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Chapter

Introductory Chapter: Distillation

Vilmar Steffen

1. Modelling, simulation, and optimization of distillation processes

Obtaining a phenomenological model of a process consists on applying law conservations, like mass, energy, and momentum balances and constitutive relations, like vapor-liquid equilibrium, chemical reaction rate, chemical equilibrium relation, etc. A mathematical model, developed to represent (approximately) the real behavior of a process, is very important to analyze an existing plant or to evaluate the technical viability of a new chemical process plant. These analyses and evaluations normally are carried out by making changes in some process parameter and measuring the results of the respective change, in other words, carry out lots of "what if" relations. The analysis of a plant, by simulation, within the development of new processes may frequently show beforehand whether it is technically and economically viable [1].

The solution process of a mathematical model is known as simulation (nowadays, simulation is synonymous of computational simulation). Analyzing a process based only in the mathematical model, is a task almost impossible, but the numerical results of simulation can be easier analyzed. The mathematical model is very important, beyond for simulation and analyses, for the optimization of a process. The mathematical model must correctly represent the quantities and reflect the state of the studied system, only so the simulation and optimization will succeed. In the step of the mathematical model construction, the engineer must analyze if some simplifications, which can make the model simpler (or much simpler), can be adopted without a significant loss in the prediction capacity of system property behavior. However complex a model may be, it cannot represent exactly the real behavior, so some simplifications can be accepted, resulting in a much more simpler model, with little loss in the result quality [2].

The complexity of a distillation column is not due to the material and energy balances that normally are simple equations. This complexity comes from the constitutive relations of chemical reaction (for the case of reactive distillation), mass transfer relation (in a more simplified way, phase equilibrium), and relations to compute the enthalpy. The chemical reaction must be analyzed for chemical equilibrium limitation and chemical reaction rates to evaluate if, in the column dimensions and operation conditions, the desired conversion will be reached. The enthalpies must be precisely evaluated, because it has influence on the heat duties of the condenser and reboiler. And, the thermodynamic property that has the greatest influence on the simulation of separation processes are those related to phase equilibria, for this part is necessary the non-idealities prediction of vapor phase (usually performed with equations of state) and liquid phase (associated with the excess Gibbs energy models). A good phase equilibrium modelling can predict limitations on the separation like those ones caused by azeotrope formation.

The distillation process is the most commonly used in industry to separate chemical mixtures; its applications range from cosmetic and pharmaceutical to petrochemical industries [3] and are responsible for a great part of energy consumption. Evaporation systems are some of the most energy-intensive parts of chemical plants [4], and the needed energy in a distillation column is used in the heat change process occurring in the reboiler. Finding solutions for energy saving has become one of the most demanding issues faced by almost all the governments, decision-makers, and stakeholders all over the world [5]. Energy saving is practiced for improving the efficiency, to minimize fossil and renewable fuels consumption, and to reduce resulting pollution and environmental burdens [4, 6]. This last item is closely related to climate change and other negative environmental impacts. But, high-energy consumption remains a challenge [7]. Fortunately, there are different ways of saving energy. In production, starting with the selection of production process thereby reducing the environmental stress [8]. The energy-efficient policies with renewable energy integration are not an actual trend; this is a requirement for sustainability [9].

A good way to reduce the environmental impacts is using solar energy. Solar distillation (solar stills that user solar radiation in the distillation process) is a method of water purification that can be implemented at low cost and less energy consumption (if compared with conventional processes) and is environmentally friendly.

Process intensification is an effective strategy to achieve increased energy efficiency. Process intensification aims at reducing the mass and heat transfer resistances while overcoming thermodynamic limitations through the integrated design and operation [10]. Recent developments in energy-related research increasingly rely upon simultaneous resource saving and pollution reduction by applying process integration [4]. Process intensification is a feasible way to reduce heat requirement [7]. One of the most common examples of the process intensification field is the reactive distillation, where the integration of reaction and separation is performed. In the cases where reactive distillation has been used, the operating and investment costs are significantly reduced, when compared to the classic set-up of a reactor followed by distillation. Reactive distillation processes offer several important advantages that include the increment of the reaction yield and selectivity, the overcoming of thermodynamic restrictions, and the considerable reduction in energy, water, and solvent consumptions [10]. So, this integration has been successfully applied in several plants. Unfortunately, the modelling and simulation (an important in the process analysis) become a quite complex.

Concluding, it is very important to well design, operate, and control (for keeping the optimal condition operation) a distillation column, which can lead to a large save on energy and raw material consumption. But, having enough knowledge for making an efficient column project and establishing the best operational conditions need much experience and lots of tests on the process in study, and this type of tests can be very expensive; this is one of the reasons that justify the usage of process simulation tools. Analysis based on numerical simulation results (various virtual tests Considering lots of changes in the process parameters) probably will lead to cost reduction or increase in profit.

Author details

Vilmar Steffen
Universidade Tecnológica Federal do Paraná—UTFPR, Francisco Beltrão, Paraná, Brasil

*Address all correspondence to: vilmars@utfpr.edu.br

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