

Tools for Computer Aided Analysis and Interpretation of Process Simulation Results

Marion ALLIET GAUBERT and Xavier JOULIA

Institut National Polytechnique de Toulouse (INPT)
Ecole Nationale Supérieure d'Ingénieurs de Génie Chimique (ENSIGC)
Institut du Génie des Procédés (IGP)
Equipe Analyse Fonctionnelle des Procédés
18, chemin de la Loge - 31078 TOULOUSE Cedex
tel. : (+33) 5 62 25 23 55 ; fax : (+33) 5 62 25 23 70 ; e-mail : Xavier.Joulia@ensigt.fr

1. INTRODUCTION

The use of process simulators is still a complex task for process engineers. It requires know-how, considerable handling and a good knowledge of modelling and simulation. The user has many problems to face: poor communications abilities at the pre-processor level, such as global process representation from predefined models; at the executive level, data transmission hazards (from simple copy-paste to simulation parameter estimation from raw data), and potential convergence difficulties; and, finally, at the post-processor level, problems of analysis and interpretation of the results. These problems occur because simulation software is highly complex. In addition, little practical help is available. The user is required to carry out many tasks unaided. Optimised use supposes a good understanding of the software's capabilities and even an in-depth knowledge of how the software actually works (algorithm details and implementation). Some of these problems may be put down to the technical nature of the actual simulators, for instance in numerical or modelling aspects. These problems will be solved as fast as technical developments proceed. On the other hand, there are many problems that ought to be able to be solved by a better representation and exploitation of the available knowledge.

The goal of our work is to build an environment to facilitate simulator use. Assistance is based on including in the environment more information than strictly necessary for simulation purposes. It also relies on an appropriate representation and use of two kinds of available knowledge: 1- general knowledge about fundamental physical and chemical laws or heuristics, 2- user-specific knowledge about the user's process captured in an appropriate structure of the environment. A good representation of this knowledge should be transparently clear for the user. The environment is devised from an object representation of the process and uses graphical and interactive techniques. In this paper, we will emphasise the use of these techniques for the analysis and presentation of simulation results. Comprehension is facilitated by the graphical interface.

Interactivity provides flexibility, while an object-oriented approach is used to ensure a better adapted representation of knowledge.

Our second part presents some recent progress in results visualisation. This is already able to help analysis by offering easy and concise access to results. The third part describes the modelisation concepts. This is the link which helps to bridge the gap between simulation results and the engineers' ideas about the process. The concepts developed of path, aggregation and functional model are shown to improve visualisation. Moreover, this modelisation is important for the analysis tool presented in the fourth part, since it allows easy communication and better use of the tool. The fourth part introduces an analysis tool which enables results and certain expected values to be compared. The expected values are either given by the user or are some general and usually admitted chemical engineering criteria. Throughout the paper, the results analysis is applied to the process of hydrodealkylation of toluene (HDA). All the necessary data for simulation can be found in Douglas (1988). In the fifth part, a summing-up of this example shows how the concepts developed can be used.

2. VISUALISATION

Graphical interfaces have come a long way in recent years and users are now much more demanding. Some commercial process simulators (ASPEN, ProVision, ...) enable the user to give the input data through adapted and interactive windows, use the graphical interface to show the simulation convergence on the flow-sheet and give access to results from the flow-sheet (a click on a stream or a unit will give its characteristics). However, the pre-processor aspect is usually more developed than the post-processor one. Some academic work (for example, Preece et al, 1991), where simulation is associated with design, is capable of producing data-sheets. Malone (Malone and Dye, 1996) proposes to show flow-rates with proportional bars and to look at aggregated units according to Douglas's hierarchical view (Douglas, 1988). These are real improvements from the old user's interface which used to be closed to

programming languages. However, it is still difficult to fully understand the process in its entirety.

