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Abstract

We present a novel steady-state model for distillation columns that allows simulation of dry and vaporless stages, a task that cannot be achieved with commercial software such as ASPEN Plus. The model employs the outer loop structure of the standard inside-out algorithm, which allows for reliable and low-cost convergence under non-ideal thermodynamics, and introduces a modified nonsmooth inner loop that can be solved using automatically-computed generalized derivative elements and direct equation-solving methods. The resulting nonsmooth inside-out model automatically resets one of the column specifications if necessary, to always provide a valid physical solution of the MESH equations even under poorly-chosen inputs. A binary distillation case study from the literature is presented to demonstrate the robustness of the algorithm to specifications that lead to liquid and vapor phase disappearance or that are infeasible.

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Distillation Simulation Robust to Liquid and Vapor Phase Disappearance

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Abstract

We present a novel steady-state model for distillation columns that allows simulation of dry and vaporless stages, a task that cannot be achieved with commercial software such as ASPEN Plus. The model employs the outer loop structure of the standard inside-out algorithm, which allows for reliable and low-cost convergence under non-ideal thermodynamics, and introduces a modified nonsmooth inner loop that can be solved using automatically-computed generalized derivative elements and direct equation-solving methods. The resulting nonsmooth inside-out model automatically resets one of the column specifications if necessary, to always provide a valid physical solution of the MESH equations even under poorly-chosen inputs. A binary distillation case study from the literature is presented to demonstrate the robustness of the algorithm to specifications that lead to liquid and vapor phase disappearance or that are infeasible.

Keywords: distillation simulation, dry and vaporless stages, inside-out algorithm, nonsmooth models.

1. Introduction

Engineering software such as ASPEN Plus and HYSYS have well-known convergence problems caused by distillation column stages becoming dry or vaporless, which not only impact standard process simulation but further preclude the convergence of flowsheets with recycle and of process optimization algorithms. For any given stage we can define 3 different phase regimes: (I) 2-phase equilibrium with vapor and liquid outlets, (II): 1-phase equilibrium, with either dew-point vapor and no liquid, or bubble-point liquid with no vapor, and (III): 1-phase non-equilibrium, with either superheated vapor and no liquid, or subcooled liquid with no vapor. The standard MESH equations do not yield a physical solution for process conditions that lead to dry/vaporless stages operating in Phase Regime III because the equilibrium and summation equations cannot be satisfied simultaneously in this case, as demonstrated by Sahlodin et al. (2016).

In order to simulate all possible regimes, we can resort to nonsmooth (i.e. non-differentiable) modeling strategies that automatically switch part of the describing equations and adapt to the regime that corresponds to process inputs, without a priori knowledge. Previous attempts at steady-state dry/vaporless distillation simulation in the literature are limited to the work of Bullard and Biegler (1993) and Gopal and Biegler (1999), which is based on a complementarity constraint formulation. These papers resort to either optimization or iterative smoothing approximations to tackle the simulation problem and report very few numerical results for dry/vaporless operation.

On the other hand, in previous work (Cavalcanti and Barton, 2018) we proposed a nonsmooth modified MESH model by replacing the summation equation with an

explicitly nonsmooth equation for each stage in terms of the mid function, which returns the median of three arguments:

$$\text{mid}\left(\frac{V_j}{F_s},\ \sum_i x_{i,j} - \sum_i y_{i,j},\ -\frac{L_j}{F_s}\right) = 0, \tag{1}$$

where V_j and L_j are the vapor and liquid outlet flow rates of stage j, $y_{i,j}$ and $x_{i,j}$ are the respective vapor and liquid mole fractions of component i, and F_S is a flow rate reference value. With the method for automatic LD-derivative evaluation of Khan and Barton (2015), generalized derivative elements for the nonsmooth MESH model can be computed reliably and used within nonsmooth equation-solving approaches, such as the semismooth Newton method (Qi and Sun, 1993), to simulate dry/vaporless columns. With detailed parametric analysis, we discovered that decreasing input parameters, such as the reflux ratio, could unexpectedly lead to a critical input value at which a continuum of infinitely many steady-state solutions exist, which range from what we call the upper critical solution (approached from above the critical value) to the lower critical solution (approached from below the critical value). This bifurcation or change in the number of solutions is associated with singular generalized derivative matrices, requiring special continuation methods for simulation at or near the critical point. Moreover, in some cases no feasible solutions exist below the critical parameter value, which then becomes a positive lower bound that cannot be predicted prior to simulation.

