USE OF ADVANCED SIMULATION SOFTWARE ASPEN PLUS AS TEACHING TOOL IN CHEMICAL REACTION ENGINEERING

USO DEL SOFTWARE ASPEN PLUS COMO HERRAMIENTA DE ENSEÑANZA EN INGENIERÍA DE LAS REACCIONES QUÍMICAS

Yeison Agudelo y Rolando Barrera Zapata
Universidad de Antioquia UdeA, Medellín (Colombia)

Abstract

A comprehensive step-by-step Aspen Plus simulation for limonene epoxidation in a batch reactor using a Langmuir – Hinshelwood – Hougen – Watson (LHHW) kinetic expression is detailed described. Model validation is presented by comparison of the Aspen Plus simulated data and laboratory-scale experimental data. The RMSD between experimental and simulated data lies around $4x10^{-4}$. Thus the presented model is a valid tool for studying and analyzing the conceptual design and scale-up for the reaction system. This work is currently used in normal sessions of a Chemical Reaction Engineering course and can be used as pedagogic tool for improving inductive as well as deductive mental processes in the Chemical Reaction Engineering students.

Keywords: Reactor modeling, Chemical Reaction Engineering, Aspen Plus simulation.

Resumen

Se describe detalladamente el "paso a paso" en Aspen plus para la simulación de la epoxidación de limoneno en un reactor discontinuo utilizando una expresión cinética Langmuir – Hinshelwood – Hougen – Watson (LHHW). El modelo se valida a través de la comparación de los datos simulados con datos experimentales tomados a escala de laboratorio. La desviación cuadrática media entre los datos comparados es alrededor de $4x10^{-4}$. Por lo tanto, el modelo presentado constituye una herramienta válida para estudiar y analizar el diseño conceptual y el escalado del sistema de reacción. El presente trabajo se utiliza actualmente como herramienta de apoyo pedagógico para incentivar procesos mentales deductivos e inductivos en estudiantes de ingeniería de las reacciones químicas.

Palabras clave: Modelado de reactores, ingeniería de las reacciones químicas, simulación en Aspen Plus.

Introduction

In the teaching of science and engineering, it is very important to provide a solid background to students. This allows a better understanding of the underlying physical/chemical phenomena and encourages students to advance their knowledge in this field of study (Mahecha-Botero, 2007). Systematic robust modeling approaches, as well as individual analyses of specific case-studies are currently found in the open literature. Mechanistic modeling appears as an iterative process of representing a system found in nature by an abstract mathematical description based on physical and chemical principles in order to make predictions and gain insights about the system's underlying phenomena. Thus this process attempts to match observations with a set of equations describing and explaining what is observed and/or measured in nature, and predicting the behavior of a system. Traditionally tasks into a robust modeling approach can include, among others, the following steps: i) system characterization, ii) Identification of state variables, iii) identification of independent variables, iv) model development, v) parameter values assignment (including design parameters, operational parameters and, phisico-chemical parameters), vi) simplifying assumptions, vii) simulations and numerical analysis and, viii) model validation (Mahecha-Botero, 2007).

Now a day, the unquestionable advances in computing has allowed the combination of numerical methods and digital computers, generating powerful tools for solving the equations describing the systems in chemical engineering. These software packages have evolved into full commercial simulators compiling a variety of algorithms, numerical methods and databases that allow solving models of unit operations and full general process. Most common software architectures used for the simulation approaches include modular-sequential simulations or simulations oriented to equations (Tarifa, 1998; Scenna et al., 1999; Seider et al., 2003). In this way, many different task that use to be common and necessary steps in a typical modeling approach has become swapped for the adequate use of specific software applications, therefore the comprehensive understanding on the use of the software application can avoid spending valorous time and effort to the engineer (Cameron et al., 2009). Unfortunately, it is common to find students who do not have skills enough for comprehensive use of some particular software; when such situation is combined with weak disciplinary theoretical fundamentals, it becomes a mistake trying to use the software for solving engineering problems.

By other side, linked to the continued progress and development of computational tools, the computational aided process engineering (CAPE), dealing in this case with the specific computational tools for the modeling, simulation and optimization of chemical engineering processes, has become worldwide in a fundamental tool for the design, control and optimization of processes. The simulation of chemical processes streamlines design tasks and increases design safety, hence resulting in lower costs. The simulated control helps improve plant safety and predicts possible variability of the process by external and internal factors. Plant optimization allow to find breakpoints process, improve efficiency in the production line, analyze downtime distributions, improve operator control system, etc. Within the wide range of specialized software for process simulation in chemical engineering, which includes from spreadsheets to full simulation and optimization programs for steady state and dynamic processes (Seider et al., 2003), the software Aspen Plus (Advanced System for Process Engineering), is positioned today as one of the best in its class and is increasingly used in industry and academia worldwide. For example, in Colombia, some of the most prestigious universities have begun to incorporate the use of Aspen Plus as academic tool from earlier courses in chemical engineering programs, offering students and researchers important elements of competitiveness for the future exercise of their profession. Similarly, important colleges around the world uses process simulator as pedagogic tools for improving inductive as well as deductive mental processes (Farrell et al, 2004).

