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Rate Based Distillation

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ABSTRACT:

Although the equilibrium model has been the basis of the simulation of distillation columns, its shortcomings are well known. The model is based on the assumption that both phases leaving a stage are in thermal and material equilibrium. In practice equilibrium is rarely attained since mass and heat transfer are actually rate processes that are driven by the gradients in chemical potential and temperature. The equilibrium models predicted results far from the practical and experience alongwith rules of thumb were used as a tool to bridge the gap, hence came the Rate based simulation into picture. There has been a lot of work into this field in the recent times as its potential has been explored by the researchers. The use of the rate based model eliminates the requirement for mass transfer coefficients, Murphree stage efficiencies, liquid holdups, residence time etc. All these are calculated by the simulation engine based on the real time performance.

The aim of the presentation will be to elaborate the differences between the two models and their comparison.

Keywords-component; formatting; style; styling

1. Introduction:
Current industry design practices feature separate process design and process control groups. Process design remains a largely sequential process with each process unit being sized individually with the emphasis on minimizing capital expenditures instead of an emphasis on overall performance. The resulting dynamic system of the connected equipment can be ill-behaved or difficult to control. Especially designs that minimize holdups may lead to severe control problems. Control engineers often are involved only after the design is already complete. This may lead to redesign of the control system or equipment, unnecessarily complicated control systems, and revenue lost due to delays or not meeting promised product deliveries.

In the process design phase, dynamic simulation is needed to determine dynamic responses to process disturbances such as surge tank levels, column sump levels, product flow rates, or product compositions required for sizing of the relevant equipment as well as for the selection and location of control sensors and actuators. Dynamic modeling can also identify whether the product goals are attainable and detect control schemes which are not adequate or appropriate for meeting given product specification goals. This is specifically of interest with the installation of advanced control algorithms. Initial tuning and optimization of control parameters can result in faster process start-up and control problems will be detected earlier when the process design can be altered without a considerable increase in costs. Controllability of alternative flowsheets can be investigated and auxiliary equipment for startup or shutdown can be located and designed. A side benefit from dynamic simulation is that process engineers will become familiar with the process dynamics and control issues (and control engineers with process design)

For process safety assessments, dynamic simulation can be used to check whether environmental constraints will be met during transitions or to test various emergency shut down procedures without performing actual experiments. Start-up and shutdown of current processes can be optimized ad while interfacing with the control structure dynamic simulation can facilitate online

process optimization and operator training. It can also be a tool for testing the controls robustness, e.g., in relation to measurement errors or valve malfunctioning.

Clearly, dynamic simulation provides process and control engineers with a powerful tool to improve process design and production in various ways which can lead to improved revenues. However, dynamic process simulation is only yet starting to become of importance due to the fact that dynamic simulation programs and packages have suffered from a number of deficiencies. Most engineers could not use them because they were geared for use by specialists , they were not user-friendly nor interactive. Usually, even the more simple models required large computer resources. Simulators were not portable, fast, flexible, extendable, maintainable, or affordable.

The immense increase in available computer power now allows the engineer to do dynamic simulations on a personal computer or workstation (instead of having to use a mainframe or supercomputer). Maintainability and extendibility is possible by use of equation oriented simulators where models are described in high level declarative languages. Examples are SPEEDUP (Perkins and Sargent, 1982, Pantelides, 1988a), ASCEND (Piela et al., 1991) and gPROMS (Barton and Pantelides, 1991). Pantelides
and Barton (1993) and Wozny and Jeromin (1994) discuss the current status and possible future of (equation oriented) dynamic simulation.

2. Equilibrium Column Simulation:

The simulation of separation processes – in particular the simulation of distillation columns – is an essential part of dynamic process simulators. Distillation is a high energy consumer in most chemical processes and the interactions between columns can be significant from the design as well as the operability point of view.

Simulation of separation processes by equilibrium stage calculations dates back to 1893 when Sorel published equations for simple, continuous, steady-state distillation. These equations included total and component material balances and a corresponding energy balance that could account for heat losses. Sorel's equations were not widely applied until 1921 when they were used in a graphical solution technique for binary systems by Ponchon (1921) and Savarit (1922), who employed an enthalpy concentration diagram. In 1925 a much simpler, but restricted, graphical technique was developed by McCabe and Thiele. The simplification was achieved by assuming constant molar overflow, eliminating the energy balance equations. Lewis and Matheson (1932) and Thiele and Geddes (1933) were the first to propose methods to solve the systems of equations in a tray by tray manner. Thiele and Geddes (1933) ere also the first to solve each type of the MESH equations in turn (MESH is the acronym referring to the different types of equations: M=Material balance, E=Equilibrium between phases, S=Summation of phase mole fraction to 1, H=Heat balance).