Since most results are just checked to see if logical (no wrong input, no physical inconsistency, ...), the user should be able to have a quick look at most variables through graphical visualisation rather than tables. For instance, the temperature, represented by a graduation, and heat flux, represented by proportional size arrows (Figure 1), allow the user to consider the hot and cold parts of the process and the locations of heat loads. The visualisation of results is not sufficient if only presented with raw data: results need to be organised and structured in order to be closer to the engineers' representation of the process.

3. SOME MODELISATION CONCEPTS

The modelisation consists in adding a new layer above simulation results. This layer is based on the engineer's view of the process. The developed concepts are path, aggregation and functional model.

3.1.Path

A way to present the functioning of a process is the streams matrix. This presentation is three-dimensional (x =streams, y =components, z =flow-rate and $z=z(x,y)$). This may not be easy to grasp. The user considers the process from two points of view. What do streams contain? And where do components go? Due to its internal architecture, a simulator only answers the first question. Components paths answer the second. The component path can be shown on the graphical interface (see Figure 4 -8). On the graph, there are two points of view on the paths. First, bars are used to present flow-rates. They present the real proportions of a component, as far as this is graphically possible. Secondly, a stream is considered to be part of a component path if its recovery rate is greater than a reference rate: 0.5 seems an appropriate rate, since it allows one single input and one single output stream, but the rate can be modified if required. This interpretation gives the ability to really see a path. It also avoids overlaps due to very large recycles (for example Figure 5). In addition, being able to visualise the path of each component allows us to understand the behaviour of components present in small amounts (biphenyl in Figure 8).

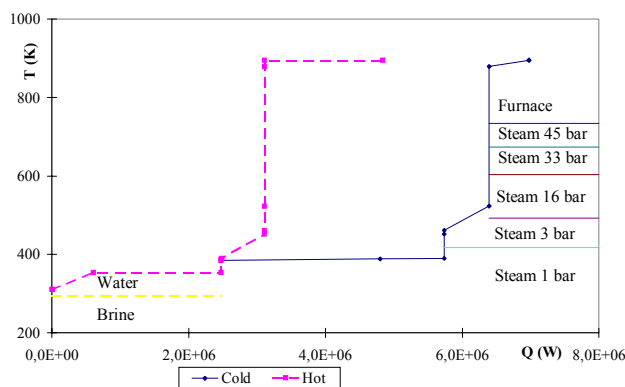
3.2.Aggregation

Chemical processes are naturally very complex because of interactions between the elements which make up the processes and because of the nature of the elements themselves. An overall view gives a better understanding of the way they work. An aggregation is a group of entities of similar type considered as a sole entity of this type. There are as many aggregation levels as necessary, ranging from global process itself to the simple elements. Three entities may be aggregated: these are units, streams and components.

Elementary units can be aggregated on aggregated units. Aggregation of units is a concept which has been

used in several chemical engineering environments (for instance, Stephanopoulos 1990). However, since unit operations can be very different, this structural modification will require some specific additional means to evaluate the aggregated structure. Malone (Malone and Dye, 1996) proposes to appraise a process by estimating its cost. He colours a unit in proportion to its cost. However, when they wish to improve a process, engineers need to consider more than simply cost alone. We propose to check if each part of the process performs the function it has been designed for. For this purpose, it is possible for a unit to be associated with a functional model (see 3.3 Functional model).

Streams are aggregated according to their nature. For aggregation, material streams are simply added together. The aggregation of material streams is associated with the aggregation of units. At the global flow-sheet level, this aggregation shows raw materials, products, by-products, gas or liquid wastes, ... (see Figure 2 and Figure 3). Such aggregation gives an accurate view of process performance in terms, for instance, of environment impact or efficiency. Aggregation of energy streams takes into account not only the amount but also the type of energy (electrical, heat...) and, for heat energy, the temperature level. Lists of hot fluids cooled-down and cold fluids warmed-up can be supplied on a table or shown on a graph (see Graph 1) with access to utilities (water, brine, cryogenics, low, middle or high pressure steam, furnace, ...). All such information is basic to any energy-savings analysis, notably pinch technology.