Regarding to the theory and general concepts on modeling and simulation of processes, there is a wealth of information at different levels of depth that can be accessed through several sources including open literature available online, specialized articles in scientific journals and academic texts. Notwithstanding, the accurate information regarding the specific use of a explicit software or the necessary modeling tasks for a particular process or equipment is often limited, either by the restrictions of software licenses, for the

typical generality that handle different manuals or tutorials or because the confidentiality intrinsic to the process or the plant that does not allow disclosure. In any case, it is not always possible to access a "step by step" manual or tutorial indicating how to develop or implement specific applications in specialized packages of process simulation. Such situation has been detected through the normal development of the full time curse Chemical Reaction Engineering (ChE program at University of Antioquia, Medellín, Colombia). Thus, the purpose of this contribution is to present a comprehensive description of the main features in the modeling of kinetic reactors using the software Aspen Plus, including tips for the reactor model selection, as well as the definition in the software of a heterogeneous kinetic expression. At the end of the document, there is a "check list" of main theoretical concepts that the student enrolled in this course should have present for understanding and interpreting the software results. Without a full understanding of such features, the student could present a poor probability of having success in the adequate use or analysis of the software response, even when he/she be able to implement and run the simulation.

The case-study selected for illustrating the use of the software deals with the liquid phase reaction for the epoxidation of limonene with hydrogen peroxide (Barrera et al., 2010; 2012); this system was chosen because the available peer-reviewed experimental data reported (Barrera et al., 2010) that allows an adequate model validation. In this work, a set of additional experimental data was acquired for model validation, as described in next section.

Methodology

Experimental: experimental set up is detailed described elsewhere (Barrera et al., 2010). 0.5 g limonene, 0.8332 g of hydrogen peroxide, 3.2 g of acetonitrile and 0.1 g of catalyst PW-Amberlite were placed in a glass flask immersed on a thermostatic bath provided of magnetic stirring (>500 RPM). Temperature was measured and controlled by means of temperature control system. Selected reaction conditions ensure the higher limonene reaction rates and avoid diffusional limitation artifacts (Barrera et al., 2006). 8 different samples were simultaneously prepared and each one

was retired from the reaction system at different times (3, 6, 9, 12, 15, 18, 21 and 24 h). After reaction, limonene concentration in each sample was determined by GC analysis using the chromatographic method reported by Barrera et al., (2006). In this way, experimental time-course reaction for 24 h was recorded.

Model description: Simulations were carried out using Advanced System for Process Engineering Simulation (Aspen Plus) version 8.0 (Aspen, 2014). Aspen Plus is a process modeling software suitable for a variety of steady state and non-steady sate modeling applications (Naveed et al., 2011; Yi et al., 2012). Aspen Plus software provides a flexible input language for describing reactant systems, including substances, connectivity, computational sequences, and extensive physical property database to model the properties for the process streams (Barrera et al., 2014). The use of Aspen Plus leads to an easier way of model development, maintenance and updating using the built-in model blocks.

The correct way of accessing to the software as well as the basic definition of a simulation, i.e., initializing the software, set up specifications, substances definition from software data-bases or thermodynamic model selection, can be found in several academic domains, i.e., University of Michigan (Umich, 2014). For this reason only the simulation specifications that require special attention will be fully described in this contribution.

After initializing a new blank simulation, the list of components should be provided. The substances present in the reactant system include limonene ($C_{10}H_{16}$) and hydrogen peroxide (H_2O_2) as reactant species, acetonitrile (CH_3CN) as solvent and water (H_2O) and limonene epoxide ($C_{10}H_{16}O$) as products (Reaction R1) (Barrera et al., 2010). Except the limonene epoxide all species are available in the software data-bases. They can be introduced to the simulation using the software interface. After introducing it, each one can be directly renamed in the "Component ID" field

$$C\_10\ H\_16 + H\_2\ O\_2\ \rightarrow C\_10\ H\_16\ O + H\_2\ O\ (R1)$$
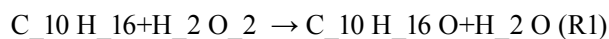
As alternative for limonene epoxide definition in the simulation, the user can choose between: i) using a probe molecule (i.e., camphor ($C_{10}H_{16}O$)) which is available in the software data-bases, or, ii) introducing

a "user defined" substance estimating its properties by a group contribution method. According to recommendations given by Barrera et al., (2009), in this work limonene epoxide was introduced as "user defined" substance by drawing its molecular structure using the software assistant (Figure 1) and establishing UNIFAC-DMD as thermodynamic model for property estimation. UNIFAC-DMD is claimed to be a suitable thermodynamic model for liquid non-ideal and non-electrolyte systems (Barrera et al., 2009). Because the presence of H_2O_2 in the simulated mixture, it is important go to the folder "Properties", the subfolder "molecular structure" and define in the Tab "group contribution" the UNIFAC-DMD groups that should be used for estimating the properties of mixtures containing H_2O_2, i.e., one group 1300 (Barrera, 2010).