Several authors discuss the assumptions used in the dynamic simulation of separation columns that introduce errors. Ranzi et al. (1988) discussed the effects of the energy balances and the way they affect the simulation. They found that the energy balances must be evaluated completely in order to predict correct behavior. Choe and Luyben (1987) conclude that vapor holdups cannot be neglected (especially for columns operating at high pressures) and that column pressures should be calculated (especially for low pressure columns, where the tray pressure has a large influence on the tray temperature).

3. Non - Equilibrium Models

Although the equilibrium model has been the basis of the dynamic simulation of distillation columns, its shortcomings are well known.

The model is based on the assumption that both phases leaving a stage are in thermal and thermodynamic equilibrium. In practice equilibrium is rarely attained since mass and heat transfer are actually rate processes that are driven by the gradients in chemical potential and temperature.

The traditional method of coping with finite rates of mass transfer in stagewise processes has been through the concept of a stage efficiency. There are various definitions of stage efficiencies, but the most popular is the Murphree (1925) component vapor efficiency. This stage efficiency reflects the ratio of actual mass transfer over the mass transfer that would be accomplished by an equilibrium stage. For lack of other information, the stage efficiency is taken to be the same for all components, obtained from some empirical correlation depending on the components in the mixture.

For a binary system both component efficiencies are equal, but unfortunately this is not the case in

systems with more than two components. Diffusional interaction phenomena (for example reverse diffusion or osmotic diffusion, have proven that mass transfer can occur against a gradient or in absence of a gradient (Toor, 1964). If a component diffuses against its gradient the component efficiency will be negative (since the direction of mass transfer is the opposite of that what the equilibrium model would predict), and, if it diffuses without a gradient, the components efficiency will be infinite (since the equilibrium model predicts no mass transfer). Because diffusional interactions influence the fluxes differently for each component, component efficiencies in mixtures with three or more components do not have to be equal. In fact they can vary over a range from –infinity to + infinity. This surprising result has been confirmed by experiment (Krishna et al., 1977). For ideal and moderately ideal systems the component efficiencies are only a weak function of the composition, in contrast to non-ideal systems where the opposite is true. Consequently, in the distillation of non-ideal systems the concentration transients could cause large component efficiency changes that might significantly alter the simulation. Therefore, any good model must be based on diffusion calculations that include diffusional interactions. However, dynamic simulators based on the equilibrium model use Murphree efficiencies which are assumed constant and equal for all components.

Efficiencies also depend on the type of operation, as they differ in distillation and absorption operations for the same mixture at hand. Plate hydraulics (including weeping and entrainment) influence the flows on a tray. Different vapor and liquid flows result into various flow regimes of the two phases on the tray (such as spray, emulsion, or bubble flow) which each have there own transfer properties (and thus, efficiencies). Thus, transients in the tray hydraulics imply possible changes in the component efficiencies but with a constant efficiency model such effects are totally neglected.

Another assumption of the equilibrium model, thermal equilibrium, forces the liquid and vapor leaving a stage to have the same temperature. In reality, heat transfer between the two phases is limited and the separate phases have their own temperatures. The assumption of thermal equilibrium makes it difficult to model the dynamics of sections in a column that are purposely used for heat transfer, or columns where feeds are normally sub cooled or superheated (such as extractive distillation or strippers/absorbers).

Thus makes the Equilibrium model inappropriate for dynamic simulations where these efficiencies are subject to change and cannot be specified beforehand. Using constant efficiencies neglects the influence of the tray hydrodynamics on the mass transfer and the consequences for the column dynamics.

To eliminate the problems discussed above we need to construct a new dynamic column model which does not employ overall thermodynamic and thermal equilibrium assumptions! A non equilibrium model was developed by Krishnamurthy and Taylor (1985a-d, 1986) (see, also, Siva Subramanian et al., 1987; Powers et al., 1988; Lao et al., 1989, 1994; Taylor and Krishna, 1993) for steady-state simulation of separation processes. The non equilibrium model splits the stage material and energy balances into balances for each phase, adding rate equations for the calculation of mass and energy interphase transfer rates. The mass transfer rates are computed through matrix routines directly from fundamental diffusion equations and mass transfer correlations. A second generation model was developed by Taylor et al. (1994) which incorporated the pressure as a variable. Taylor et al. (1992) have demonstrated application of the non equilibrium model to industrial column operations. Since the non equilibrium model avoids the use of tray efficiencies and includes the column hydraulics (which are very important in dynamic column simulation) it is suitable as a basis for developing a better dynamic column model.

As very few unsteady-state column data is available, dynamic simulations of columns or linked columns provide an ideal opportunity to study and analyze the dynamic behavior when no other model is available. However, it also makes it difficult to validate the results of a dynamic simulator other than by checking general trends. (Harry Kooijman).

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