international journal of
ADVANCES IN
SOFT COMPUTING
TECHNOLOGY

Editor-in-Chief
Dr.Vaka Murali Mohan

Object-Oriented Analysis and Design to Simulate Chemical Process Equipment

Ahmad J. Rusumdar[1]*., Sujatha.V[2] and Rajendra Prasad.P[2]

1.Dept. of Modeling, Leibniz Institute for Tropospheric Research, Leipzig, Germany

2.Andhra University College of Engineering, Vishakhapatnam-03, AP, INDIA

ABSTRACT: *A detailed representation of the process structure and of the transformations that the material in the structure undergoes is presented using an object-oriented (OO) modeling approach through the illustrative example of a jacketed reactor. The structural decomposition of the process devices gives intensification to the concepts of fundamental devices and ports. The associated elementary model results, from combining this structural decomposition with a material object and a set of hypotheses. The complete process model is then generated by aggregation of the available elementary models. By defining models on the level of technological components smaller than the classical unit operations, this modeling approach aims to meet the challenge of the model adaptability to process diversity and complexity. Implementation of this modeling is greatly facilitated by new computer technology and tools, and notably the methods and languages associated with object-oriented analysis and design.*

1. Introduction:

Research and development processes consist in general of the enrichment of existing knowledge, i. e. research done previously by other researchers is used as fundament for further investigations that deliver new results. Nowadays chemical engineering is associated with core competencies in four major areas: reaction engineering, transport phenomena, separations science, computational and systems science. Several paradigm shifts have taken place in this discipline over the years. These include the introduction of mathematical modeling in its various forms (including process control, systems approach, etc.), the shift from unit operations to transport phenomena, the recent transition towards bio systems, etc. However, one fact of chemical engineers remains unchanged, namely, that they have a responsibility of integrating the chemical engineering core constituencies with economic parameters so as to achieve commercial success. Simulation is based on models, real tools of knowledge savings on physicochemical phenomena and unit operations levels. These days, it clearly appears that the main obstacle to a larger use of simulation in the industrial community is the lack of models really suited to the user's specific needs.

*Ahmad J. Rusumdar
Department of Modeling
Leibniz Institute for Tropospheric Research,
Permoser Sraße 15, 04318 Leipzig, Germany.
Ph. No.: 004917637735149
E-Mail: ahmad.jhony@gmail.com

This is particularly true for chemical industrial equipments (i.e. distillation, reactors). Reactor modules available in simulator libraries suffer from their generality and hypotheses. The end user, who demands a better representation of the physico chemical phenomena and a perfect match for this application field (refining, petro chemistry, fine chemistry, polymers, biotechnology, food industry, etc.) and for this specific technology, cannot include this know-how and the specificity of this process.

In process engineering new findings are often achieved by computer simulation, which in many cases means to solve large equation systems numerically. This goes along with analytic determination of derivatives and with programming of functions and derivatives. New results are achieved by alternating equations or by adding new ones. All these steps are time consuming and error-prone (Grossmann & Westerberg, 2000). The same applies to keeping documentation and process methodology up to date and consistent with the program code. The problem is that the mathematical information and its equivalent programming code are kept in different documents and that these documents are updated independently and without an enforced systematic (Brandt et al., 2008).

On the other hand, the simulation problems are fully described in the literature or documentation in the form of symbolic equations and programming is thus only an auxiliary procedure. After a short overview about existing modeling tools, an object-oriented (OO) modeling approach based on a sequential decomposition of the process is presented.

Concepts of elementary device, port, material object and elementary model are defined and illustrated by a unit operation, a jacketed vessel.

2.Description of established modeling tools

To facilitate mathematical modeling, many software tools and standards have been developed. A thorough overview over modeling aspects and approaches addressing the respective difficulties is given in Zerry (2008). The most basic approach of computer modeling is using a plain programming language such as FORTRAN, for writing the equations and Jacobian matrix in a problem statement, which is subsequently solved by numeric methods taken from a library or by iteration algorithms developed especially for the problem at hand. Apart from that commercial software tools like AspenPlus or ChemCAD provide readily tested models for most of the equipment used in process engineering. While the approach of programming directly has the advantage of giving freedom in the problem description, readily programmed models are easy to use and available for more and more equipment and modeling approaches. However, it is often desired to adapt or extend existing models such that standard models in flow-sheeting tools like AspenPlus or ChemCAD cannot be used.