Figure 1. Software assistant for drawing non-available substances in Aspen Plus
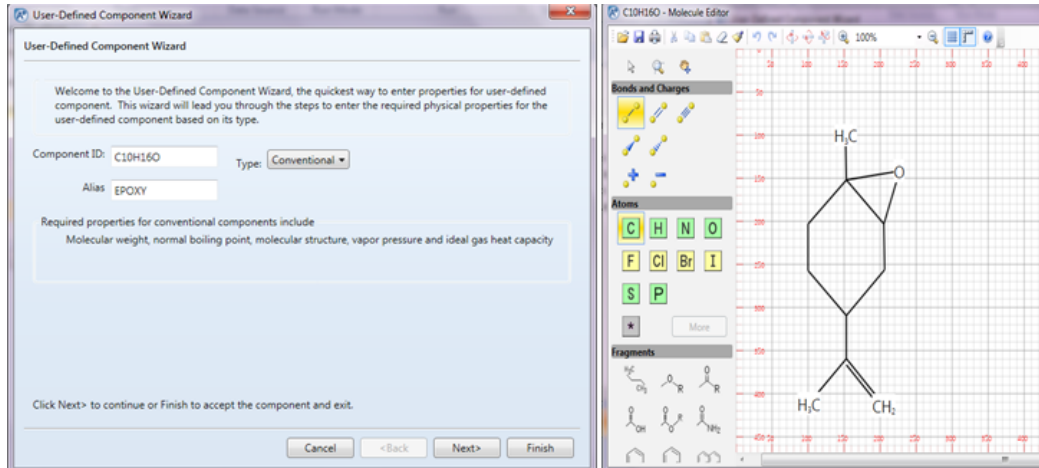
Once the substances and property estimation method have been specified, next step is going to the simulation environment (unless the user decides to analyze and explore the software possibilities for the pure substances and the mixture properties estimation). In the simulation environment, the correct definition of the flow sheet (graphic representation of the unit operations and its stream connections) involves the reactor model selection. Aspen Plus includes seven different built-in block models for reactor modeling that can be used according to the characteristics of the modeled process: RSTOIC for stoichiometric-based reactors; RYIELD for yield-based reactors; REQUIL for equilibrium-based reactor, RGIBBS for Gibbs free energy minimization reactors; RCSTR for rigorous model of continuous stirred tank reactors; RPLUG for rigorous model of plug flow reactors; and RBATCH for rigorous model of batch or semi-batch reactors, i.e., unsteady-state processes. Tip questions for the adequate model selection are given in Figure 2:

Figure 2. Tip questions for adequate reactor model selection
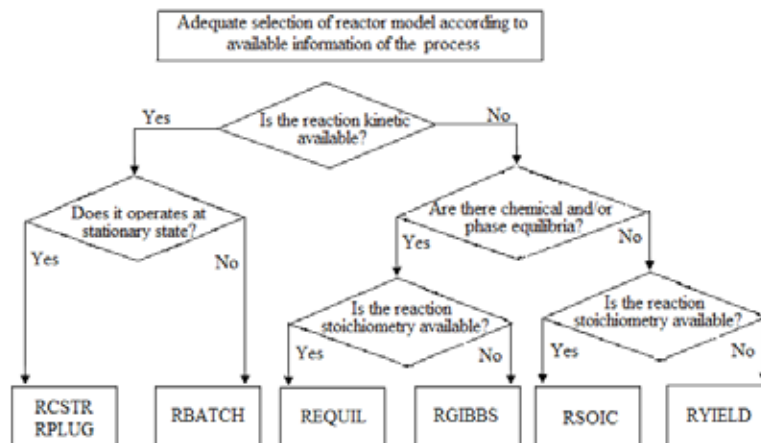
In this work, the flow-sheet used includes a batch reactor (a built-in model of Aspen Plus libraries), an inlet stream (FEED) for feeding the reactor and an outlet stream (PRODUCT) for products discharge, Figure 3. By definition, Batch reactor is a non-stationary model, thus the inlet stream (FEED) does not represent a continuous stream into the reactor. It is used for feeding reactants (charge) to the batch unit. Feeding time, batch reaction time and discharging time are further specified in the model reactor definition.

Figure 3. Flow-sheet for the batch reactor simulation
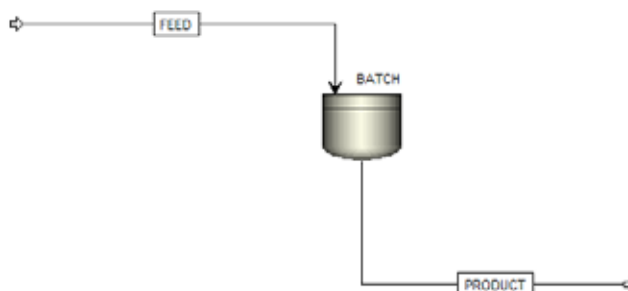
After introducing the flow sheet, the software will require the specification of the inlet stream. For model validation proposes, thermodynamic conditions on the feeding stream were specified equal to the reported experimental conditions, i.e., 33°C, 1 atm, 0.5 g of limonene, 0.833 g of 30 % wt. aqueous hydrogen peroxide (stated as 0.58329 g of water and 0.24996 g of pure hydrogen peroxide), and 3.2 g of acetonitrile. As previously described, a flow rate should be specified. It is important to remember that time units in such flow make no sense, as long as the feeding time is not included in the batch operation. In this simulation the flow rate is defined using kg. s^{-1}. Once the inlet stream is defined, the block reactor should be detailed. The first tab allows introducing temperature (33°C), pressure (1 atm) and valid phases. In this case, considering the thermodynamic state of all the substances at the operation conditions, the reaction takes place only in the liquid phase.

