Mejoramiento de la Enseñanza en Ingeniería a Través de Software de Dinámica de Fluidos Computacional

Enhanced Engineering Teaching Through Computational Fluid Dynamics Software

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Resumen

El curso de ingeniería de las reacciones químicas, una de las piedras angulares del programa de ingeniería química, e incluso ingeniería ambiental, se ha impartido a través de cursos introductorios que no necesariamente tienen en cuenta los conceptos de reactores no ideales, los cuales son la base para el análisis de sistemas reales como los reservorios o las lagunas aireadas. En este trabajo se presenta una estrategia para optimizar la enseñanza de la Ingeniería de las reacciones químicas por medio de software de dinámica de fluidos computacional. La inclusión de dichas herramientas computacionales permite introducir conceptos de reactores no ideales en una forma más amigable, ya que es muy fácil observar perfiles de velocidad, concentración y temperatura en geometrías bidimensionales. Al mismo tiempo, la construcción del modelo garantiza el establecimiento de conexiones con otros cursos de ingeniería, tales como transferencia de calor y dinámica de fluidos, de manera que el software no se convierta en una caja negra.

Palabras clave: estrategias de aprendizaje activo, ingeniería de las reacciones, CFD

Abstract

The chemical reaction engineering course, one of the cornerstones of chemical and even environmental engineering programs, has been taught through introductory courses that do not necessarily have into account non-ideal reactors concepts, which are the basis for the analysis of many real systems such as reservoirs and aerated lagoons. In this work, a strategy to enhance the reaction engineering teaching by means of computational fluid dynamics software is presented. The inclusion of such software tools allows introducing concepts of non-ideal reactors in a more friendly way, as velocity, concentration and temperature profiles in two dimensional geometries can be easily analyzed. At the same time, the model construction guarantees the establishment of connections with other engineering courses such as heat transfer and fluid dynamics, so that the software does not become a black box.

Keywords: active learning strategies, reaction engineering, CFD

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Introduction

It has been shown that active learning strategies help students to developed better thinking, synthesis and evaluation skills, which are the engineering essence [1]. The simulations are an effective technique to create a class environment that leads to such learning, because it brings a reality sense to the activities and promotes the formation of more active and interested studies. At the same time, these activities help the students to recognize connections between courses, the curricula and the profession, fostering the development of autonomous learning strategies.

With the introduction of software packages extremely powerful and user friendly, such as the computational fluid dynamics (CFD) programs, is possible to approach the solution of engineering problems in a more effective way, in other words, recognizing the complexity of the modeled situation as a coupled multiphysics phenomena where the momentum, heat and mass transfer mechanisms with convective and diffusive contributions are present.

Traditionally, the chemical reaction engineering teaching, one of the cornerstones that hold the chemical engineering profession because distinguishes it from other engineering professions, has been relegated to introductory courses, where the diffusive contributions of the transport mechanisms are assumed insignificant in comparison to the convective part of the equations in order to get an analytical solution of a system of ordinary differential equations. This approach, although generally accepted, brings a lack of connection with the introductory courses of fluid mechanics and heat and mass transport, in a course where the simultaneous study could be easily taken advantage of due to the wide spectrum of diverse situations that at industrial level can be explored for the formation of scientific-engineers.

Accordingly, In this paper is discussed the implementation of the CFD package Comsol Multiphysics 3.3 as a tool to improve the teaching of the chemical reaction engineering course according to the guidelines of the active learning strategies. The described case studies can be implemented as lab practices for students taking the reaction engineering course in the non-ideal reactors section. Each group can perform a parametric analysis of the system, such as the effect of the spatial time and Reynolds number in the streamlines or the stagnant region formation, and discuss the obtained results in class.

Computational fluid dynamics software

During the last years the use of computational fluid dynamics software such as Fluent®, Ansys®, Comsol® and Flow3D®, has been integrated to the modeling of non-ideal reactors in the chemical engineering curricula of American universities in major of postgraduate studies [2], [3], [4], [6], [1]. Its use is promoted by the benefits that for the teaching activity has the complete simulation of flow, temperature and concentration profiles in a chemical reactor, in bidimensional or tridimensional geometries, which can be easily visualized through color variations in the variables as a tool for the leaning process. In addition, this activities allow exploring the effect of change in system geometry or the initial conditions through the type of questions what if?.

