Modified Bounded Newton Homotopy Method in Solving Sidestream Column Configurations

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Abstract

This paper illustrates through distillation examples how the bounded Newton homotopy method considerably extends the area of convergence compared with the unbounded one. Sidestream column configurations with exact mole fraction specifications are used as demonstrative test cases. Starting point multiplicity is found to be a real challenge when solving distillation problems with Newton homotopy-based solving methods. When these methods cannot approach the solution from the trivial starting point, flow ratios are used to generate a more favourable initialization.

Keywords

Bounded Newton homotopy; Continuation methods; Convergence property; Sidestream distillation columns

1. Introduction

According to the statistics gathered by Taylor [1], research work carried out lately on developing algorithms and solving methods especially in distillation seems to be fairly minor. Evidently, the reason for this scant interest is that nowadays the solving methods available in simulators are capable of solving the great majority of simulation problems. In addition, the need to develop fast algorithms has diminished with advances in computer technology. Therefore

reliability, i.e. robustness, is now the main reason for studying and developing new solving methods in chemical engineering.

This paper introduces how the bounded Newton homotopy method extends the area of convergence compared with the unbounded one. Both liquid and vapour sidestream column configurations with exact mole fraction specifications are used as test problems. Ternary and quaternary component systems consisting of both zeotropic ans azeotropic mixtures have been selected to demonstrate the performance of the methods considered.

2. Background

The manual iterative solving strategy is still widely utilized when determining the desired state distribution for distillation column configurations. In several cases flows and flow ratios are used as well-behaved manipulative variables in the determination process when some local Newton-Raphson type solving method is applied. In such cases, a desired solution sufficiently close to the pre-specified product flow purity requirements is approached using the successive solving of a column configuration model. This is done by properly modifying, step by step, the values of the selected manipulative variables. This kind of solving strategy is, however, not only laborious and time consuming, but also inaccurate.

Homotopy continuation methods (continuation, embedding or homotopy methods) may be used to extend the area of convergence. Thus, the rigorous solution for a distillation column configuration with tight and rarely used design specifications may be approached robustly without manual iteration work. But even though homotopy continuation methods have the property of global convergence, difficulties may arise if the homotopy path runs outside the problem domain. This is problematic especially in chemical engineering problem solving. If a non-acceptable variable value, e.g. a negative mole fraction or temperature, is substituted into a thermodynamical calculation routine, it may generate an error stop.

To overcome homotopy path unboundedness, Paloschi [2, 3] has proposed a class of bounded homotopy methods. These methods limit the homotopy path to ensure it stays inside the problem domain, thus preventing the appearance of non-acceptable variable values.

Malinen and Tanskanen [4] have recently presented suggestions, which increase the usefulness of the bounded homotopy methods in chemical engineering. The power of the modifications is based on the variables mapping strategy enabling the flexible tracking of the homotopy path very near the problem domain boundaries. The suggested modified bounded homotopies have been extended to apply also when large and sparse non-linear equation sets are being solved. The methods developed offer the possibility to track the homotopy path in real space and inside the strictly specified problem domain, thus providing an efficient tool to solve complex distillation column configurations robustly.

3. Convergence properties with exact mole fraction specifications

In the following some sidestream column configuration examples with exact mole fraction specifications have been considered. The three examples have been selected to illustrate the general observations made of the convergence properties of the studied Newton homotopy based solving methods.

In these cases the full set of MESH equations and nonlinear thermodynamics have been used. The thermodynamic models and parameters are based on the Wilson thermodynamic package and on the database of the commercial simulation program HYSYS. The column models and the problem-independent equation-oriented solving approaches have been implemented in the MATLAB environment. Molar flow values of 1 mol/s, reboiler and condenser duties of 20,000 Watts, reflux and reboil ratios of 1, and mole fraction and temperature values of the column feed have been used as the trivial starting point selection for the homotopy path tracking procedure, and are denoted with #1 in the text.

3.1. Convergence of the Newton homotopy method (Case 1)

The first example illustrates nicely the strong convergence property of the classical Newton homotopy method. The exact mole fraction specifications and the structure of the selected column configuration are illustrated in Fig. 1. The existence of the azeotrope and the distillation boundary (separatrix) have been noted when specifying quaternary acetone/chloroform/benzene/toluene separation.