For introducing the reaction, it is necessary go to the folder "Reactions" (Figure 4), were reaction stoichiometry and reaction kinetic can be defined. The kinetic expression for limonene epoxidation (Equation (1)) is taken form literature (Barrera et al., 2010) and corresponds to a Langmuir Hinshelwood Hugen Watson Kinetic expression (LHHW).

Figure 4. Reaction definition
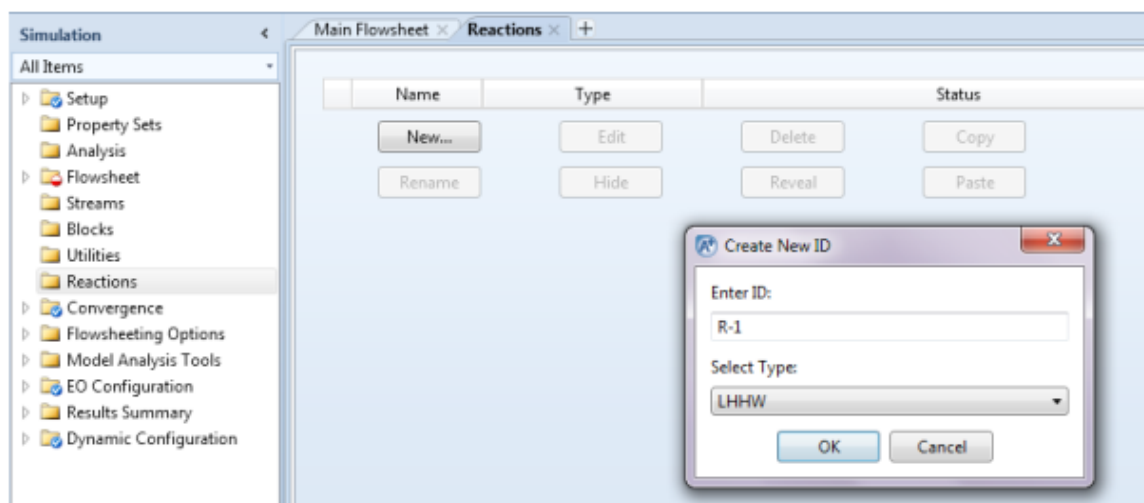
$$-r_L = \frac{k_3 k_H k_L C_T C_H C_L}{1 + k_H C_H + k_H k_L C_H C_L + \frac{k_3 k_H k_L}{k_4} C_H C_L + \frac{1}{k_E} C_W C_E + k_S C_S + k_W C_W} \quad (1)$$

Where the limonene reaction rate (-r_L) is expressed in mol. s^{-1}. g_{cat}^{-1}, Concentration C_i in mol. l^{-1} with i = H for hydrogen peroxide, L for limonene, E for limonene epoxide, W for water, S for solvent (acetonitrile), and T for total catalyst active sites. For 0.1 g of catalyst used in the laboratory scale experiments, C_T corresponds to 0.01 mol. l^{-1} (Barrera et al., 2006). Description and values for constants K_i is given in Table 1.

Table 1. Description of constants K_i from Equation (1)

Parameter	Description	Units	Value
	Equilibrium adsorption constant for hydrogen peroxide	L mol^{-1}	12.5
	Equilibrium adsorption constant for limonene	L mol^{-1}	19.0
	Equilibrium adsorption constant for acetonitrile	L mol^{-1}	1.1
	Equilibrium adsorption constant for water	L mol^{-1}	0.21
	Equilibrium adsorption constant for limonene epoxide	mol^2 L^{-2}	3.1x10^{-5}
	Pseudo-constant of reaction	L s^{-1} g^{-1}	0.97
	Products desorption constant	L s^{-1} g^{-1}	5.8x10^{-5}

Pseudo-constant of reaction, k_3 is assumed to be temperature dependent according to the Arrhenius law (Fogler, 2008), Eq, (2)

$$k_3 = k_0 e^{-E_A/RT} \quad (2)$$

with k_0 frequency factor (17873 l. $s^{-1}.g_{cat}^{-1}$), E_A the activation energy (25000 kJ kmol^{-1}), R universal constant (8.314 J mol^{-1} K^{-1}) and T absolute temperature (306.15 K) (Barrera et al., 2010). Reaction stoichiometry (Reaction (R1)) is defined in the corresponding tab, Figure 5, being in this case all coefficients = 1. After that, the kinetic can be introduced, Figure 6. The kinetic factor should be provided, that means, appropriate values for the frequency factor (k) and the activation energy (E). As temperature reference for the kinetic values from Table 1 was reported to be 33°C (Barrera et al., 2010), the T_0 label remains in blank, i.e., no temperature corrections are required for the kinetic factor.

