Teaching Laminar-Flow Reactors: From Experimentation to CFD Simulation*

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An integrated chemical engineering lab experiment is described in this paper. It makes use of a laminar-flow tubular reactor (LFTR) through consecutive lab sessions. In a first session (not described here), the pseudo first-order kinetic constant for the reaction between crystal violet and sodium hydroxide is determined at different temperatures in a batch reactor. Then a tracer experiment is used to characterize the flow pattern in the LFTR, and finally the steady-state conversion of crystal violet in the reactor is measured. For computing the theoretical reactor conversion, students must use the previously collected kinetic and tracer data, in a concept-integration exercise. A computational fluid dynamics (CFD) code (Fluent) is also used to simulate both the tracer and the isothermal reaction experiments performed in the LFTR. A very good agreement is obtained between experimental and simulated results and both only differ slightly from the theoretical predictions. The use of the CFD program is particularly noteworthy. For instance, transient simulations allow a very nice visualization of the tracer concentration front evolution, while the steady-state profiles along the axial position provide a good perspective of how reactant concentration varies within the reactor.

Keywords: chemical reactors; computational fluid dynamics; simulation

NOMENCLATURE

C	concentration of tracer, reactant or product (mol.m^{-3})
$\overline{C_{out}}$	average exit concentration of the reactant (mol.m^{-3})
E_a	activation energy (J.mol^{-1})
$ei(\lambda)$	exponential integral function
$E(t)$	residence time distribution function (s^{-1})
$F(t)$	Danckwerts' F curve
$H(t)$	Heaviside function
k'	pseudo first-order rate constant (s^{-1})
k	second-order rate constant (m^3 mol^{-1} s^{-1})
k_o	pre-exponential factor (m^3 mol^{-1}s^{-1})
L	length of the reactor (m)
Q	volumetric flow rate (m^{3}s^{-1})
r	radial position in the tubular reactor (m)
$(-r)$	reaction rate (mol.m^{-3}s^{-1})
R	internal radius of the reactor (m)
t	time (s)
$u(r)$	fluid velocity at the radial position r (m.s^{-1})
u_{max}	maximum fluid velocity (m.s^{-1})
u_{mean}	mean fluid velocity (m.s^{-1})
V	reactor volume (m^3)
X	conversion
$\overline{X}$	average conversion
$X_{overall}$	overall experimental conversion (considering both reactor and tube)
X_{tube}	experimental conversion reached in the connection tube
z	axial position in the tubular reactor (m)

Subscripts

CV	crystal violet
in	inlet conditions
out	outflow conditions
$batch$	batch reactor

Greek symbols

τ	space-time (s)
λ	$\dfrac{kL}{u_{max}} = \dfrac{k\tau}{2}$

INTRODUCTION

REACTION BETWEEN CRYSTAL violet and sodium hydroxide has been widely used for pedagogical purposes. Some important reasons are the change in colour as the reaction progresses, which is a visual reinforcement of the measured results, and also the fact of being operable at room temperature, thus reducing the complexity and cost of the experimental apparatus [1, 2]. It is well known that this hydrolysis reaction is second-order (first-order towards each reactant) [1, 2], but, if sodium hydroxide is present in great excess, it can be assumed to be pseudo first-order:

$$(-r)_{CV} = kC_{NaOH}C_{CV} \approx k'C_{CV} \qquad (1)$$

where k' is the pseudo rate constant.

Crystal violet is a highly coloured dye with a maximum absorbance at a wavelength of 588 nm. On the other hand, both sodium hydroxide and the hydrolysis product (carbinol derivative) are colourless, the corresponding aqueous solution

having an absorbance similar to that of water. So, it is possible to follow this reaction by spectrophotometry. Direct visualization is also of interest, as it provides an intuitive qualitative description of the hydrolysis progression.

This reaction was conducted by Hudgins and Cayrol [2] in a tubular reactor. The authors reported that students were very interested in the experiment, which led us to adopt it. However, we have incorporated tracer experiments for flow pattern characterization in the laminar-flow tubular reactor (LFTR). The idea is to obtain an integrated chemical reaction engineering lab experiment [3]. Indeed, during the first semester of the fourth academic year, in the current curricula of our ChE study plan, students have a laboratory course where they operate, among other experimental projects, batch and continuous-flow reactors. Using conventional tracer experiments, they characterize the flow pattern in the open reactors. The residence time distribution (RTD) then determined is used in a subsequent lab class, together with reaction kinetics data collected in a batch reactor, to predict the theoretical conversion in the same reactor, which is compared to experiment results. This experiment work is performed in three consecutive lab classes, each three hours long (one for the kinetic analysis, the second for RTD determination, and the final one for measurement of steady-state conversion).