Graph 1: External heat loads and utilities

Finally, components may be aggregated into macro-components. Indeed, in order to determine the role of components, it is useful to group them together into solvents, gasoline, aqueous phase, wastes, products, raw materials, heavy, light... At the higher level, a macro-component groups all the components. At the lower level, macro-components are the components themselves. They may be defined for the global process (raw materials, products), for a part of the process (reactants of reaction part) or for specific units (lights in a distillation column). These macro-components can then be processed by the path.

3.3. Functional model

Functional models may be associated with elementary or aggregated units. Input and output streams are aggregated according to the given functional model. These aggregations may be modified by the user. In functional models, macro-components may be considered as well.

A functional model looks at a part of a process from the point of view of a given function. A set of performance evaluation criteria is associated with each functional model. These variables give qualitative interpretation of the functions of components and they evaluate the efficiency of the given function. There are a number of different functions in chemical engineering, such as heating, reacting, splitting... The two main functions are production (reaction) and purification (separation). These functions are the most important, and even the objectives of chemical plants. Other functions, such as heating, cooling, mixing, splitting, recycling, pumping, ... are sub-functions of the primary objective of obtaining a given quantity of a product with a given quality. Thus, the global objective of a process can often be appraised in terms of reaction and separation.

For the reaction function, components are classified into three categories: reactants, products and invariants. A component is said to be a reactant if its total inlet flow-rate is higher than its outlet flow-rate, a product if the opposite is the case, and an invariant if inlet and outlet flow-rates are equal. The reaction functional model of the overall HDA process (see Figure 2) is able to supply the following information: 1. the global reaction equation (resulting equation) which can be scaled according to one reference reactant or product (in this case, benzene), 2. conversion rates for reactants and production rates for products.

In the same way, the separation functional model gives the recovery rate and the purity of each component in each outlet since both variables characterise a good separation (Figure 3). A difficulty in using this separation functional model comes from the fact that it can be applied to any aggregated unit. This aggregated unit may include some reactors. Due to reaction, some components which are going out are not coming in (since they are produced). The recovery rate of these products is infinite. In order to avoid this kind of problems, two pseudo-streams, Production and Consumption, are generated. These pseudo-streams are streams of material only and they are build in order to have equilibrated material balances.

The first advantage of these modelisation concepts is to improve the presentation of results. Another advantage is that other tools, such as the comparison of results with expected values, can be implemented.

4. CHECKING.

Engineer require easy access to results in order to be able to compare the actual results with the original conception of the process. These ideas about the process can be of different kinds: order of magnitude,

inequality, range, Comparisons are long, tedious and error-prone. That is why we consider that an automatic process would be preferable.

Some of the variables can be checked automatically, from a physical or expert point of view. For examples : 1-, is the second thermodynamic law satisfied (The minimum difference of temperature in a heat exchanger should be higher than its default value of 5°C)? 2- is distillation column functioning satisfactory (The recovery rate of a key component in the associated output stream should be higher than a default value)? This knowledge is embedded in the model of the flow-sheet. However, some constraints are difficult to evaluate automatically. The difficulty of having a constraint for each parameter comes from the fact that some functions are hard to guess. For example, products are diverse in character; they may be objective or waste products. An objective product should have a high coefficient of global reaction (benzene in Figure 2), whereas a waste-product should have a low one (biphenyl). Even if there are some relations between product price, outlet purity and its character, the relation is not necessarily obvious and systematic. This means that it is up to the user to supply certain information. In the previous example, the engineer is familiar with the products used in the process and can easily enter the data in the model in order to have their characteristics estimated.

If before the simulation, the user has to manually input all the constraints to be automatically checked on completion of the simulation, then this automatic checking has limited interest. That is why adequate modelisation is important. Aggregations allow the user to give high level constraints to be checked on normal level results. For instance, there may be a constraint relating to the recovery rate of the macro-component on the global flow-sheet. This would imply an aggregated unit, input stream and component, i.e. three components and two input streams, that is searching for and manipulating nine values. Constraint checking gives a warning message whenever the constraint is not verified. Over and above allowing the user to input less constraints, this high level modelisation works the way the user is thinking, so that users do not need to transform their knowledge into the format of the simulator data.