Another important aspect of distillation simulation is that simultaneous convergence of the MESH equations in their original or primitive form can be unreliable and highly dependent on a good initial guess, especially with complex non-ideal multicomponent systems. To overcome this problem, Boston and Sullivan (1974) introduced the inside-out method, an algorithmic strategy that creates 2 nested iterative loops to improve reliability of convergence and reduce the cost of repeated thermodynamic property evaluations. However, dry/vaporless solutions cannot be obtained and arbitrary scaling factors must be adjusted heuristically to avoid near-zero or negative flow rates. In this work, we develop a nonsmooth inside-out method that can retain the desirable convergence reliability under non-ideal thermodynamics and at the same time overcome the issues associated with liquid and vapor phase disappearance, to provide a physical solution robustly even in the face of infeasible specifications.

2. The multistage inside-out algorithm

The inside-out algorithms do not manipulate the physical or primitive variables (temperatures, flow rates, etc.) directly to converge the set of MESH equations. Instead, two nested outer and inner loops are created, each with its respective set of outer and inner iteration variables. In the outer loop, the complex thermodynamic property models for the equilibrium $K_{i,j}$ values and for the vapor and liquid phase enthalpy departures Δh_j^V and Δh_j^L are used to generate simple approximate local models:

$$\ln K_{b,j} = A_j + B_j\left(1/T_j - 1/T_j^*\right), \tag{2}$$

$$\Delta h_j^V = C_j + D_j\left(T_j - T_j^*\right), \tag{3}$$

$$\Delta h_j^L = E_j + F_j \left(T_j - T_j^* \right), \tag{4}$$

where $\ln K_{b,j} = \sum_i w_i \ln K_{i,j}$ and w_i are weighting factors, and T_j^* is a reference temperature; the parameters A_j to F_j, together with the relative volatilities $\alpha_{i,j} = K_{i,j} / K_{b,j}$, are the outer loop variables for each stage j, with $1 \le j \le N$. Unlike the primitive variables, the outer loop variables do not require precise initialization.

The inner loop employs the approximate property models to converge a rearrangement of the MESH equations. First, the mass balance, equilibrium and summation relationships are combined to create a tridiagonal linear system in terms of the component liquid flow rates $l_{i,j}$, which is solved with the Thomas algorithm. Second, the residuals of the energy balances and of column specification equations are computed and iteratively driven to near-zero values with a quasi-Newton method. The main inner loop variables are derived from the stripping factors for each stage,

$$S_j = \frac{K_{b,j} V_j}{L_j}. \tag{5}$$

From Eq. (5) it becomes evident that a dry stage ($L_j = 0$) leads to an undefined value of S_j, creating a fundamental problem with the multistage inside-out algorithm and preventing convergence to the dry MESH solutions in Phase Regime II. In order to avoid near-zero and negative flow rates, scaling factors $S_{b,j}$ are introduced and heuristically adjusted, and $\ln(S_j / S_{b,j})$ become the actual inner loop iteration variables.

The original inner loop of Boston and Sullivan (1974) relies on all product rates being specified and is amenable to direct substitution methods. This way, Broyden's method can be used with the identity as the initial Jacobian matrix and the inner loop can be converged at very low cost. However, their formulation does not allow for other specifications such as component purities and recoveries, which motivated Russell (1983) to propose a modified inside-out method that converges the set of energy balances and general specifications simultaneously. An approximation to the Jacobian matrix is computed and subsequently updated with Broyden's formula. Several other versions of the inside-out method have been proposed, such as adaptations to reactive distillation systems (Venkataraman et al., 1990); in particular, RadFrac and related models of ASPEN Plus are proprietary modifications of the Boston-Sullivan method.