Figure 5. Stoichiometry definition

Figure 6. Kinetic factor definition
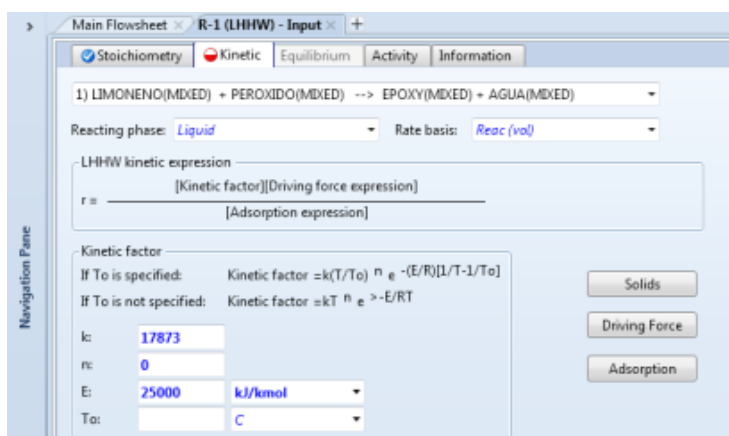
Since the kinetic expression correspond to a LHHW heterogeneous mechanistic pathway (Equation (1)), is necessary to define the driving force term and the adsorption term (Figure 6). The driving force term represents the numerator of Equation (1) excluding the k_3 value (previously introduced in the kinetic factor definition, Figure 6). In Aspen Plus is necessary to specify the driving force for forward reaction (Term 1, Figure 7) and backward reaction (Term 2, Figure 7).

Figure 7. Driving force definition
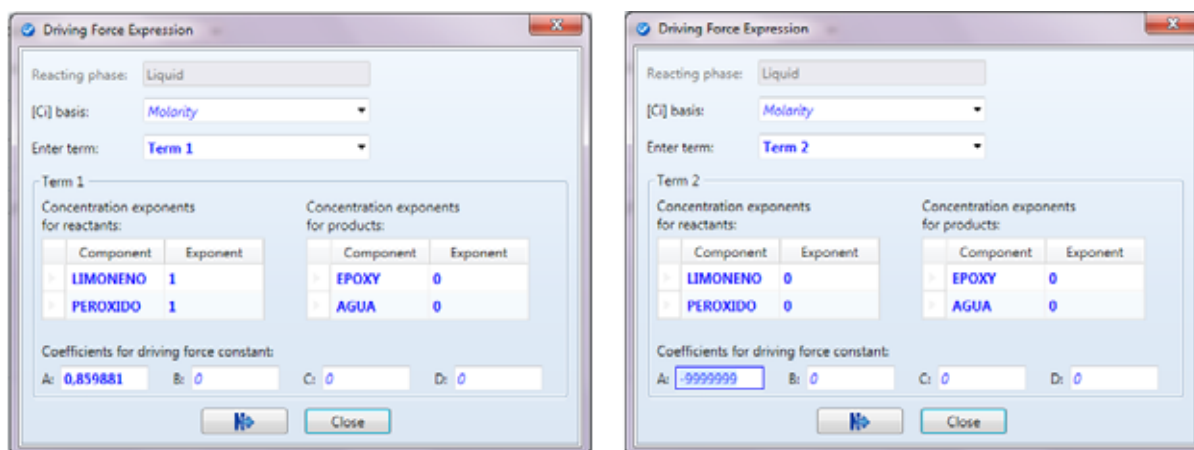
As noticed from Equation (1), the driving force for Term 1 (forward reaction) will include a coefficient estimated as the product of k_H, k_L and C_T. According to data from Table 1, this coefficient has a numerical value of 2.3629. The value introduced in Aspen (Figure 7) is 0.8599. This is because Aspen requires the value of the natural logarithm of the constant to be introduced ($e^{(0.8599)} \approx 2.3629$). The only substances present in this Term 1 are limonene and hydrogen peroxide, Equation (1), for that reason their corresponding exponents are settled in 1, while the exponents for limonene epoxide and water are settled in 0. The limonene
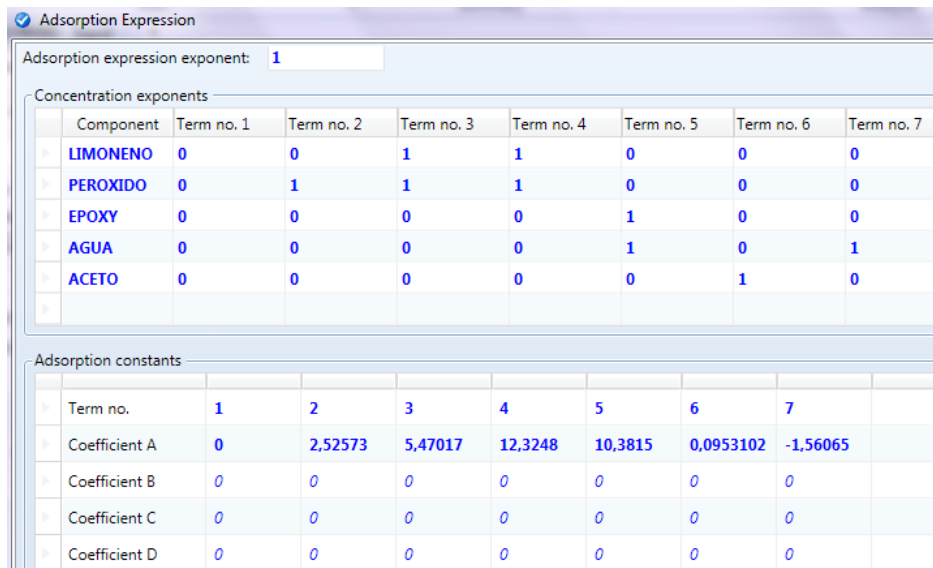
epoxidation reaction is introduced as an irreversible reaction, thus there is no backward reaction in the driving force (Term 2). In Aspen Plus, this is defined by introducing 0 in the exponent for all species and a high negative number in the coefficient for driving force constant ($e^{(-9999)} \approx 0$), Figure 7.