5. EXAMPLE OF USE.

As an illustration of these principles, we give below one possible user's thought processes:

Since there are only five components, they are not aggregated into macro-components. Benzene is given as the reference product for the reaction functional model.

The simulation is run, and the following are checked :

1. Global process objectives through reaction and separation functional models. This is applied to the whole process (Figure 2 and Figure 3).
2. Temperature (Figure 1) and pressure orders of magnitude.

3. Components paths (Figure 4 to Figure 8).

4. External heat loads (Graph 1 and Figure 1).

This small amount of information will elicit the following remarks from the user. We give these below in order to illustrate the point:

1. The global objective of the process seems correct ; there is efficient use of toluene (99.56% is consumed). It is nearly totally transformed into benzene (1.031 toluene gives 1.0 benzene). Little biphenyl is produced. Product purities are good (0.997 for benzene and 0.990 for biphenyl)

2. Some thermal integration is already done in the reaction section. Integration could be improved: the heat produced by the Biphenyl column condenser and the reactor could be used to heat-up other parts of the process (columns boilers). Water can be used to cool down the flash and columns condensers.

3. The conversion rate of hydrogen is 58.31% which means that 41.69 % of this raw material is eliminated with the waste products. Since the preliminary studies were made to ensure the conversion rate for given temperature, pressure and reactant proportion inlet, this conversion rate could be improved by a lower feed and a higher recycle. However, a look at recycle stream G3 shows that the recycle is already very high since 699% of methane is recycled (methane is recycled 7 times before being removed by the purge stream).

4. The biphenyl path shows that biphenyl is recycled. This was not expected by the user, who then takes a closer look at the Biphenyl column. Interactivity allows a separation functional model to be applied to the Biphenyl column (Figure 9). It can be seen that 72.85% of the biphenyl that comes into the column goes into the recycle. This can be explained by the high purity required for the biphenyl component in the Biphenyl output stream (0.990), and by the fact that the biphenyl is recycled in order to limit its production. This is done by moving the reactional equilibrium.

5. These two remarks on the recycled streams lead the user to have a look at the reactor. Applying a reaction functional model (Figure 10), it can be seen that the global reaction is (hopefully) the same. However, the differences between local and global conversion rates (14.32% and 58.30% for hydrogen, 75.00% and 99.56% for toluene) show the need for recycling. The differences between local and global production rates (11.50% versus 91.83% for methane, ...) show the size of recycle loops.

6. Little hydrogen and methane (0.28% and 5.59%) escape in the H2CH4 outlet. The stabilising column is there to take what remains of these components. This is in order to avoid uncondensable gas problems in the next two columns.

The user could thus have seen the main functioning aspects of this process with only one graph, ten views (eight original ones and two requested ones) and half a page of comments.

6. CONCLUSION

A process modelisation for results analysis is presented. This modelisation has recovered concepts already used for design (aggregation of units, pinch technology, ...) and come up with specific ones of its own (aggregation of components, process objectives, ...). The understanding of the process has been enhanced by means of objective functions and path visualisation. General or user-specified automatic checking constraints allow the engineer to concentrate on important features of the process. These techniques may be extended to other procedures (test of alternatives, ...). A prototype containing the ideas presented in this paper is processed. The next step of the concepts development is a closer study of sub-functions, and an extension of constraints checking using automatic consistency checking.