The inclusion of teaching activities supported in these simulation packages also responds to the Accreditation Board for Engineering and Technology (ABET) criteria for chemical engineering when specifies that majors have a knowledge in modern techniques of computation, without specifically mention programming as it did in the past [3].

The computational fluid dynamics packages solve the generalized balance equations of momentum, heat and mass transfer through the finite element method (Comsol) or finite volume (Fluent). The modeling process consist on the creation of a geometry, assignation of initial and boundary conditions and the definition of the finite element method mesh. Comsol includes a chemical engineering module where the transport equations are already defined and can be easily accessible. The modeling process constitutes an efficient learning exercise because the designer has to choose the appropriate boundary conditions for the heat and mass transfer, such as insulated wall, thermal symmetry, temperature or constant heat flow and boundary conditions for the momentum transport such as non-slip or symmetry. This exercise guarantees the software does not become a black box but a tool to understand easier the transport mechanism. At the same time, the complete simulation requires to estimate the mixture parameters such as thermal conductivity, viscosity, heat capacity and diffusivity, which enables to explore the different
theoretical or empirical models available in literature and acknowledge the limitations that there exist for such purpose.

Results and Discussion

1. Case study: Anhydride acetic production

In this case study the software Comsol was used to model to anhydride acetic production from acetone in a tubular reactor. This is a class problem formulated in the book Elements of Chemical Reaction Engineering [6]. In order to point out the advantages of the software implementation in the course, an evolutive process that starts with the ideal solution described in the book and ends with a rigorous simulation is carried out.

The ideal solution does not have into account the diffusive transport mechanisms, i.e. no radial or axial dispersion and therefore the concentration and temperature variations depend only in the global movement of fluid through the reactor as a piston. This assumption is based on the turbulent flow behavior; however, this is not verified in the classical books of reaction engineering. In Comsol the ideal solution is obtained when the conductivity and diffusity are defined as zero in the heat and mass balances, and the flow velocity is assumed constant along the reactor, so that no momentum balance is included. Figure 1, shows the ideal solution for the conversion and temperature profiles.

![Figure 1 Ideal isosurface conversion (up) and temperature profiles inside the reactor](image)

Figure 1, shows that the piston flow behavior inside the reactor is valid for constant velocities, even near the reactor walls, which is not necessarily true due to existence of a stagnant layer that causes a velocity and thermal boundary layers where the viscous effects are important. The piston flow shown allow making a more concise analysis on the assumptions on which the model is supported and the validity to approach a solution.

The rigorous solution includes the momentum balance along with the heat and mass transfer balances. The thermal conductivity and diffusivity of the mixture is calculated by means of correlations reported in literature [7]. Figure 2, shows the two-dimensional rigorous simulation results for the conversion and Figure 3 for temperature.
In Figures 2 and 3, it is evident that the velocity profile calculated with the momentum equation affects considerable the conversion and temperature profiles, so that the piston flow assumption is no longer valid. Since the temperature and conversion are not constant in the reactor cross section because of the velocity profile is necessary to integrate to obtain the punctual values in the reactor outlet. Comsol includes a tool to integrate over the surface the variable value. The integrated values for the conversion and temperature are 0.11 and 952 K, which are not very different from those previously obtained with the piston flow assumption, 0.146 and 960 K. This result can be attributed to the high Re number around 5000 and the high feed temperature that promotes the convective effects, decreasing the boundary layers thickness.

In this point of the simulation is appropriate to explore the behavior of the reactor in different situations by means of what if? Questions. The effectiveness of these kinds of questions when consolidating theoretical-practical concepts has been widely acknowledged by the academic community [8,1]. In the case study of the anhydride acetic the conversion is severely limited by the strong endothermic reaction, so that the addition of a heating medium in the reactor walls in order to increase the outlet conversion can be explored. There are two possibilities to have into account in the boundary conditions of the heat balance: constant heat flux and constant wall temperature. The constant heat flow is presented with resistive heating media and the constant temperature takes place with a heat exchange fluid condensing at constant temperature of a very high fluid flow, so that the temperature change is insignificant. Figure 4 shows the simulation results for the constant temperature boundary conditions T=1035 K.
Figure 4. Constant temperature boundary condition, $T=1035 \, \text{K}$

Figure 4 shows the conversion is higher near the walls due to the low flow velocities, whereas is practically zero in the maximum velocity region. The constant wall temperature condition produces and outlet conversion of 0.29, which is higher than the obtained without external heating.