The adsorption expression corresponds to the denominator of the Equation (1). It is noticed that this expression includes 7 terms, the first one correspond to a constant and it does not multiply the concentration of any specie. By other side, limonene

appears in Terms 3 and 4, hydrogen peroxide in Terms 2, 3 and 4, limonene epoxide in Term 5, water in Terms 5 and 7 and acetonitrile in Term 6. The corresponding exponent for each substance in any of the Terms is introduced as shown in Figure 8. The adsorption constants represent the coefficient of any Term, estimated from values from Table 1 and being carefully of introducing in Aspen the natural logarithm of each corresponding value. Notice for example that coefficient for Term 1 should be 1, but it is introduced 0 ($e^{(0)} = 1$). By other side, the number 1 in the "adsorption expression exponent" corresponds to the global exponent of the entire adsorption term (i.e., denominator on Equation (1)).

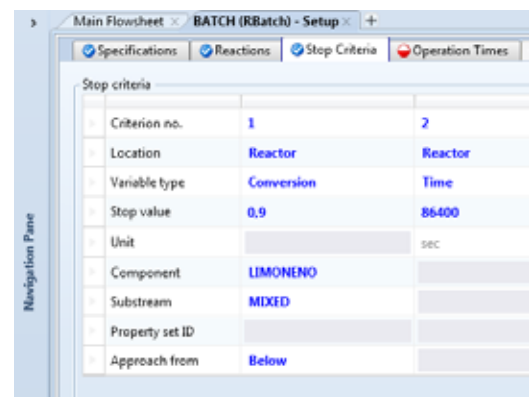Figure 8. Adsorption term definition.

Once the reaction is fully specified, is necessary to go back to the batch reactor unit, to load the reaction and specify the software stopping criteria. This is necessary because the transient nature of the simulated block. For illustrative proposes, in this simulation two stopping criteria were defined (Figure 9); thus the simulator will stop when any of them is reached. The selected stopping criteria was the 90 % conversion of limonene (criterion number 1) or 24 hours of reaction (criterion number 2), Figure 9. Finally, the operation times should be specified. According to values introduced in this Tab, Aspen will include or not the time required for loading the reactor in the batch operation cycle. In this Tab is also possible to define the time intervals for tabulating results. For this simulation, 24 h of total cycle time, 24 h for maximum calculation time, and 1 h time interval for profiles are defined.

Figure 9. Definition of stopping criteria for simulation.


Results and discussion

The software uses internal algorithms for calculations, thus no programming is necessary for modeling or

simulating the phenomena. In the stream results, it is possible to find the values for the stream mixture composition, temperature, pressure, average density, among others (Figure 10a). Figure 10b includes results for time-profiles in the reactor. The block (batch reactor) results include mass and energy balances, as well as estimation of the required heat or power for carrying out the reaction (Figure 10c).

Figure 10. Simulation results: a) stream results; b) time-profile results; c) reactor (block) results
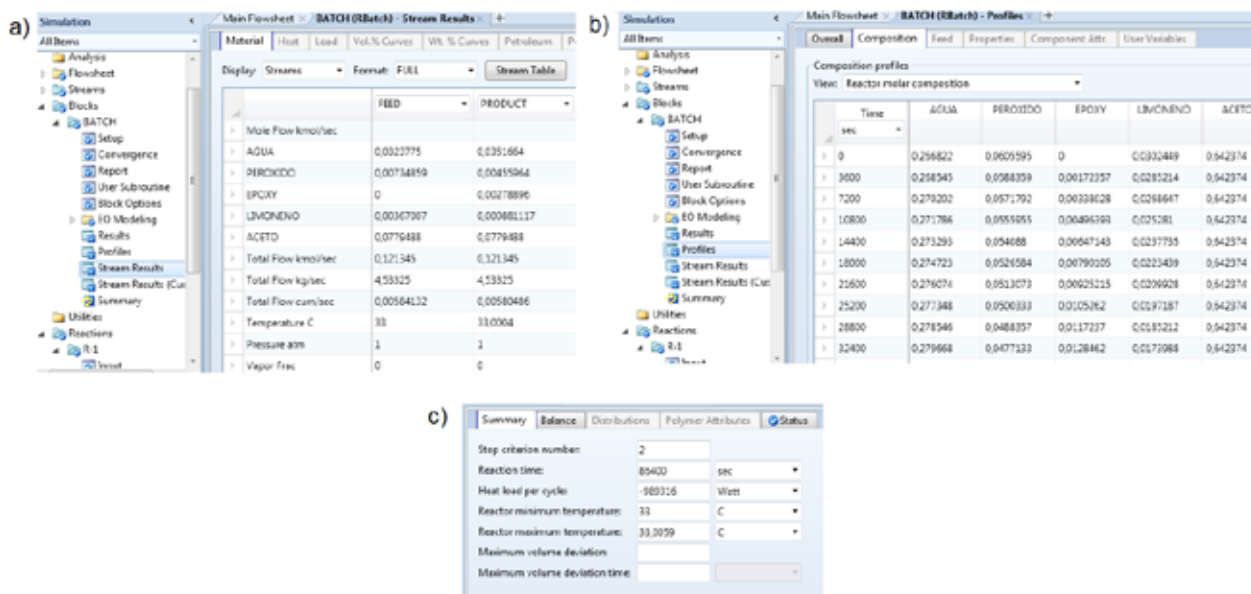