3. The proposed nonsmooth inside-out algorithm

We propose two main structural modifications to the inner loop of the multistage inside-out method of Russell (1983). The end result is a nonsmooth inside-out algorithm that enforces the MESH equations at the final solution, is capable of converging to dry and vaporless solutions in Phase Regime II without running into singularities, and automatically resets input specifications that are infeasible or cannot be satisfied by the MESH equations to always yield a physical solution.

The first modification involves the specification equations, included in the set of inner loop residuals. The user chooses one of the column specifications to be flexible, say, the reflux ratio R. The standard specification equation $R - R_{spec} = 0$, which would enforce the user-specified value R_{spec}, is substituted by the nonsmooth equation

$$\min\left(R - R_{spec}, \min\left(\min_{1\le j\le N} V_j, \min_{1\le j\le N} L_j\right)\right) = 0, \tag{6}$$

which involves nested minimum operations. This ensures that specified values R_{spec} greater than the critical value R_{cr} are enforced to yield a vapor-liquid solution in Phase Regime I, but any smaller values $R_{spec} < R_{cr}$ (either infeasible or leading to a feasible solution in Phase Regime III) are overridden and the reflux ratio R is automatically set to its critical value to yield the upper critical solution in Phase Regime II.

The second alteration allows the algorithm to deal with zero and negative flow rates and to converge to dry/vaporless solutions in Phase Regime II. Instead of the stripping factors, the inner loop variables are chosen to be what we denote the vapor-ratio factors

$$\phi_j = \frac{K_{b,j} V_j}{K_{b,j} V_j + K^0_{b,j} L_J}, \tag{7}$$

where $K^0_{b,j}$ is a reference value of the same magnitude of $K_{b,j}$. The ϕ_j factors are analogous to the inner variables in the Boston and Britt (1978) single-stage flash inside-out method; they are physically bounded between 0 and 1 but remain well defined for near-zero or negative flow rates and can be manipulated directly instead of their logarithm values. Additionally, in order to maintain well-defined mole fractions for absent vapor and liquid phases, the tridiagonal linear system in the inner loop is reformulated in terms of the alternative variables $p_{i,j}$, which are direct proxies to the liquid-phase mole fractions and are related by

$$l_{i,j} = p_{i,j}(1 - \phi_j). \tag{8}$$

The resulting inner loop contains a single nonsmooth equation and preserves the original loop size. In this work, the set of energy balances and specifications are converged simultaneously with a semismooth Newton method, with exact generalized Jacobian matrices computed with the automatic LD-differentiation method of Khan and Barton (2015). The initialization procedure of Boston and Sullivan (1974) is employed and the outer loop is converged with direct substitution.

4. Case study: binary distillation

We illustrate the performance of our algorithm with a case study considered by Bullard and Biegler (1993) and Gopal and Biegler (1999). A saturated liquid stream with 70% benzene and 30% toluene (% mol) is fed to Stage 20 of a column with $N = 27$ stages, with a linear pressure profile from the total condenser (Stage 1) at 1.05 bar to the reboiler (Stage N) at 1.2 bar, and a feed-to-distillate ratio of 0.5. Here, the Peng-Robinson equation of state is used to describe the liquid and vapor phases.

Figures 1 and 2 present the results of a parametric analysis in which we vary the specified reflux ratio R_{spec} and plot the above-feed liquid flow rates L_{19} and L_8, respectively, as obtained with 4 different models: (1) ASPEN Plus' RadFrac inside-out model, (2) the standard MESH equations, solved simultaneously with Newton's method, (3) the nonsmooth MESH model represented by Eq. (1), solved simultaneously with the semismooth Newton method and continuation methods (Cavalcanti and Barton, 2018), and (4) the proposed nonsmooth inside-out model. For high values of reflux ratio, all stages operate with vapor and liquid in Phase Regime I and all models yield the same unique solution. As we decrease the reflux ratio and approach its critical value $R_{cr} \approx 0.0101$, which is not known prior to simulation, the liquid phase directly above the feed stage disappears ($L_{19} = 0$) and we obtain the upper critical solution, in which Stage 19 is the only dry stage and operates in Phase Regime II.