On the conceptual level, and consequently on the numerical level, two approaches historically conflict in process modeling and simulation: the so-called module-oriented (MO) approach and the so-called equation-oriented (EO) approach. The MO approach is used in the majority of commercial software, such as Aspen PlusTM, PRO/IITM, HysysTM and ProSimTM. In this approach, the basic element in building the model of the process is the unit operation (UO) model, called module. This corresponds to the classical and perhaps outdated view of a flow sheet. To model this process, the user selects the elementary standard modules from the simulator library, provides design and operating parameters and connects them by streams corresponding to material, energy and information flows circulating between units of the real process. The flow sheet is seen as a graph, where the nodes are the modules, and the arcs the streams. Experts in modeling have developed modules, even though the end user cannot really insert this own knowledge and the specificity of this process into them. The basic element for decomposing the process, the unit operation, corresponds to too large a scale and does not allow variety. These simulators suffer from their generality, which, after having been their strong point, has proved to be ill adapted to the present demand.

The EO approach is used in most dynamic simulators, such as gPROMSTM. These EO simulators appear above all as differential algebraic equation (DAE) numerical solvers in an environment offering an advanced modeling language. They are renowned for their numerical efficiency. Unfortunately, their UO model libraries are poor, and the user has to play the role of modeler. In the EO approach, the basic elements for building the process model are the equation and the variable, that is to say a numerical view of modeling. This numerical view limits access to these simulators to a small group of experts and not to process engineers. The enthusiasm that followed the advent of dynamic simulators in the early eighties therefore quickly disappeared.

In summary, it clearly appears that the existing modeling environments do not satisfy the appropriateness between available models, due to the diversity and complexity of physicochemical phenomena and technology. Moreover, they are incompatible with specific interfaces for integrating user models. This last point is the main motivation of the Global CAPE-OPEN project that is in the continuity of the European CAPE-OPEN project (Braunschweig et al., 1999). Standard interfaces have been defined for the four key software components of a modeling environment: unit operation module, physical properties (thermodynamics) package, numerical solver and simulation executive. The objective is to be able to define tailored simulators by assembling software components from various sources. Defining standard interfaces for the key components of existing simulators is major progress in responding to the diversity and complexity of the user's needs, but it is not sufficient. It appears necessary to adopt a new conceptual approach and especially to put aside the unit operation concept without going into a numerical and mathematical view of process modeling. The fundamental aspect for process modeling is the definition of the technological scale of the elementary components, which, by aggregation, allow the creation of unit operation, process and plant models. This goes through a hierarchical decomposition of the process structure in which the building block moves from unit operation to technological elements of the devices. This process structure hierarchy is based on an object-oriented approach.

3. Addressed Aspects in Modeling

3.1 Symbolic modeling

As described in the introduction, the transfer of mathematical equations from symbolic formulation in literature into a code that can be evaluated by a computer is very important in modeling. The process of documentation can be considered as another transfer process of information, which is as important as the former one. The optimization of these transfer process are not yet addressed by current software. The project presented in this work aims

to facilitate this part of modeling. The first step to do this is to work with symbolic description of equation systems in order to avoid differences between the display in literature and in the computer code. Several tools on the market already offer symbolic presentation of equations in numerical software. The aim in this paper is to establish a conceptual model for the evaluation of symbolic equations.

3.2 Problem reformulation

One difficulty encountered when programming equation systems in languages like C or FORTRAN is that the decision for the iteration variables and design values is a fixed part of the code. In general, a reclassification, i. e. making one or more iteration variables design values, and replacing them by former design values, takes much programming effort and testing time. In the tool proposed this step takes place before automated programming and can be undertaken without much work of the engineer.