The following semester, students deal with another kind of experimental set-ups, some of them at a pilot-scale, and handle some software tools that might be used in industrial practice. In this respect, the use of computational fluid dynamics (CFD) codes has been implemented, because these have been successfully used in practice to design commercial-sized reactors, usually with complex flow processes [4], and have a significant pedagogical potential [5, 6]. However, CFD cannot be adequately used without continued reference to experimental and/or analytical validation of numerical results [7]. Therefore, we propose that students use a CFD code to simulate the laminar-flow reactor that they studied in the previous lab course, and compare the simulated data with their experiment results (both flow pattern characterization and steady-state conversion data). Since analytical solutions are available for either the RTD or the steady-state conversion, these are an important tool for students to check the validity of their simulation results. Most of the computational work is carried out in two classes, each one being three hours long. Additional simulations can, however, be performed at home, or using the computers in the faculty computing rooms.

LAMINAR-FLOW TUBULAR REACTORS: THEORETICAL BACKGROUND

Operation of tubular reactors at high flow rates may necessitate the use of long vessels to ensure that sufficient retention time is provided for the reaction mixture. Otherwise, low conversion values are obtained. To avoid this, operation is frequently done at low flow rates (in some cases under a laminar regime), as such rates allow a greater reaction time for a given reactor, or allow the design of a shorter reactor to perform a desired conversion. Apart from the recognized industrial interest of LFTRs, particularly in processing polymer, food or other types of viscous fluids [8, 9], or in emerging areas such as monolith reactors or micro-process engineering (because flow in the channels is laminar) [10], this type of reactor has been widely used for instructional purposes [2].

In this section we present the main equations that students need to use in order to: (i) verify if the flow pattern in the tubular reactor can be modelled as a laminar-flow tubular reactor (LFTR) and (ii) predict the steady-state conversion in the real reactor.

In an LFTR with radius R, the velocity profile is parabolic and can be mathematically described by the well-known Hagen-Poiseuille equation:

$$u(r) = u_{max}\left[1 - \left(\frac{r}{R}\right)^2\right] \qquad (2)$$

where u_{max} is the fluid velocity at the centre of the pipe ($u_{max} = 2u_{mean}$). From this profile, and assuming negligible molecular diffusion of the species, the residence time distribution in an LFTR can be easily deduced [11, 12]:

$$E(t) = \frac{\tau^2}{2t^3}H\left(t - \frac{\tau}{2}\right) \qquad (3)$$

where τ is the space-time and $H(t)$ the Heaviside function. Integration of this equation provides the well-known Danckwerts' F curve, which is the normalized reactor response to a step change at the entrance:

$$F(t) = \frac{C_{out}(t)}{C_{in}} = \int_0^t E(t)\,dt$$

$$= \left[1 - \left(\frac{\tau}{2t}\right)^2\right]H\left(t - \frac{\tau}{2}\right)$$

$$= \begin{cases} 0 & t < \tau/2 \\ \left[1 - \left(\frac{\tau}{2t}\right)^2\right] & t \geq \tau/2 \end{cases} \qquad (4)$$

In the pure convection regime (negligible molecular diffusion), each element of fluid follows its streamline with no intermixing with neighbouring elements. In essence this gives macrofluid behaviour, for which the average conversion ($\overline{X}$) can be predicted by the total segregation model [11, 13]. This model assumes that fluid elements having the same age (residence time) 'travel together' in the reactor and do not mix with elements of different ages until they exit the reactor. Because no mass interchange occurs between fluid elements, each

one acts as a batch reactor and the mean steady-state conversion in the real vector is given by:

$$\overline{X} = \int_0^\infty X_{element\ of\ fluid}E(t)\,dt = \int_0^\infty X_{batch}E(t)\,dt \tag{5}$$

For first-order kinetics, conversion in a batch reactor is given by:

$$X_{batch} = 1 - e^{-k't} \tag{6}$$

where k' is the appropriate first-order rate constant (in our case $k' = kC_{NaOH_{in}}$, which must be determined at the reaction temperature and can be assumed to be constant because NaOH is considerably in excess compared with the dye). If the flow pattern in the real reactor corresponds to an LFTR, equation (3) can be used in the integration of equation (5). Otherwise, the experimental $E(t)$ data must be used.

In addition to the total segregation model, other approaches can be used for prediction of the reactor's conversion which include the mass balance or the maximum mixedness model (Zwietering equation) [11, 13]. Since the reaction is first-order (linear system), all models provide the same result, so students may freely choose which one to use.