Model 1 fails to find any solutions for $R_{spec} \leq 0.01012$, with severe error messages stating that stages are dried up. ASPEN Plus aborts all flowsheet computations if flow rate values or ratios between vapor and liquid flow rates within the column fall below an arbitrary small positive value. Model 2 yields the upper critical solution at R_{cr}; for smaller values $R_{spec} < R_{cr}$ we obtain a unique nonphysical solution characterized by negative liquid flow rates $L_{19} < 0$. Model 3 exhibits a continuum of infinitely many physical solutions at R_{cr}, evidenced by the vertical graph segment in Figure 2. These solutions range from the upper critical solution, with only Stage 19 being dry and in Phase Regime II, to the lower critical solution, with Stages 3-19 being dry in Phase Regime III and Stage 2 dry in Phase Regime II. Model 3 has a unique physical solution for $0 \leq R_{spec} < R_{cr}$ corresponding to Stages 2-19 all dry and operating in Phase Regime III, and no solution for $R_{spec} < 0$, which reflects the actual physical behaviour of the system. On the other hand, the proposed Model 4 provides a unique physical solution for all specified values of reflux ratio, including poorly-chosen negative values, and automatically returns the upper critical solution for $R_{spec} \leq R_{cr}$. As expected, the MESH Model 2 exhibits smooth solution curves with respect to the reflux ratio, while the nonsmooth models originate graphs with kinks (Model 4) or discontinuities (Model 3) at the critical reflux value.

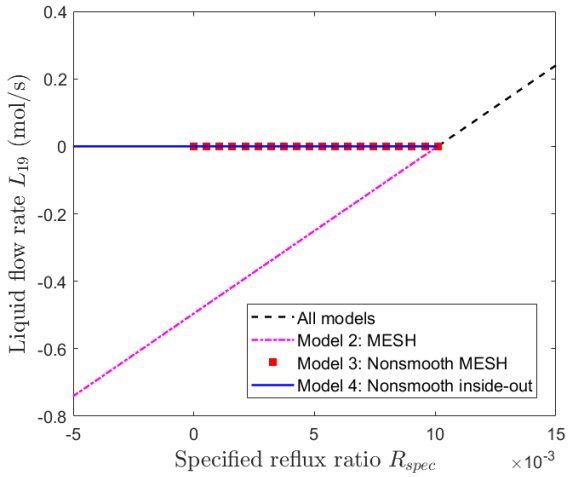

Figure 1: Liquid flow rate L_{19} versus specified reflux ratio for each of the 4 models.

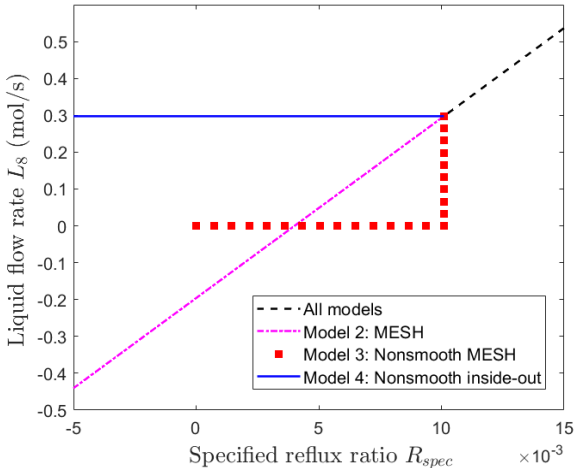

Figure 2: Liquid flow rate L_8 versus specified reflux ratio for each of the 4 models.

5. Conclusions

We have presented a novel inside-out model for steady state distillation simulation that is robust to liquid and vapor phase disappearance and to infeasible column specifications. The Russell (1983) inside-out algorithm was restructured to employ new inner loop iteration variables that allow convergence to solutions with dry and vaporless stages and do not require heuristic scaling factors. The new inner loop contains a single nonsmooth equation that automatically bounds the column to operating conditions at which the MESH equations are valid, without resorting to inequality constraints. As a result, a valid physical solution is obtained by nonsmooth equation-solving methods even if column specifications are unpredictably infeasible or poorly chosen.

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