	0.855	0.832	0.832
$Q_{condenser}$ (kW)	-3626.4	-3594.5	-3639.9	-3591	-3375.2	-3378.7
$Q_{reboiler}$ (kW)	2307.9	2272.2	2300.6	2245.7	2366.8	2366.4

5.1 Optimal design problem

The problem for the optimal design of a distillation column has been formulated as follows:

$$\min_{RF,RB,\, feed\ tray, N_{trays}} \quad 10^3 \left(\sum_{i=1}^{N_{trays}} x_{bypass,i}\right) + (Q_R + Q_C)$$

s.t.: $x_{D,benzene} \geq 0.95$; $x_{B,toluene} \geq 0.95$; $RF \leq 4$; $RB \leq 4$ (2)

The objective function minimizes a capital cost (number of active trays) and an operating cost (reboiler and condenser duty). The number of active trays is multiplied by a cost coefficient of 1000 to scale it to the same range as that of the condenser and reboiler duties to ensure equal weights to the capital and operating cost in the objective function. The feed conditions are the same as that used for simulation studies outlined in Table 1 (Ideal case). For the NLP framework, the model was initialized with 35 active trays (feed tray = 10) and initial values for the decision variables were unchanged from the simulation case study. The solver used was IPOPT with MA 27 as the linear solver. The optimal solution using the NLP framework is outlined in Table 2 and it can be seen that the total number of trays is an integer value (11 in this case) even though the bypass variables were declared as continuous variables. Also, the optimal feed location is tray 6. The same aforementioned solution was obtained when the model was initialized with 15/20/50/60 active trays or when the feed location was changed to 10/15/25/30 in the superstructure respectively. The GDP model was solved using the GDPopt solver in Pyomo, which implements LOA and uses both Gurobi and IPOPT as sub-solvers. Even though the formulation with the bypass framework consists of a larger NLP model, it required 597 function evaluations to determine the optimal solution. In comparison, the GDPopt terminated after 20 master iterations requiring 2057 NLP function evaluations in total mainly due to weak linear approximations. However, this can be avoided with better reformulation techniques. Table 2: Optimal solutions from NLP and GDP frameworks

Optimal solution	**NLP framework**	**GDP framework**
Objective	19430	19450
No. of trays	11	10
Feed tray	6	5
Reflux ratio	2.07	2.45
Reboil ratio	2.13	2.39

$x_{D,benzene}/ x_{B,toluene}$	0.95/0.95	0.95/0.95

Both the NLP and GDP frameworks yield similar solutions. The NLP framework solution includes one extra tray to reduce column duties, making a slightly different capital vs. operating cost trade-off compared to the GDP framework.

6. Conclusions

This work presents a tray-by-tray distillation column model using MESH equations within the IDAES modeling framework that is suitable for both simulation and deterministic optimization studies. For solving the conceptual design problem for distillation columns, both NLP and GDP frameworks are available and a comparative case study is presented in this work. In the case study considered here, while the NLP and GDP frameworks yield similar solutions, the NLP framework using bypass streams requires fewer nonlinear function evaluations when compared to the GDP solution but a robust initialization scheme was necessary. On the other hand, the main limitation of the GDP framework in this case study was the quality of the linear approximation, leading to slower convergence. This may be addressed by adding support for stronger GDP to MILP reformulation techniques in GDPopt, improving the bounds via automatic bound-strengthening tools, and adding logical propositions to screen out structurally redundant configurations. At the same time, the impact of the reduced space sub-problems in LOA can be seen, as only a few function evaluations are required for each subproblem, even without a complex initialization scheme. A thorough comparison between the two frameworks will be considered in the future especially with more rigorous property models like the cubic equation of state.

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