The problem of optimizing the outlet conversion is explored by means of what if questions such as what if the residence time is decreased?, what if the inlet temperature is increased? When answering these questions the inductive capacity is consolidated, essential skill when making decisions on the possible effect of the temporal variations of the operating conditions of a process.

2. Case study: Residence time distribution

It is well known that the residence time has an important effect on the performance of some non-ideal reactive systems such as the stabilization lagoons. The geometry of these systems affects the residence time distribution (RTD). Therefore, it is important to carry out experiments with tracers or estimate the RTD in order to design better treatment plants. However, the tracer experiments can be impractical due to the elevated residence time in certain geometries, so that RTD pilot plant experiments are carried out and scaled. Another possibility is to derive the RTD distribution by means of the Navier-Stokes equation and the convection-diffusion equations that the students learn in the fluid mechanics courses. All of the CFD packages (Fluent, CFX, Fidap, Phoenics, Flow3D, Comsol etc.) can accomplish this task easily [8].

The case study considers a two-dimensional reservoir with a length to height ratio of 3. Water in laminar flow and isothermal conditions are considered for the simulation. The inlet and outlet have a length of 30 cm. The simulations are carried out with Re variations, which in practical terms correspond to increase the inlet flowrate. Figure 5 shows the streamlines as a function of Re and Figure 6 shows the velocity distribution for Re 3000 and an inlet velocity of 0.1 m/s.
Figure 5 shows the stagnant region of the reservoir increases with Re, whereas at low Re the creeping flow conditions is attained. The stagnant regions characterize an inefficient system because the flow is retained longer than the average fluid residence time, and therefore stagnant regions are wasted space and most of the fluid spends a shorter time than the theoretical residence time in the reservoir (V/Q). Figure 6 shows that the velocity in the stagnant regions is practically zero.

In order to simulate a tracer experiment a step injection of a tracer component in steady state in the reservoir system was carried out. The tracer concentration was 5 mol/m³. The diffusivity of the component in water was assumed as 0.01 m²s⁻¹ so that a fast diffusion of the tracer in the stagnant zones could be observed without an excessive computational effort of several hours. Figure 7 shows the tracer concentration in the reservoir with time.
Figure 7 shows the tracer is detected in the outlet after 25 s. For 100 s the tracer concentration is not uniform due to the presence of the stagnant zones. The concentration is uniform for 200 s. With a real tracer the time to achieve an uniform concentration can be of several hours or even days because in the stagnant zones the tracer moves only by diffusion. However, the analyzed situation allows explaining the concepts of RTD. With the tracer outlet concentration with time a mathematical analysis can be posed:

$$F(t) = \frac{C_{out}(t)}{C_{in}} \quad (1)$$

$$E(t) = \frac{dF(t)}{dt} \quad (2)$$

And the average residence time can be calculated:

$$t_r = \int_0^\infty t \cdot E(t) dt \quad (3)$$

The average residence time is important to assess the operation of a reactor or reservoir. The difference between the CFD calculated values with the spatial time V/Q indicates the existence of bypasses or dead zones.

**Conclusion**

The simulation is an ideal technique to improve the students learning. These activities help to recognize connection between courses, the curricula and the profession.

The chemical process simulation is currently sub used in the chemical engineering curricula. The present paper shows a scheme to introduce concepts of non-ideal reactors to the students, which can be improved with the inclusion of simple experiments that allow comparing the theory with the simulation.

The use of CFD software in the engineering classes is advantageous because it allows the students to easily visualize and understand the involved concepts, mainly in the study of non-ideal reactors.

The residence time distribution concepts and non-ideal reactors are not familiar to major students, so that their inclusion can be difficult. The explanation of tracer simulated experiments provides the theoretical foundations for rigorous reactors performance analysis in real life applications.

**Bibliographic References**