4. OO MODELLING

As first proposed by Nilsson (1993), an OO modeling approach was adopted to define a general and open OO modeling and simulation environment for dynamic simulation of chemical processes. This environment is based on three main OO software components (Fig. 1), as follows:

ATOM: Applied Thermodynamic Object-Oriented Model, which defines a hierarchical structure of material for physicochemical properties and phase equilibria calculations (Jourda, 1996; Jourda et al., 1996).

DISCo: Object-Oriented numerical kernel devoted to the dynamic simulation of hybrid dynamic systems. This kernel notably includes a DAE numerical solver (Sargousse, 1999).

Odysseo: Object-Oriented Dynamic Simulation Software Environment, which notably defines the process structure hierarchy based on a direct abstraction of the real world (Moyse et al., 1999). This paper focuses on process structure hierarchy and the associated concepts.
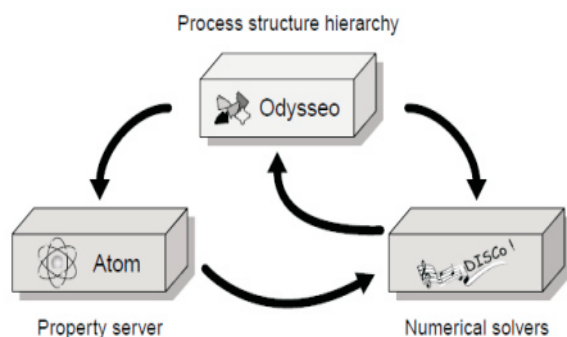

Fig.1. OO software components of the modeling and simulation environment

The Odysseo modeling approach aims to associate a detailed representation first of the process structure, and second of the transformations that the material in the structure undergoes. The proposed strategy for process modeling can be formalized by the following steps:

- ✓ The structural decomposition of the process into building blocks in a chain of command. This gives rise to the concepts of elementary devices and ports;
- ✓ The creation of the elementary model associated with each triplet: elementary device, material system, set of hypotheses;
- ✓ The aggregation of the elementary devices and consequently of the elementary models to generate the unit operation models and so on until the complete process model is established.

5. PROCESS STRUCTURE HIERARCHY

The abstraction of the process is created via a structural decomposition into meaningful physical components in a hierarchy. Uncoupling structure, or topology, material and phenomena are a basic concept. The structural decomposition of chemical processes is accomplished on two levels. The first is the process or flow sheet level and the second results in elementary devices.

5.1 Flow sheet Decomposition into Units

The structural description or topology of a chemical plant is commonly described in a flow sheet. Flow sheet describes the whole process with different subsections for reaction, separation, etc. It displays the unit operations, such as reactor, heat exchanger, and control system, used in the chemical process and how these units are connected to each other. Thus, a flow sheet represents the first level of breaking chemical processes down into units, which are the basic and classical predefined building blocks.

5.2 Unit Operation Decomposition into Elementary Devices

Depending on their complexity, the units can have an internal structure of units or subunits and so can be further decomposed. Classical examples of such complex units are distillation columns and reactors. This leads to a hierarchical decomposition and the definition of composite and elementary devices. An elementary device is defined as a simple unit or control volume, which is not or cannot be further, divided on a structural level. A composite device is defined as a recursive assembly of other composite or elementary devices. As an illustration, decomposing a batch or continuous jacketed stirred tank reactor (STR) composite device (Fig. 2) is presented. The elementary devices identified are shown in Figure 2b. These are: vessel, agitator, wall and jacket. Just to give an idea of the combinatorial explosion due to technology. The same applies for vessels and cooling systems. Technology has an impact on

physicochemical phenomena and must be taken into account. Thus, a unit operation appears as a combination of elementary devices and means of communication with the surroundings. These media are technological elements, such as flange, interface, wire respectively used for material, heat and information transfer with other elementary devices. By decomposing one unit operation into its technological elements, the internal details of the unit are abstracted and the structure becomes more comprehensible. Elementary devices of one unit can be reused as parts of other units. Elementary devices are the new key building blocks proposed for process modeling. They correspond to components smaller than the unit operations and aim to increase modelling power and thereby provide a solution to technological combinatory explosion. Elementary devices must be analyzed under different aspects:

