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DYNAMIC NEGATIVE LIQUID-LIQUID FLASH

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ABSTRACT

After reviewing different previous contributions in the proposed field, a rigorous mathematical model of dynamic behaviour for batch distillation column stage with possible occurrences of several liquid phases is presented. The generalized model is based on an interesting extension of the concept of negative liquid-liquid phase to the more complicated case of dynamic application. Great care is taken in the model formulation in order to take into account the different possibilities and in order to smooth the internal and potential discontinuities involved in the system due to phase distribution uncertainty. In the proposed algorithm based on gear_s method appied to DAE systems (index 1 and index 2), discontinuities which appear in course of the calculation due to model change and phase splitting are treated by a special procedure in order to insure initial consistency, automatic initialization or re-initialization and smooth integrator behaviour.

Illustrative applications to liquid-liquid phase split and liquid-liquid- vapor phase situation on a single stage are presented and compared with previous results.

SCOPE

Batch distillation is still an interesting field of research due to the great flexibility of this system. When combined with extractive and azeotropic distillation, the process becomes even more complex.

In such a case, as observed in conventional distillation of heterogeneous azeotropic mixtures, pattern distribution could change drastically on individual tray and from tray to tray at each time sample. Namely, the liquid phase could split into two phases and not only at the

overhead. It induces that such systems are often found to behave erratically and are exceptionnally difficult to operate and to control. More as a complete campaign of a batch distillation comprises several steps (startup period, change in phase pattern,...) as well as change in control actions (heat supply, reflux ratio,..), it induces different physical and numerical discontinuities.

That the reason why it appears extremely important to perfectly detect phase splitting and to model the resulting system. Also, this contribution is much more devoted to the development of a generalized rigorous dynamic model for a generic single stage which should be used as basic block for extractive batch distillation column.

This model should be able to smoothly handle a whole batch campaign and allows phase pattern change on each stage. For this objective, dynamic models for column stage, reboiler and a combined condenser-decanter system are developed and presented in detail with respect to the different phase situation which may occurred. It is based on an extension and adaptation to dynamic context of the so -called negative flash calculation. Discussion is done on the opportunity to use this concept presented by Michelsen for steady-state calculations and its potentialities to the present goal are enlighted. It results in an unique and uniform formulation able to simulate in the same row the behaviour of multiple liquid phase systems, i.e single liquid phase, or liquid-vapor/ liquid-liquid phase, or liquid-liquid-vapor phase.

Then, paper is devoted to the presentation of the algorithm used to solve the resulting set (s) of Differential-Algebraic systems by a global simultaneous approach. The proposed one is based on an efficient implementation of Gear's method applied to solve up to index two systems. It deals with time and state event detection and discontinuity management occurring due to model change. The proper detection and treatment of such discontinuities are well described from a physical and numerical point of view. Reliability and accuracy of such features are very important in order to insure the smooth behaviour of the integrator and in order to insure the system to change adaptively during the course of the integration.

Finally, some applications are given in order to illustrate the system capabilities, in particular some results presented by Eckert (1984) are compared with our approach.

CONCLUSIONS AND SIGNIFICANCE

This contribution is an interesting and successful attempt to the use of dynamic negative liqui-liquid flash calculation in view to solve the very complex problem of phase distribution changes which may occurred in the more general context of azeotropic and extractive batch (or continuous) distillation. Development of the proposed methodology are applied to the case of a generic generalized model for an individual stage and further work are currently performed to the case of the dynamic simulation of heteregeneous azeotropic distillation columns as well as to perform the real start-up of such complex columns.