DISTILLATION PROCESSES MODELING AND DYNAMIC SIMULATION – A CRITICAL SURVEY

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Abstract: A distillation plant is one of the basic functional components for a refinery. While steady state modeling and simulation tend to become a standard today by using well-known software tools like PRO/II®, 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, which is usually induced by the dynamics of individual sub-processes in combination with the unit topology. Also, it serves to investigate suitable operating strategies, including closed-loop operation at the nominal point, load and specification changes, startup procedures and so on.

It is not possible to formulate general principles on how to build-up a simulator, but some basic guidelines, remarks, problems and main goals may be emphasized. However, following a correct way from the system abstract description to the software simulator implementation proves to be not only a technique, but also a real "simulation art".

Keywords: distillation columns, mathematical model, simulation.

1. INTRODUCTION

The distillation process is one of the most important processes in any refinery. Due to its own place (its products becoming either final products or feedstock for other processing units), complexity and taking into account the highly energy-consuming process feature, it is very important to have powerful instruments to intimately study it.

A software simulator, focused (if possible) on the process dynamic behavior may be one of these analyzing tools. Obviously, for research purposes, a special dedicated tool is required, it having different features from the "general applications" simulators. But in order to get the benefits of such a simulator it is necessary to formulate a mathematical model for the process, then to find an appropriate method to solve it and finally to display the simulation results in an accessible form for the user.

After experiments in this field, the authors present in this paper an overview on how to build-up a software simulator, from a few basic principles on the distillation process modeling to some guidelines in the simulator implementation.

2. THE DISTILLATION PROCESSES MODELING: PRINCIPLES AND GOALS

In general, 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 distillation processes topic, first, a model could be used to simulate a particular distillation column or even an entire plant. The 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).

Then, slightly different types of models are used as an intrinsic component of the control systems. Generally, the advanced control algorithms (i.e. Feed-forward Control, Internal Model Control, Model Predictive Control) are derived or even include these "control mathematical models". In this case, the model mainly "tells" what inputs are required to get the desired system outputs (in a specific time), in respect with a set of process constraints (Chung and Riggs, 1995; Hsie, 1989; Gani, *et al*., 1986; Rădulescu, 2002).

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

A. Steady state vs. dynamic models.

As shown above, 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 makes use only steady state models to determine the column geometry and operating parameters, as the design specifications would be accomplished. The researchers in this field use classical software tools (PRO/II®, for example) and they affirm there is no need for more complex environments.

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. Let take into account just a very simple example. Supposing a given change on a sensitive operating parameter (the main column reflux rate, for example), both steady state and dynamic models show that the distillation plant evolutes from the "A" state to the "B" state, both situated in a vicinity of the main operating point (considered as the safe operating region). But only the dynamic model is able to show if the trajectory between "A" and "B" does not pass through the "C" state – which may be not respecting the safety operating rules of the plant (see figure 1). And it is well known that the major technical problems arise not in the steady state, but in the transient regime of the system!

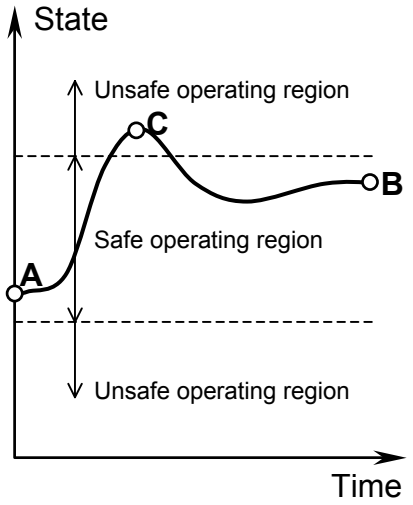

Fig. 1. A possible state trajectory for a real system.

As an opinion, the steady state or dynamic type of the model may be decided only by taking into account the application type, but the authors do believe that, in the future, the dynamic models will cover most of the interest area, replacing in many situations the classical steady state models

(which could be even obtained from the dynamic models).