✓ The structural aspect, with the topological description of the elementary device which notably defines the boundaries or control volume and communications with the outside world. This last point leads to the concept of ports:

✓ The material aspect, with the description of the material system that the elementary device contains;

✓ Lastly, the phenomenological aspect, with a mathematical description of the physicochemical phenomena which take place. This phenomenological descriptio depends on structure and material but also on the hypotheses made.
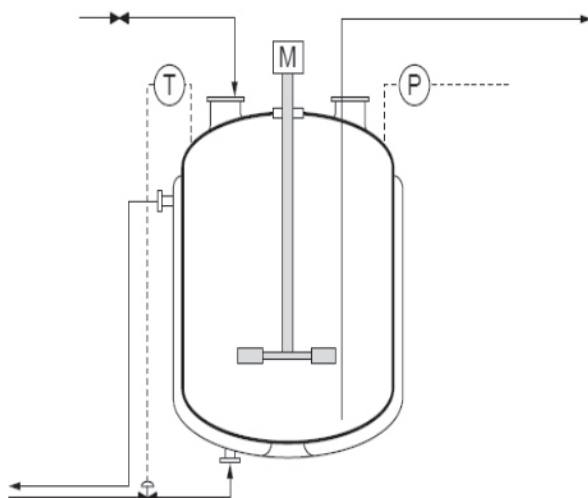

Fig.2a. Jacketed stirred tank reactor

6. CONCEPTS
6.1 Ports
As mentioned earlier, elementary devices have different means of communicating with the surroundings such as a flange for material flow, a wall for heat transfer, a driving shaft for mechanical energy and wires for measurements from sensors or actions from control systems. All these technological components allow an elementary device to exchange information with one or possibly several other elementary devices. On the conceptual level, a port is defined as an abstraction of a location on a physical device, where material, energy, or information enters or exits.
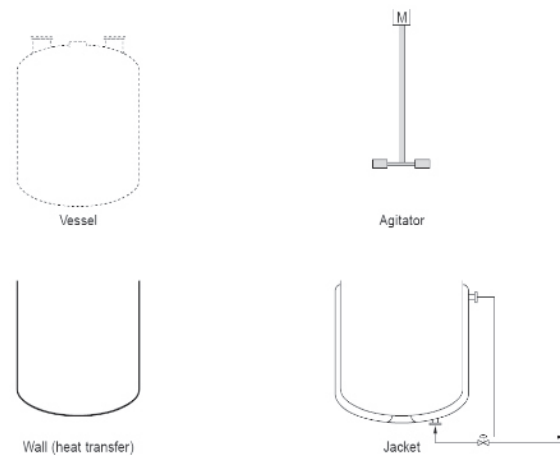

Fig.2b. Elementary devices of the jacketed STR

All connections between different unit operations, composite devices or elementary devices are accomplished with ports. Ports can be described along two axes. The first is modelling causality (inlet or outlet), and the other is the functionality of the connection: a port can be a communication port where the exchange of typed data is similar to a digital connection, or a transport port, where the exchange is qualified by a flux and a potential. Thus, there are four kinds of generic ports that can be clearly typed for specific content.

The connection between an input port and an output port is made by sharing content reference. Only the output port hosts the shared object. Communication ports (Fig. 3a) share a variable or a more complex object. An output communication port can be connected to several input communication ports: they all share the same references. There is no concept of flux, and thus their content can be broadcast to many inlet ports. On the other hand, transport ports (Fig. 3b) share a flux and a variable or a more complex object such as material or energy. The flux is defined as a function of the difference of potential variables (output input) of the two interconnected transport ports. The

potential of a transport port is a weight that determines towards which ports a real flux can be considered. The difference in potential is the driving force for the flux. This flux is defined by convention to be positive when it goes from an output port to an input port. The connection between an input transport port and an output transport port gives visibility to both in and out potentials (Fig. 3c).

