Current Problems in Reactive Distillation Process Control

Ioana Georgescu[*], *Gabriel Rădulescu*

Petroleum – Gas University of Ploieşti, ROMÂNIA

E-mail: ioana.georgescu@gmail.com

Abstract: A reactive distillation plant is one of the most important and "delicate" functional components of a complex chemical plant.

While steady state modeling and simulation tend to become a standard today by using some well known dedicated software tools, only little is known about the dynamic simulation in the open literature. Due to the process complexity, the references in this field mention many difficulties in building-up a dynamic model that could be appropriate for numerical integration.

The (dynamic) simulation is useful in understanding the behavior of such a complex plant. But the most important goal by using an appropriate simulation tool would be to design and set up a control system for such a reactive distillation process**.**

Keywords: reactive distillation, mathematical model, simulation, control.

1. Introduction

The reactive distillation process has a high complexity compared to classical distillation processes. It also has a major advantage: the reactor and the distillation column are no more needed as two separate entities, their role being taken up by a distillation column, where both the reaction and separation processes take place.

By analyzing the current state of the reactive distillation modeling and simulation, the authors reached to a conclusion – at present two models are mainly used: equilibrium (EQ) and non-equilibrium (NEQ) models, both having their own characteristics and constraints.

This paper intends to offer an overview on the actual state of reactive distillation modeling and simulation techniques as well as some personal remarks emphasizing the problems that may occur when simulating such a process.

[*] Corresponding author

2. The Reactive Distillation Processes Modeling Principles and Goals

Generally, a model is a schematic representation of a (real) system, which describes in a given manner the system behavior. Usually the model consists in a set of mathematical equations, so it being called a “mathematical model”; this work also focuses only on this type of models.

There are several situations requiring the use of a mathematical model. Related to the announced reactive distillation processes topic, first, a model could be used to simulate a particular distillation column or even an entire plant. Simulators are the most used tools in research activities with a wide coverage area of interest: process intimacy investigation, plant structure and control systems design and test, state estimation (inferential measurements), plant operators training and so on. These models, well known as “simulation models”, describe the process behavior (internal state and outputs evolution) for a specific set of input variables, taking into account the time (dynamic models) or not (steady state models) (Grüner et al., 2003; King, 1980; Rădulescu, 2000, 2002).

The mathematical models may be categorized according with many criteria, but only a few are significant when applied to the reactive distillation process models. Thus, the authors want to emphasize three of the most used types.

A. EQ vs. NEQ models

For equilibrium (EQ) models, the vapor and liquid streams leaving the stage are assumed to be in equilibrium with each other, while the non-equilibrium (NEQ) models follow the philosophy of rate-based models for conventional distillation. In addition, in the NEQ model, hardware design information must be specified so that mass transfer coefficients, interfacial areas and so on can be calculated. In addition, physical properties such as surface tension, diffusion coefficients and so on for calculation of mass (and heat) transfer coefficients and interfacial areas are required.

B. Steady state vs. dynamic models

These two types differ in the manner the time is taken into account or not. Of course, a dynamic model is supposed to better describe the process behavior than a steady state one. But there are many situations that do not require such a complexity; a well-known example is the distillation column design, which use only steady state models to determine the column geometry and operating parameters, as the design specifications would be accomplished.

On the other hand, a dynamic model is strongly required for post-design studies, when testing the plant behavior (before building it up). Even if the authors met a few different opinions, they do believe that only a dynamic simulation can offer a complete overview on the distillation plant.

C. Rigorous vs. empirical models

A mathematical model may be formulated mainly through two techniques. First, using some basic principles leading the real system behavior (i.e. mass and energy conservation, liquid-vapor equilibrium), with usual simplifying assumptions, adequate relations between inputs, outputs and state variables are established. The used principles are chosen in a manner that can globally characterize the system (the reactive distillation process in our case), so the obtained equations system being that way a mathematical model for it. This is a so-called "rigorous model".

On the other hand, for many applications such a "complete" and complex model is not useful. The training software simulators and advanced control systems, for example, are based on reduced-scale models, still giving an acceptable overview on the reactive distillation plant behavior (input-output correlations) but without any details about "what is inside".

Usually, these models are obtained through identification (observing the real plant or making use of a software simulator based on a rigorous model) or other reduction techniques and mainly do not take into account the physical principles leading the reactive distillation process, so being called "empirical models". This type is very useful when a fast simulation is required, as in real-time systems (Grüner et al., 2003).

Because the EQ are the most frequently used and studied models, the remarks on our paper refer only to that model.

3. The Dynamic Simulation of the Reactive Distillation – Still a Challenge?

To simulate a given physical system means in fact to use a representation for this one, which can offer a qualitative and/or quantitative image over the real system behavior when a set of inputs changes. This representation must have at least two functional sections: a model for the physical system and a “simulation engine” (see figure 1). There also must be a correlation between the physical system inputs/outputs (real inputs/outputs) and the simulator inputs/outputs (modeled inputs/outputs).

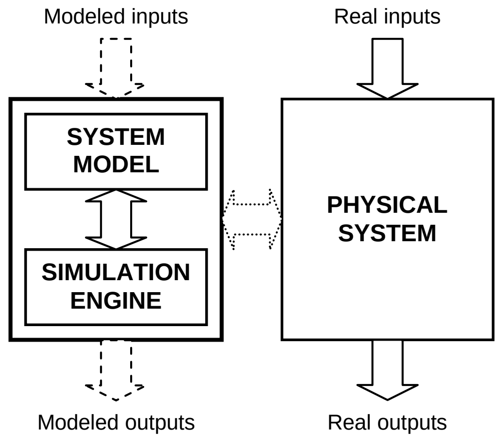

Fig. 1. The general simulator architecture.

In order to implement such a simulator structure, the authors suggest a versatile and powerful software oriented on dynamic simulations for industrial plants, DIVA (Dynamische Simulation Verfahrenstechnischer Anlagen), developed at the Stuttgart University. This simulation environment runs under Linux operating system and integrates some sets of high-level routines to solve/integrate complex algebraic and differential equation systems (Mangold et al., 2000).

Some problematic aspects in the dynamic simulation. First, it must be mentioned the mathematical model translation, from standard equations to a computer-coded representation. Even if in general it seems to be not any problem, regarding the model for the reactive distillation process the simulation environment must have such a very important facility as equation indexing, meaning in fact an automated model generation by a re-scaling operation (Rădulescu et al., 2000).

Then, the model equations being a differential algebraic system, the main problem is to determine consistent initial values for the integration.

Another problem could be how to choose an appropriate integration method. Most of the software simulation environments provide different solutions, suitable for some type of applications.

Nevertheless, the hardest to solve problem is to answer the question: are the simulation results systematically correlated with the real system response or these are only the simulator response? Many others also ask themselves about this (Mohl, 1999). The authors of this work do strongly believe that being able to give this answer, when simulating such a complex process like reactive distillation, means in fact to pass from the simulation usual techniques to the simulation art.

4. Conclusions

The reactive distillation process, having a high complexity compared to classical distillation processes, needs appropriate and powerful tools in order to study the process behavior. This paper briefly presented the actual state of reactive distillation modeling and simulation techniques. In addition, based on authors experience in this field, some remarks regarding the problems that may occur when simulating such process are emphasized.

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