B. 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 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".

Generally, for a particular distillation plant, such a (dynamic) model consists in hundreds or even thousands of algebraic and differential equations (Rădulescu, *et al*., 1998, 2000). It should be used only when a deep "look inside the process" is needed (for fundamental research topics), as time as it usually requires top-level hardware and software environments to be put into value. The simulation time is long enough to prohibit the use of this model in real-time systems, designed for advanced control purposes. But the model has a unique feature: it best describes the process intimacy behavior and offers significant information related to the real plant that could not be revealed even on the physical system, through classical measurements.

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 distillation plant behavior (input-output correlations) but without any details about "what is inside" (Chung and Riggs, 1995; Hsie, 1989; Kienle, 2000; Rădulescu, 2002).

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 distillation process, so being called "empirical models". This type is very useful when a fast simulation is required, as in real-time systems (Kienle, 2000; Rădulescu, 2002).

It is very interesting that, sometimes, a particular application requires a hybrid model (typical in the advanced control area), with both rigorous and empirical components. And, in the same time, the application itself even imposes the modeling technique and the final complexity; in this field it does not exist a methodology suitable for all situations.

At this point, it must be revealed that, if a rigorous dynamic model for the distillation process is available, there are several ways to obtain from it both dynamic and steady-state reduced-scale models, as the specific application requires. This is the major reason why the authors have focused their work on how to obtain and truly put into value a complex dimensional dynamic model for this process in general (and in particular for the crude oil plant). Based on their experience and taking into account the major directions in this field quoted in the open literature, some guidelines on how to build-up such a model have to be emphasized in this paper, the interested reader being invited to consult the references for more details.

Basic principles. The main problem when modeling a distillation unit is to find the best model for the columns. Considering a classical plant aggregated from a few coupled columns with trays, a good compromise between the results accuracy and a reasonable model dimension in order to require a non-prohibitive execution time for the integration routine may be made by using some classic simplifying assumptions (Chung and Riggs, 1995; Gani, *et al*., 1986; Strătulă, 1986):

- The plant feeds may be divided in NC pure components or pseudo-components (for complex mixtures like crude oil, for example), with known physical properties.
- The (pseudo) components are always perfectly mixed on the column trays.
- The trays are ideal (theoretical trays), between the vapor and liquid phase being an equilibrium state.
- The vapor holdup on each tray is negligible.
- The pressure profile is constant.
- The condensers from the plant are considered total condensers with "perfect" controlled condensed liquid temperature.

The model for the entire plant, which may consist in several columns, sidestripers, pumparounds, condensers and accumulation tanks, is usually obtained from the models for each particular element, this technique being called the "structural approach" in the industrial plant modeling (Chung and Riggs, 1995; Holland, 1981; King, 1980).

Usually, the model for the columns and the sidestripers is the same, the only thing that differs being the number of trays NT (considered as a "structural" parameter for the model) and is obtained by coupling the independent models for each tray. Such a model is detailed in past authors' papers (Rădulescu, *et al*., 1998, 2000; Rădulescu, 2002) and mainly contain:

- NC equations derived from the independent components material balance.
- NC equations for the liquid-vapor phase equilibrium.
- One equation for the total material balance.
- One equation for the energy balance.
- One equation for liquid holdup on tray.

Other additional equations are also required (some summation conditions, for example). To give a short overview on the model dimensions, for an industrial crude oil distillation column with NT=30 trays, the feed being divided in 37 pseudo-components (including added water), the total number of equations is 1290, as shown in the references (Rădulescu, 2002). In the same work are also detailed the models for a total condenser with accumulation tank (based on total and component material balance equations) and for a heat exchanger from the pumparound line (based on total material balance, component material balance and energy conservation equations). If the model for the aggregated crude oil unit includes sections for the liquid accumulation level controllers and an auxiliary module for product quality estimation, the mentioned plant is represented through 9125 equations, with 1598 differential and 7527 algebraic equations!

Some problems. Obviously, such a complex model is oriented only to research purposes, as time as it can give all significant information about the plant state (liquid accumulation on each column tray, internal/external liquid and vapor flow rates, temperatures, component mole fractions in each particular point of the plant, products quality and so on). As mentioned above, only a small part from these numerical values are needed in other usual (industrial) applications.

But the model formulation is just a small problem; many others must be revealed when analyzing the resulting model characteristics. First, the system is non-linear and stiff, due to the different time scales in the model, imposing serious limitations for the integration step in order to have a stable numerical solution. In the authors' opinion, the best solution possible is to use a variable step routine that permits a significant number of step size reductions (Rădulescu, *et al*., 1998, 2000; Rădulescu, 2002).