Six kinds of ports can be defined:

- ✓ Material input and output ports: these ports allow material transfer. They contain an ATOM phase object. By including the phase object in the material port, not only the set of independent variables defining the intensive state of a material system (i.e. for normal fluids: composition, temperature and pressure) are accessible but also all the methods for calculating thermodynamic properties. The flux is a material flow and the potential is the pressure in the device at the port. Material ports transfer only a single phase (solid, liquid or vapour);

- ✓ Energy input and output ports: in this case, the flux is a power variable and the potential, in the case of thermal energy, is the temperature of the device at the port. Note that the attribute output denotes that the heat flux is determined by the associated elementary device and an input energy port receives the heat flux from an output energy port;

- ✓ Communication input and output ports: these ports exchange any variable or more complex object. This can be temperature, pressure, operating parameters or any other distinctive object from a device. They are useful for some specific devices such as controllers and transmitters for example. Communication ports can be specialised to exchange specific types of objects.
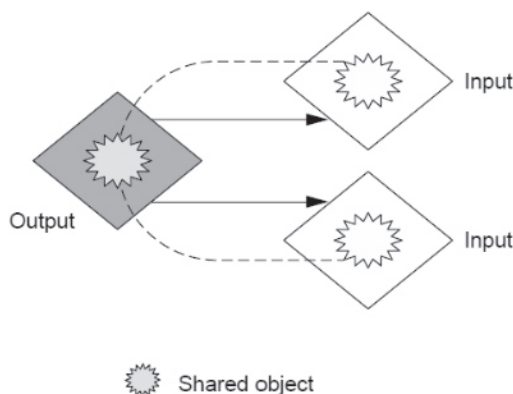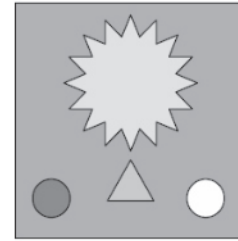

Fig.3a. Communication ports.

Fig.3b. Input & Output transport ports connected.

Material port
Shared data = flux and material object
Potential   = pressure

Thermal energy port
Shared data = flux and thermal energy object
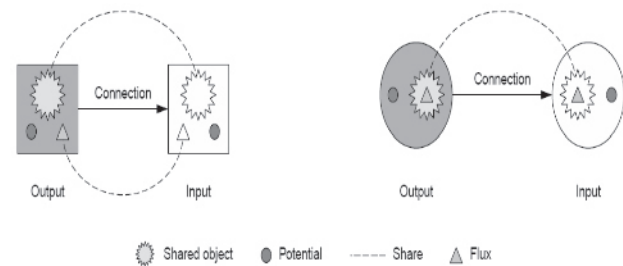Potential   = temperature