When starting point #1 is selected, the homotopy path runs towards the solution shown in Table 1 without crossing the problem domain boundaries. If starting point #1 is slightly modified by specifying the temperature values as T=340 K, the solution is approached without crossing the domain boundaries by tracking the homotopy path first in the negative direction.
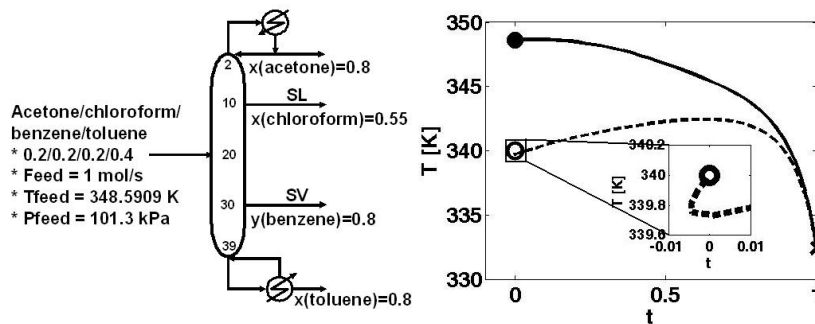

Fig. 1. On the left the column configuration studied in Case 1. On the right the Newton homotopy paths for the condenser temperature when the starting point temperature for every column stage is 348.5909 K (●) and 340 K (○). The final solution (×) is 332.4023 K.

3.2. Convergence of the modified bounded Newton homotopy method (Case 2)

The ternary acetone/benzene/toluene example illustrated in Fig. 2 demonstrates a situation where the unbounded Newton homotopy path runs partly outside the problem domain boundaries. The modified bounded Newton homotopy method restricts the homotopy path to running inside the problem domain boundaries and the solution presented in Table 1 is approached without crossing the problem domain.

The modified bounded homotopy methods enable the use of an extremely narrow bounding zone; $1 \cdot 10^{-10}$ of the problem domain width has been specified herein. This property has been found to be vital when solving chemical engineering problems.
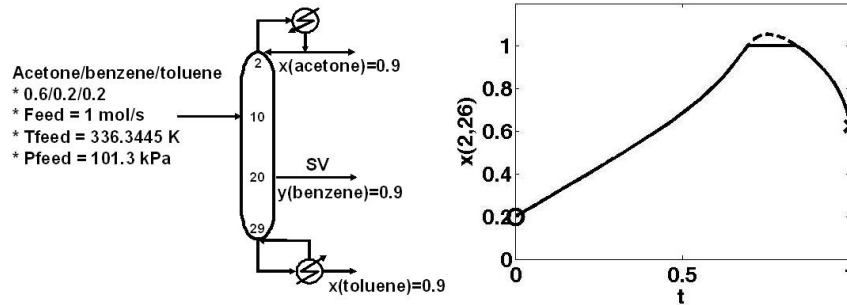

Fig. 2. On the left the column configuration studied in Case 2. On the right the unbounded (--) and bounded (—) Newton homotopy path for benzene liquid mole fraction in stage 26. The trivial starting point #1 (○) and the final solution (×).

3.3. Starting point multiplicity (Case 3)

In some situations neither the unbounded nor bounded Newton homotopy methods are able to guarantee the approached solution. The effect of the starting point selection on the convergence property may be illustrated with the ternary azeotropic acetone/chloroform/benzene example shown in Fig. 4. When the homotopy path is tracked from starting point #1, some of the variables strongly run towards infinity (or towards an unacceptable solution), and a feasible solution is not approached. Fig. 3 shows, however, that the solution shown in Table 1 may be approached from the other (multiplicity) points formed at $\theta = 0$.

This kind of starting point non-uniqueness is a universal disadvantage of the Newton homotopy method [5]. Fixed-point and scale-invariant affine homotopy methods have been proposed as alternative methods to avoid starting point multiplicity. With these methods, however, the homotopy paths may consist of branches that are only connected at infinities or by branches in the complex domain [6].

Starting point multiplicity has been found here to be one basic fundamental restriction why a converged result cannot be regularly approached for column configuration with Newton homotopy based solving methods. The convergence property may be improved significantly, however, with a more favourable starting point. For example in the case in hand, instead of the trivial starting point #1 it is useful to calculate the initial state distribution for the column system, and use that as the favourable starting point. The initial state distribution is calculated here based on the reflux and reboil ratios with a value of 0.1, and specifying the liquid sidestream flow to be as large as the molar flow down from the side draw stage.