Another problem is that the system dimension is very large and may lead to memory management problems when using it in some software environments. Without changing the model order, some dimensional reductions must be operated (i.e. for the distillation column not all trays have external feeds and sidedraws, so these variables should be eliminated).

Obviously the model had to be validated, in order to be sure it can give solutions with practical relevance. In the same time this is a way to evaluate how the simplifying assumptions affect the modeled system response. In a "normal" situation, having reasonable dimensions and complexity, there are available a few analytical methods to study the inherent model properties: its solutions existence, uniqueness, continuity depending on the input data and especially their behavior in correlation with the physical sense. But unfortunately it is not our case: the model is quite large and complex even for a regular computer-coded representation, not only for a human researcher! This way, the only method to validate the model is to study very carefully its behavior during a significant number of simulations; the authors' opinion is that such a model has a good accuracy when there is an obvious concordance between the obtained results and the data directly taken from the real plant, taking into account the good sense remarks from the plant operators too (Chung and Riggs, 1995; Hsie, 1989).

Goals. As mentioned, once all these problems are overridden, the validated model should be put into value. It must be fitted to an appropriate software environment, with powerful integration

routines, able to provide feasible numerical solutions; the resulting dynamic software simulator becomes itself a dedicated tool for research activities. As a remark, any distillation plant complete and complex dynamic model has not an intrinsic value (of course, excepting the value of some years of experiments!), but its value comes from the benefits that could be obtained from the built-up software dynamic simulator: new reduced-scale models identifications, operating strategies tests over the simulated plant, advanced control systems design and so on.

3. THE DYNAMIC SIMULATION – 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 2). There also must be a correlation between the physical system inputs/outputs (real inputs/outputs) and the simulator inputs/outputs (modeled inputs/outputs).

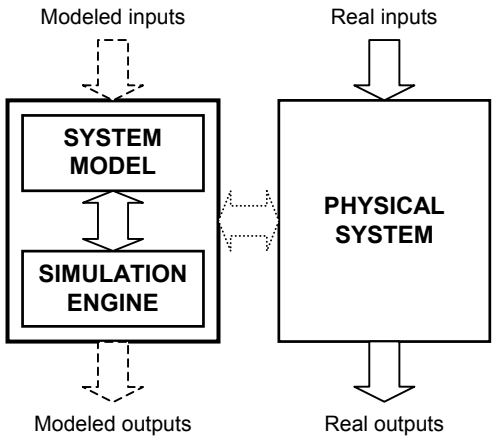

Fig. 2. The general simulator architecture.

When a mathematical model characterizes the system and the "engine" is a software environment, this is the case of a typical software simulator. Of course, in the past, when the digital technique performances did not permit such a complex task, other ways to simulate the real systems were used (i.e. by using analog computers based on operational amplifiers), but this is not a topic for present work.

Whenever a problem has to be solved by a simulation, an answer to the question „what kind of simulator is more appropriate?" has to be found, taking into account a few attributes characterizing a software simulation environment.

If the problem is enough simple and the human solver is well trained, a "full hand-made" simulator may be used. This is a typical situation for student laboratory works, when each subject must formulate an adequate mathematical model, choose a solving method and then "translate" the model and the numerical method in a computer program, using a high-level programming language (C++, Pascal, FORTRAN) or other software environment. In the present days, this manner of work is in fact only an applied teaching technique, not a real manner to solve a simulation problem, because it seems to be a "wheel re-invention"! But, as re-inventing the wheel helps to understand why it turns round, re-building "by own hands" at small scale a software simulator is a compulsory stage to climb for those who want to have future significant results in the area of systems modeling and simulation.