Fig.3c. Transport ports

6.2 Material System

An elementary device has to be associated with a material system. Figure 4 shows the simplified unified modelling language (UML) diagram giving the hierarchical structure of material as proposed by Jourda et al. (1996) in ATOM. Note that the UML class diagrams represent the software architecture and are used as a tool for OO analysis and design. A material system contains all the information concerning the description of matter. These are the state variables (for normal fluids: composition, temperature and pressure) and the different phases existing in the material system. The material system is associated with different thermodynamic models that can calculate the phase physicochemical properties, such as density, enthalpy, and phase equilibria. An extension of the ATOM phase system that supports chemical reactions has been suggested by Moyse et al. (1999) and a specialisation for polymerisation reactions by Skowrowski (2000).
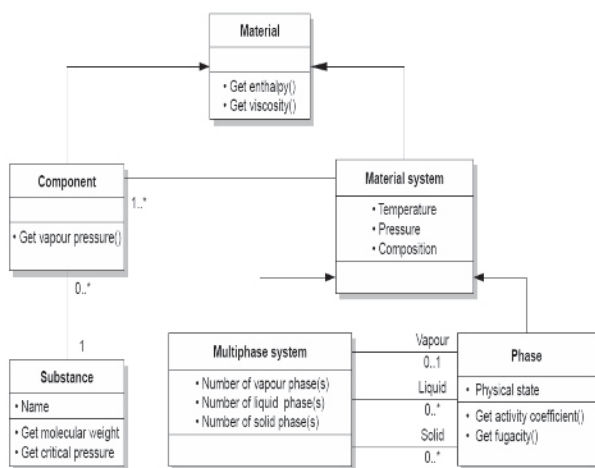
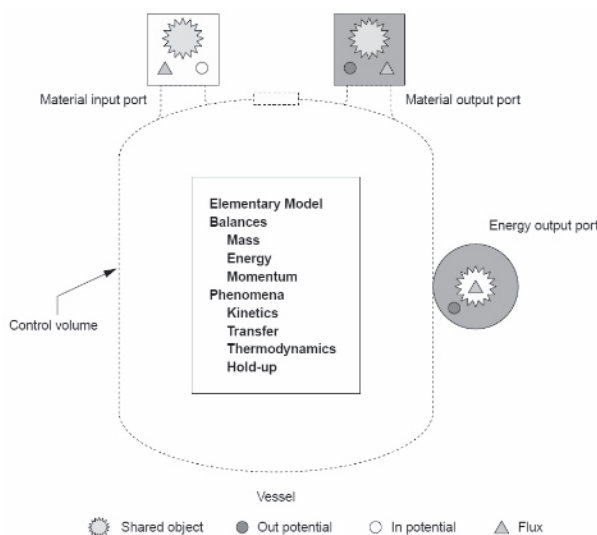Fig.4. Hierarchical structure of material (simplified UML class diagram).

Fig.5. Elementary model associated with the vessel elementary device.

6.3 Elementary Model

The elementary device is associated with an elementary mathematical model to describe the physical behaviour of the process. Elementary devices are control volumes on which balances are defined. Global and partial material balances are generated in accordance with the physical state and the causality and number of its material ports. An energy balance is generated in accordance with the causality and number of material and energy ports. All balance equations are automatically generated for any elementary device. The formulation of this mathematical model, including the overall and partial mass, energy and possibly momentum balances, must be as general and flexible as possible. The model contains additional algebraic equations associated with kinetic, transfer, holdup and thermodynamic terms. Generally, one algebraic equation links one physicochemical property to the independent variables (i.e. temperature, pressure, composition) defining the material system via a model. More specialised equations can also be introduced for specific devices. The complete elementary model is built on the triplet basis: elementary device (control volume and ports), material system, and set of hypotheses. As an illustration, the elementary model associated with the vessel elementary device of the jacketed STR is shown in Figure 5. The material object corresponds to one liquid phase and the vessel is assumed to be perfectly stirred. The vessel has one input and one output material port as well as one energy output port.

7. COMPOSITE DEVICES & AGGREGATION

Composite devices, such as unit operations, result from the aggregation of elementary devices or other composite devices. Aggregation is the connection of ports of elementary devices to generate a new building block, the composite device. The visibility of composite devices is limited to their defined boundaries, and communication with other devices is achieved by means of ports. The composite device ports are only references to the inner non-connected ports of the elementary devices. The composite device receives all the information needed from its elementary devices. The composite device model results from the aggregation of its elementary device models and some specific model equations can be added on the composite device level. The jacketed STR composite device model is presented in Figure 6.
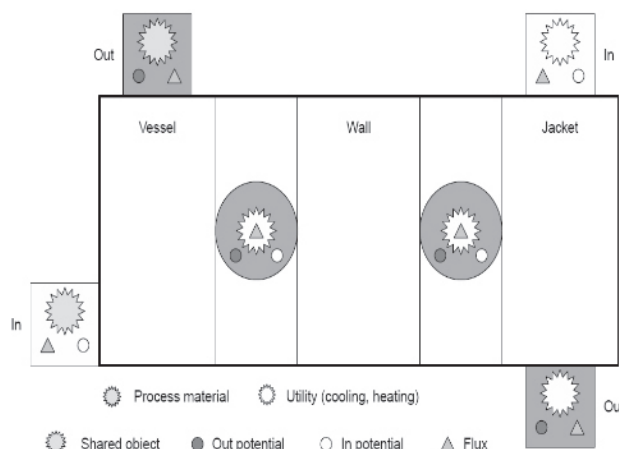

Fig.6. Jacketed STR composite device.