As Fig. 4 shows, the unbounded homotopy path of the liquid sidestream flow runs partly outside the problem domain when starting from the calculated starting point. With the modified bounded Newton homotopy method the homotopy path may be kept inside the problem domain, and the final solution shown in Table 1 can be approached without crossing the problem domain.
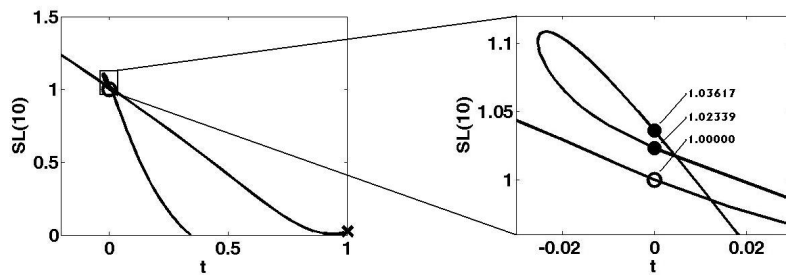

Fig. 3. Homotopy paths for the liquid sidestream flow studied in Case 3. The trivial starting point (○), the solution (×) and the starting point multiplicities (●).
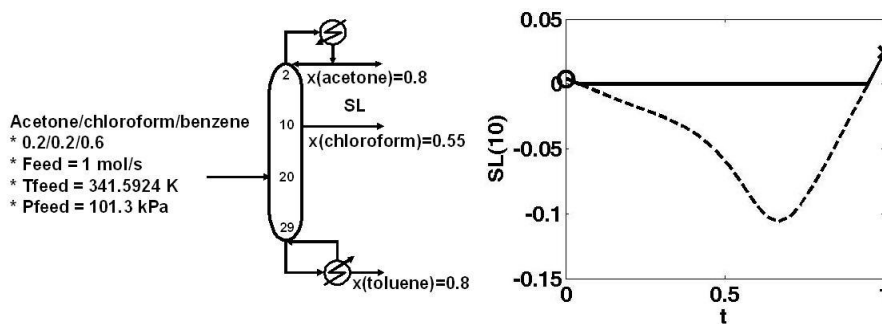

Fig. 4. On the left the column configuration studied in Case 3. On the right the unbounded (--) and bounded (—) Newton homotopy path for the liquid sidestream when a favourable starting point is used. The favourable starting point (○) and the solution (×).

Table 1. Characteristic results of the sidestream column Cases 1-3.

	Feed composition (mole fractions)	Product flow compositions: distillate sidestreams (liquid **L**, vapour **V**) bottom product	Reflux ratio Reboil ratio	Reboiler & Cond. duties (Watts)
1*	0.2/0.2/0.2/0.4	**0.8000**/0.1849/0.0151/0.0000 0.3629/**0.5500**/0.0871/0.0000 (**L**) 0.0002/0.1044/**0.8000**/0.0954 (**V**) 0.0000/0.0009/0.1991/**0.8000**	18.135 4.056	66,090 61,595
2*	0.6/0.2/0.2	**0.9000**/0.0998/0.0002 0.0145/**0.9000**/0.0855 (**V**) 0.0000/0.1000/**0.9000**	0.759 5.633	39,611 34,388
3*	0.2/0.2/0.6	**0.8000**/0.1882/0.0118 0.3883/**0.5500**/0.0617 (**L**) 0.0008/0.1922/**0.8000**	13.928 4.440	101,060 100,680

* Columns have a total condenser and partial reboiler. Pressure 101.3 kPa and saturated liquid feed.

4. Conclusions

The selected examples show that starting point multiplicity is a real challenge when solving distillation problems with Newton homotopy-based solving methods. A favourable initial state distribution based on flow relations has proved to be a good practice for improving the convergence properties of these methods.

The examples also illustrate that the suggested modified bounded Newton homotopy method considerably enhances the chances of solving non-linear equation sets by enlarging the area of convergence. This decidedly increases the robustness thus diminishing the need for manual iteration work. Although the advantages of the suggested modified bounded Newton homotopy method in solving sidestream column configurations are clear, the authors expect that the benefits are even more significant when more complex column configurations are studied.

References

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