Totally opposed is the situation of a very complex problem and a human solver novice in the field of modeling and simulation methods. This is a typical case when a dedicated software simulator is required, providing both the mathematical model and the simulation routine for a particular situation. The user just has to choose an adequate model from a complete library, the appropriate solving routine and then analyze the simulation results from his point of view. In this situation, the human subject is only a simple client of a complex software environment, dedicated to a specific class of applications, and his abilities are not focused on how to best describe the physical system by a model, but on how to best use the environment facilities to cover his research interest area. For example, PRO/II® is one of the most used tools in the complex petrochemical processes simulation (including distillation), oriented to specialists in this field of activity, not for experts in computer-aided modeling and simulation (Simulation Sciences, Inc., 1998 a, b, c). It offers a huge database with plant models, component physical properties as well as solving

numerical methods, all accessible from a friendly graphical user interface (see figure 3).

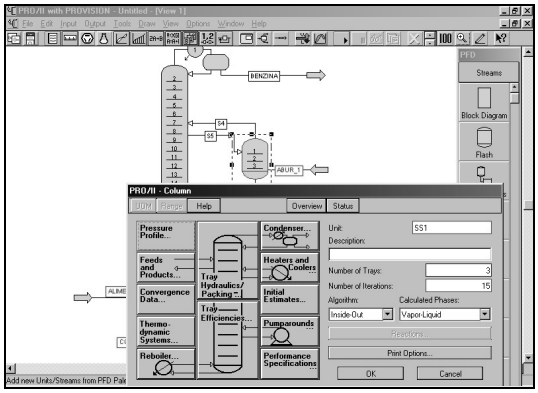

Fig. 3. The PRO/II® user interface.

Of course, the simulation becomes an easy-to-solve problem, which is the main advantage when using such a software environments like PRO/II®. But this could not be satisfactory for a researcher who wants to test its own plant model or make improvements for the existing one, as time as the models from the system database are quite stiff and not full documented in the open literature. More, these models are fitted to a particular situation by modifying only a set of parameters (i.e. for a distillation column model: number of trays, diameter, other geometrical elements, some important operating parameters and so on), being not permitted to make any change in the model equations, which are inaccessible. This is why the advanced researches in the field of distillation process modeling and simulation require other software tools, full adaptable to the researcher needs.

In the authors' opinion, the best compromise between a "hand-made" simulator and a totally dedicated one could be a so-called "large-scale application" software simulation environment. It puts together the benefits of a flexible modeling tool and the power of a state-of-art numerical methods implementation. In this case, the user is full responsible for the plant model formulation and its specific software codification, but the environment has already built-in a comprehensive solving algorithms library, which can be freely tested until the best results are obtained.

The authors want to give as example Simulink® and DIVA, among several well-known environments for large-scale application dynamic simulations. Simulink® has the great advantage of a nice and intuitive graphical user interface, as well as a complex "object library" (standard mathematical models for usual systems, which can be combined to aggregate almost any type of a real system model). Whenever a model cannot be formulated via these standard simple models, it can be written "by hand" (but this is not a facile operation). The objects are connected in a diagram, this being a helpful manner of work in a better system behavior understanding (see figure 4). After building the model, some solving routine parameters have to be established and then the simulation may be started. The simulation results are usually displayed "on-line" by the scope-objects, during the simulation (The MathWorks, Inc., 2000 a, b).

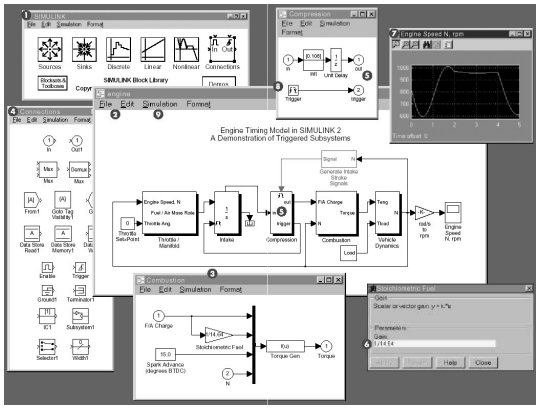

Fig. 4. The characteristic Simulink® connection diagram.

But this is just a nice hypothetic situation, which cannot be met when trying to build-up a software simulator for a distillation column, for example. It is not easy at all to graphically aggregate a mathematical model with about 1300 equations (as shown above), even if these equations are not too complicated. The resulting diagram would be more complex than the modeling problem itself! Or, more probable, the diagram complexity would generate so much memory management problems as the Simulink® will systematically fail to provide relevant simulation results (as proved by tests). And this is just the case of a simple distillation column, without saying any word about a complex plant, with more 9000 equations in its model (like the crude oil unit)! As a personal authors' conclusion, Simulink® appears to be a feasible solution for small and medium

applications, not exceeding its capabilities, which unfortunately is not the case of the distillation processes.