For validation of the model, the limonene mole fraction estimated with the software through reaction time (Figure 10b) was overlapped with experimental reaction data acquired in the Lab. Results are displayed in Figure 11. It is observed a good prediction capability of the model for estimating the composition of limonene during reaction. The Root Mean Squared Deviation (RMSD) between estimated and experimental data, calculated with Equation (3) lies in the order of 4×10^{-4}.

$$(3) \quad RMSD = \sqrt{\frac{\sum_{i=1}^{n}\left(X_{i,exp}-X_{i,mod}\right)^2}{n}}$$

Where X represents the limonene mole fraction; the sub index i, each one of the n samples; and n = 8, since data for t = 0 were not included in the RMSD calculation.

Figure 11. Comparison between experimental and simulated data for limonene epoxidation.
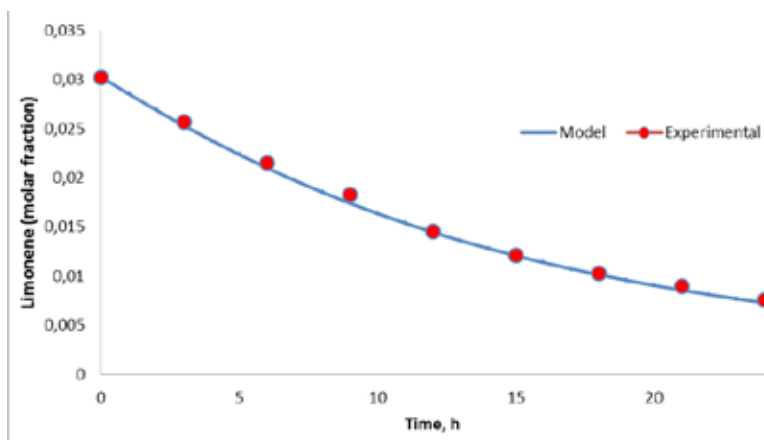
Once the model has been validated with experimental data (as previously shown) or with additional data (for example, non-isothermal reactor operation) reported in Barrera et al., (2010), it is used in the Chemical Reaction Engineering class for exploring and analyzing different reaction system features. Students are asked to formulate specific chemical reactor engineering questions and solve them exploring the software analysis tools. These questions should be responded using trial and error in the model definition; or using analysis tools of the software as sensitivity analysis. Typical questions deal in an implicit or explicit way with questions of the type "what happen if…?", for example:

- How much can be increased the limonene conversion if isothermal temperature is raised to 50°C?. It is expected that the higher limonene epoxide production compensates the implicit higher production cost related with the use of a higher operation temperature?
- What should be the amount of inlet reactants if it is desired a limonene epoxide batch production of 1 kg?
- If a continuous limonene epoxide production is desired, and a CSTR reactor will be used, what volume of reactor should be used for producing 1 kg/h of limonene epoxide?
- How many reactors CSTR operating in series are required for obtaining 24 kg/day of limonene epoxide if volume and residence time for all of them is 10 liter and 2 h, respectively?
- In terms of the reactor volume, for obtaining 1 kg/h of limonene epoxide, it is better using a CSTR reactor or a PFR reactor operating at similar conditions?
- What happen if UNIFAC-DMD thermodynamic model is changed by other model?. Why is necessary to specify the group contribution for H_2O_2 molecule (i.e., one group 1300) for running the simulation with any UNIFAC-type contribution method?

For advanced students, even more complex tasks can be derived from the model and can include introducing additional unit operations (bombs, valves, distillation towers for recovering limonene epoxide, etc.); analyzing property estimation for the multicomponent mixture; include process design, process control, process energy analysis and (or) process economic analysis.

Going back to the basic model development, it is necessary to verify that students already have capabilities to understand, at least in a basic level, the following items, otherwise, the student could present a poor probability of having success in the adequate use or analysis of the software response, even when he/she be able to implement and run the simulation:

- Basic definition of modeling and simulation
- A basic software usage: create a simulation; create a flow sheet, saving a model, etc.
- To explore software data bases for substance properties estimation
- Drawing molecular structures
- The importance of choosing an adequate thermodynamic model for the properties estimation
- The difference between typical reactor models (batch, CSTR, PFR)
- The concept of "die-time" in a batch operation unit
- The structure of non-elementary kinetic expressions (i.e., heterogeneous kinetic expressions)
- The concept of Arrhenius-temperature dependence on kinetic expressions
- The transient nature of batch processes

Conclusions

It was developed the modeling of a batch reactor using the software Aspen Plus. Such model is typically used in the chemical reaction engineering class for improving deductive and inductive mental process in students. It is assumed that students know the basic software usage, so only those items that require special attention are described in detail.