It results from the aggregation of the three elementary models associated with the vessel, the wall and the jacket, respectively. The wall elementary model has one input and one output energy port connected to the output energy port of the vessel elementary model and to the input energy port of the jacket elementary model, respectively. Consequently, the wall receives the heat flux from the vessel and transmits it to the jacket. The jacket elementary model has one input energy port, one input and one output material port. The material associated with the jacket elementary device corresponds to the thermal fluid while the one associated with the vessel corresponds to the process fluid.

8. CONCLUSION

In this paper, a hierarchy of chemical process structure has been presented through an illustrative example, a jacketed stirred tank chemical reactor. The basic element, the elementary device, has been characterized by its ports, its phase system, its hypotheses and its associated elementary mathematical model. Once the elementary devices are specified, decomposition is reversed by aggregating the elementary devices to make up composite devices, unit operations and finally the chemical process. By defining models on a level of technological components smaller than the classical unit operations, this Object-Oriented modeling approach aims to meet the challenge of model adaptability to process diversity and complexity. The elementary device model library is progressively becoming richer. This should considerably shorten the development time for new unit operation and process models. Implementation of this type of modelling is greatly facilitated by new computer technology and tools, and particularly the methods and languages associated with object-oriented analysis and design. The proposed approach increases model reusability and extendibility and thus allows construction of tailored simulation packages, perfectly adapted to the user's needs. Futhermore, the proposed modeling concepts can also applied to the other major chemical process equipments like, reactive distillation column, plug flow reactor, fluid catalytic cracking ...etc.

9. REFERENCES:

1. Brandt,S.C., Morbach,J., Miatidis,M., Thießen,M., Jarke,M., & Marquardt, W. (2008) An ontology-based approach to knowledge management in design processes. Comp.Chem.Engg., 32 (1-2), 320-342.
2. Grossmann, I.E., & Westerberg, A.W. (2000). Research challenges in process systems engineering. AIChE., 46, 1700-1703.
3. Jourda, L. (1996) Composants logiciels orientés objet pour la modélisation et la simulation des procédés chimiques. PhD Thesis, INPT.
4. Jourda, L., Joulia, X. and Koehret, B. (1996) Introducing ATOM, the Applied Thermodynamic Object Oriented Model. Computer & Chemical Engineering, 20A, 157-164.
5. Kuipers, J. A. M., et al., (2000) OO Concepts for Process Modelling and Simulation. Oil & Gas Science and Tech. - Rev. IFP, 55(4): p. 447-456.
6. M. Jarke, J. Koeller, W. Marquardt, L. von Wedel, and B. Braunschweig (1999). CAPE-OPEN: Experiences from a standardization effort in chemical industries. Technical report, Lehrstuhl fr Prozesstechnik, RWTH Aachen.
7. Moyse, A., Le Lann, J.M., Jourda, L. and Joulia, X. (1999) Object Oriented Framework for Process Dynamic Simulation. ECCE2 CD Rom.
8. Nilsson, B. (1993) Object-Oriented Modeling of Chemical Processes. PhD Thesis, ISRN LUTFD2/TFRT-1041-SE.
9. Sargoussse, A. (1999) Noyau numérique orienté objet dédié à la simulation des systèmes dynamique hybrides. PhD Thesis, INPT.
10. Skowronski, M. (2000) Object Oriented Software Components for the Modelling and Simulation of a Styrene Polymerisation Reactor. PhD Thesis, INPT.
11. Zerry, R., (2008), MOSAIC, Eine webbasierte Modellierungs- und Simulationsumge für die Verfarenstechnique. Shaker Verlag, Aachen, ISBN 978-3-8322-7148-0.