Thus, the authors suggest another versatile and powerful software oriented on dynamic simulations for industrial plants, DIVA (Dynamische Simulation Verfahrenstechnischer Anlagen), developed at the Stuttgart University (Mangold, 2000; Marquardt, *et al*., 1987; Kröner, *et al*., 1990; Tränkle, *et al*., 1997). This simulator runs under Linux operating system and integrates some sets of high-level routines to solve/integrate complex algebraic and differential equation systems. Being oriented on simulations over the industrial plants, DIVA works also with the concept of "block device": the entire plant is divided in relevant parts in accord with topologic and functional rules. Every block is described by its own model and external connections, giving a natural way to aggregate the entire plant, in a structural approach.

DIVA cannot be characterized as a too friendly environment at the present, as time as the user interacts with it via terminal command lines and standard formatted text files. More, the simulation results may be analyzed only "off-line". But these disadvantages are overridden by the real amazing computing power and an optimized memory management. This could be proved by all the results obtained in the dynamic simulation of an industrial crude oil plant, first in open-loop configuration and then equipped with an advanced product quality control structure (Rădulescu, *et al*., 2000; Rădulescu, 2002). In fact, DIVA was the only way to solve in an adequate manner such a complex modeling and simulation problem, described in the quoted references.

Some problematic aspects in the dynamic simulation. Regardless the chosen software environment, there are some common problems in the simulator implementation that have to be emphasized. 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 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. To be concrete, as mentioned, the model for a distillation column is obtained by coupling the quasi-independent NS stage models, which must be not re-written by NS times!

Then, the model equations being a differential algebraic system, the main problem is to determine consistent initial values for the integration (in fact to compute values of the algebraic variables which are consistent with the given initial values of the dynamic variables). A distillation plant "true" steady state, with practical relevance, is a special case where this is satisfied. But how can be obtained this state? One possible answer should be: by an arbitrary initialization of the dynamic variables followed by a long time horizon simulation, supposing it will lead to a "true" plant steady state. This manner of work may be suitable for simple systems, but in the case of the mentioned crude oil plant it systematically fails to provide relevant results, this being a typical non-minimum phase system. For these complex plants, the authors still have not found a robust way to get this "true" steady state using only the plant dynamic model. However, a hybrid methodology was adopted, by using a derived steady-state model to get initial values for a sub-set of the state variables, then initializing the dynamic simulator with these values and simulating the system until a real steady state is obtained (Rădulescu, 2002).

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. Obviously, an explicit "recipe" on "how to generally choose" cannot be formulated, but some criteria may be taken into account: the system order, sensitivity, maximum error tolerance, the simulation hypothesis (with/without known consistent initial values), the inputs dynamic changes amplitude (requiring fixed/variable integration step size), inherent stability and so on. Routines as Runge-Kutta and Euler implicit type (like SDASSL, LIMEXS, RADAUS, EULERB, SDIRK4) are mentioned as best suitable for usual applications by the literature, in particular for the distillation process simulation (Mangold, *et al*., 2000; Tränkle, 1997).

But 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? Too many aspects are implied here: the solving algorithm relevance, the mathematical model validation (but how to exactly know if a mistake comes from an inappropriate model or from the integration method?) and, not at last, the human expert subjectivity. The authors do strongly believe that being able to give this answer, when simulating such a complex process like distillation, means in fact to pass from the simulation usual techniques to the simulation art.

4. CONCLUDING REMARKS

The software simulation, especially focused on the process dynamic behavior, tends to become in the present days one of the most used analyzing tools for the distillation process. For research purposes, which need a very close "look inside the process", a special dedicated tool is required, it having different features from the general simulators. The authors presented in this paper a short overview on how to build-up such a software simulator. The basic principles, problems and goals on the distillation process modeling are emphasized and then some guidelines in the simulator implementation are presented. This way to follow proves an extraordinary complexity and hides many problems and real traps, this is why the authors do believe the distillation process modeling and simulation migrates from a technique to the real art.

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