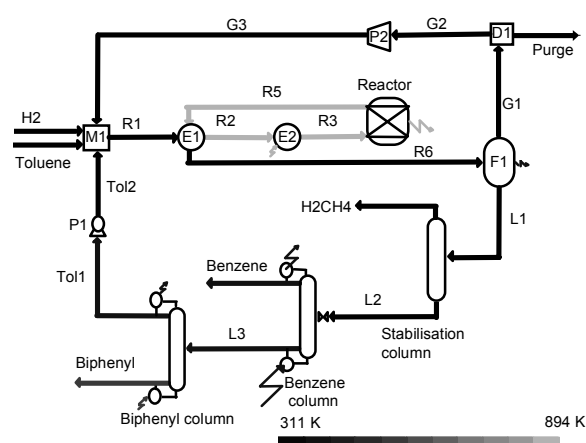


Figure 1 : Temperature path and heat loads.

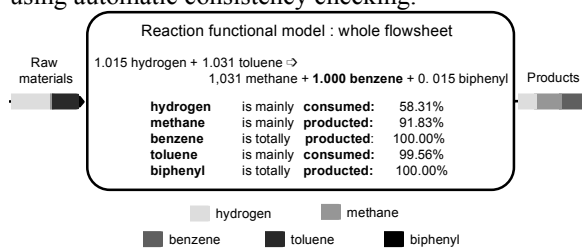


Figure 2 : Reaction functional model for the HDA process.

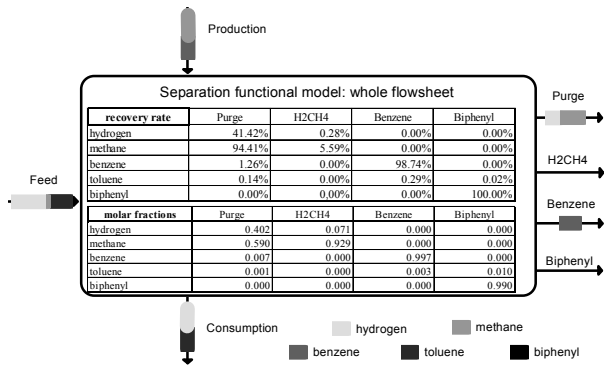


Figure 3: Separation functional model for the HDA process.

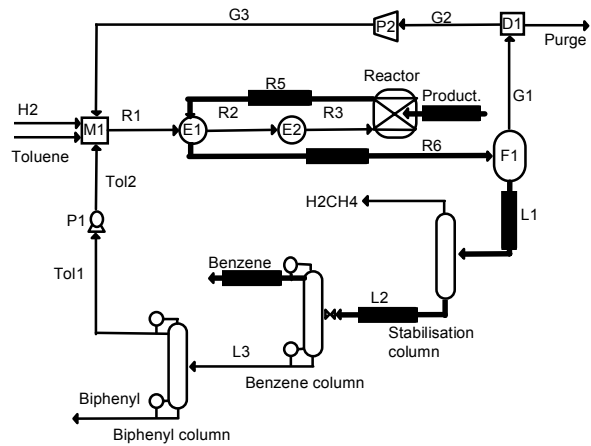


Figure 6 : Benzene path.

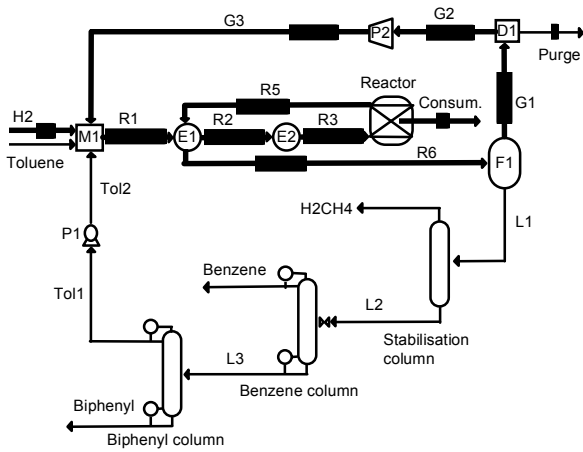


Figure 4 : Hydrogen path.