The model is validated with experimental data acquired in the lab and the RMSD between experimental and simulated data is lower than $4x10^{-4}$. Thus, the model becomes a software tool that can be used for studying and analyzing process features such as process control; process design; process scale-up; among others. With pedagogical purposes, the model can be used for studying many different chemical engineering concepts

that can include from basic theoretical frameworks (i.e., mass and energy balances, property estimation, among others), until detailed and advanced analysis of design and control. Different activities that involve deductive and inductive mental processes are compromised in the adequate analysis of the simulation results and related phenomena, the incidence of variation in selected variables on specific results, and the proper assimilation of concepts from chemical reaction engineering, as reactor and kinetic issues. The software's reasonable usage is necessary if it is used for improving typical modeling approach tasks. Thus it is important ensure in class that students have skills enough for using and interpreting the computational tool.

Acknowledgments

References

Aspen Plus TM. (2014). *Aspen Engineering Suite*, Cambridge MA, USA. Aspen Technology Inc. Recuperado el 04 de febrero de 2014 de http://www.aspentech.com.

Barrera, R., Villa, A.L., Montes, C. (2006). *Limonene Epoxidation: Diffusion and Reaction over PW-Amberlite in a Triphasic System. Industrial & Engineering Chemistry Research*, Vol. 45(13) p. 4589 – 4596.

Barrera, R., Villa, A.L., Montes C. (2009). Measurement of Activity Coefficients at Infinite Dilution for Acetonitrile, Water, Limonene, Limonene Epoxide and their Binary Pairs. *Fluid Phase Equilibria*. (275), 46 – 51.

Barrera, R. (2010). *Modelado, simulación y diseño del reactor y el proceso de separación para la producción de epóxido de limoneno*. Tesis Doctoral, Departamento de ingeniería química, Universidad de Antioquía, Medellín, Colombia.

Barrera, R., Villa, A.L., Montes, C., Ricardez-Sandoval, L., Elkamel, A. (2010). Dynamic Modeling and Optimization of a Batch Reactor for Limonene Epoxidation. *Industrial & Engineering Chemistry Research*, 49(18), 8369 – 8378.

Barrera, R., Villa, A.L., Montes, C. (2012). *Modeling and simulation of a batch distillation column for recovering limonene epoxide. Revista EIA. Escuela de Ingeniería de Antioquía*, 18, 131–141.

Barrera, R., Salazar, C., Pérez, J. (2014). Thermochemical Equilibrium Model of Synthetic Natural Gas Production from Coal Gasification Using Aspen Plus, *International Journal of Chemical Engineering*, 2014, (Electronic publication, Article 192057, DOI: http://dx.doi.org/10.1155/2014/192057.

Cameron I., Lewin, D. (2009). *Curricular and pedagogical challenges for enhanced graduate attributes in CAPE. Computers & Chemical Engineering*, 33(10), 1781–1792.

Farrell S., Hesketh, R.P., Savelski, M.J., Slater, C.S. (2004). *Process simulators in the ChE Curriculum*, Proceedings of the 2004 Western Simulation Conference, paper I051, San Diego, CA.

Fogler, H.S. (2008). *Elementos de ingeniería de las reacciones químicas*, (4ta Ed.), México: Prentice Hall.

Mahecha-Botero, A., Grace, J.R., Elnashaie, S.S., Lim, C.J. (2007). A Comprehensive Approach to Reaction Engineering. *International Journal of Chemical Reactor Engineering*, 5, (Electronic publication, Article 17, DOI: 10.2202/1542-6580.1399).

Naveed, R., Asma, A., Shahid, N., Abdullah, M. (2011). Simulation of hybrid biomas gasification using Aspen plus: A comparative performance analysis for food, municipal solid and poultry waste. *Biomass an Bioenergy*, 35, 3962 – 3969.

Qun Yi, Q., Feng, J., Ying, L. (2012). Optimization and Efficiency Analysis of Polygeneration System with Coke-Oven gas and Coal Gasified gas by Aspen Plus. *Fuel*, 96, 131–140.

Scenna, N.J., Aguirre, P.A., Benz, S.J., Chiotti, O.J., Espinosa, H.J., Ferrero, M.B., Montagna, J.M., Mussat, M.C., Pérez, G.A., Rodríguez, J., Salomone, H.E., Santa Cruz, A.S.M., Tarifa, E.E., Vega, J., (1999). *Modelado, Simulación y Optimización de Procesos Químicos*. Universidad Tecnológica Nacional, Argentina. Recuperado el 13 de agoto de 2014 de http://www.modeladoeningenieria.edu.ar.

Seider, W., Seader, J.D., Lewin, D., (2003). *Product and Process Design Principles. Synthesis, Analysis, and Evaluation*. (2nd Ed.). New York, NY: John Wiley and Sons.

Tarifa, E. (1998). *Simulación de Sistemas Químicos*. Universidad Tecnológica Nacional, Argentina.

Recuperado el 09 de julio de 2014 de http://www.modeladoeningenieria.edu.ar.

Umich (2014). *Introduction to Aspen Plus™ 2006.5*, University of Michigan. Recuperado el 16 de septiembre de 2014 de http://www.umich.edu/~essen/html/help/software/html/aspen/intro.htm.

Sobre los autores

Rolando Barrera Zapata

Ingeniero químico, Magister en Ciencias Químicas, Doctor en Ingeniería. Profesor Asistente, Departamento de Ingeniería Química, Facultad de Ingeniería, Universidad de Antioquia.

Yeison Agudelo

Ingeniero químico, Departamento de Ingeniería Química, Facultad de Ingeniería, Universidad de Antioquia.