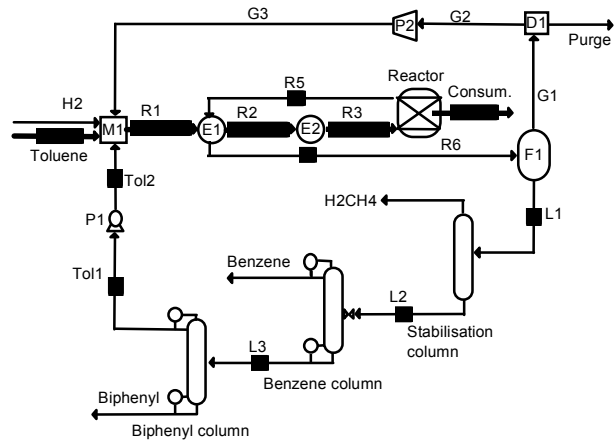


Figure 7 : Toluene path.

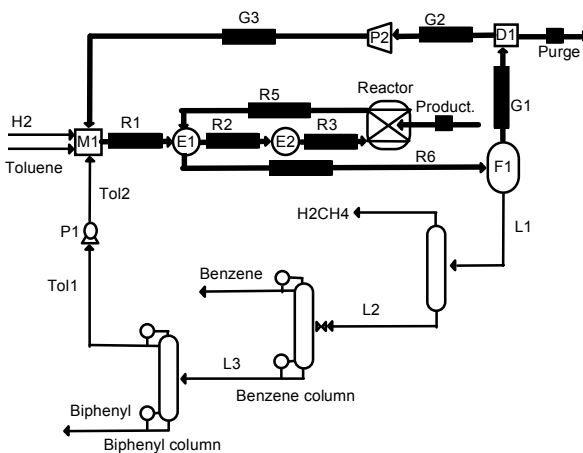


Figure 5 : Methane path.

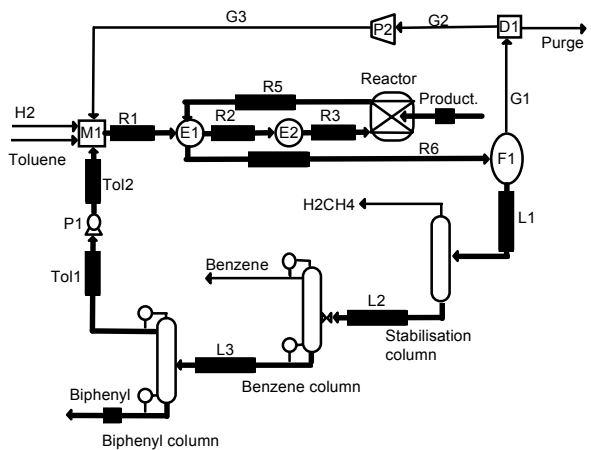


Figure 8 : Biphenyl path.

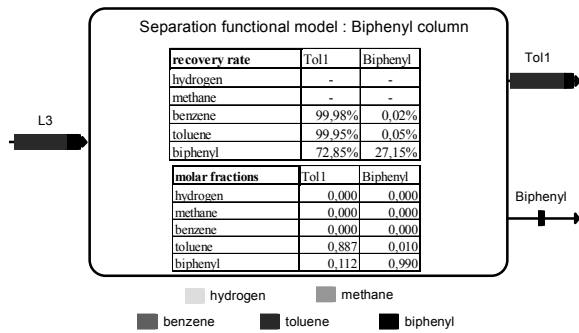


Figure 9 : Separation functional model for the Biphenyl column.

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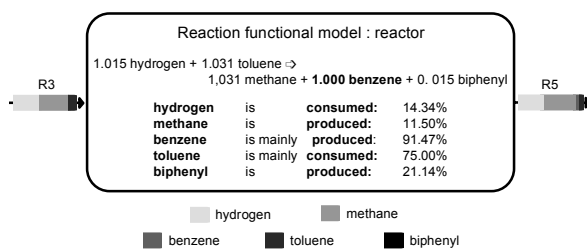


Figure 10 : Reaction functional model for the reactor.