EXPERIMENT SET-UP

The experiment set-up used for the tracer and conversion experiments is basically composed of a transparent acrylic jacketed tubular reactor (length = 1.01 m; internal diameter (ID) = 2.2×10^{-2} m), which is connected to a thermostatic bath with heating and cooling system (Huber, Polystat cc1). Solutions are fed to the reactor using a peristaltic pump with eight rolls and two channels, from Ismatec (model Reglo-Analog MS-2/8-160), and the exit stream is directed to a flow-through cell of a Jenway 6300 spectrophotometer, operating at 588 nm. Connection of the RS232 port of the spectrophotometer to a computer allows for absorbance data to be collected, saved and displayed in the monitor, at a frequency of 0.5 Hz. A simple data acquisition program was developed for this purpose in LabVIEW (National Instruments). It is noteworthy that a static mixer was introduced at the reactor's inlet (bottom) for homogenization of the reactant streams and to ensure a good distribution of the feed through the entire reactor cross-section (Fig. 1). This mixer consists of a small cylinder (20 mm length and 8 mm ID) filled with small glass beads (with diameters in the range of 850–1230 μm), followed by a conical tube (with internal diameters of 3 mm and 22 mm and a length of 10 cm), containing glass beads with $d_p \approx 3$ mm. At the reactor outlet, an identical conical tube containing glass beads ensures good mixing of the exiting streamlines.
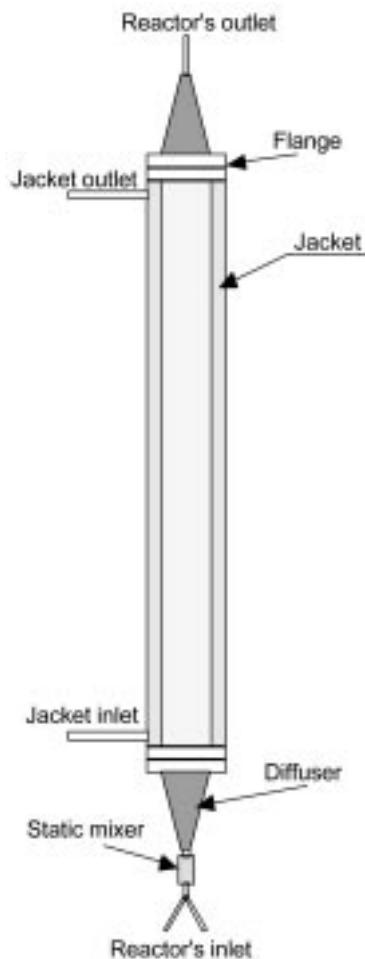

Fig. 1. Sketch of the tubular reactor.

For the flow pattern experiments, a tracer step input is made at the reactor inlet. The tubular reactor is first filled with distilled water and then one switches to the tracer solution (crystal violet at a concentration of about 1×10^{-5} M), which is fed until absorbance at the reactor outlet approaches the value previously recorded for that solution. Students' attention is drawn to the fact that a much diluted tracer solution must be used, so that its density is close to that of water and therefore does not affect the reactor hydrodynamics. Otherwise, the expected laminar profile will not be obtained, due to the action of gravity. Another crucial point is that the temperature of both solutions and that of the reactor's wall must not differ by more than about 0.5°C. Higher differences will lead to natural convection streams induced by the temperature gradients, which would also significantly affect the parabolic velocity profile.

During the tracer experiment the outlet flow rate must be determined at least three times. For the data herein provided, $Q = 0.879 \times 10^{-6}$ m^3/s. The time required for the tracer solution to reach the reactor inlet (i.e., the time spent along the path vessel $\rightarrow$ reactor), as well as the time spent between the reactor outlet and the detector, must be known

to correct the $F(t)$ curve. These values are about 48.8 s and 18.4 s, respectively. Moreover, this last value is also crucial to rectify the steady-state conversion, once reaction progresses in the connection tubes. This issue will be discussed further below.

For determination of the steady-state conversion in the continuous-flow tubular reactor, the two reactant solutions (sodium hydroxide 0.05 M and crystal violet 2.0×10^{-5} M) are fed to the bottom until a constant absorbance is recorded at the reactor outlet. The solutions were fed at a total flow rate of 0.849×10^{-6} m³/s ($\tau = 452.2$ s, which includes the time spent by fluid elements in the reactor and in the inlet and outlet static mixers/diffusers; see Fig. 1). The ratio between the two individual volume flow rates is slightly different from unity, since the two heads of the peristaltic pump are not absolutely identical (for the data herein presented, $Q_{NaOH}/Q_{CV} = 1.124$). Students are warned about this, so they should correct the absorbance of the fed crystal violet solution and the inlet sodium hydroxide concentration. It should be noticed that the basic solution is present in a concentration about 2500-fold in excess, so that equation (1) applies; i.e., the reaction can be considered as pseudo first-order. The jacket of the reactor is filled with water at a temperature close to room temperature. In the present case, the experiment was performed at 19.45°C.

CFD SIMULATIONS

Simulations of both the hydrodynamics and chemical reaction were run with the commercial package Fluent 6.0, from Fluent Inc. Although the software is quite user-friendly, it is advisable that a brief tutorial is provided so that students can quickly familiarize themselves with the program. In this tutorial, the essential steps that must be followed for any simulation should be outlined, preferably giving an example. Then different exercises can be provided for groups of two or three students, who should finally compile their results into a written report (usually of less than 10 pages), or they could discuss them in an oral presentation of no longer than 15 minutes. In any case, students should include simulations of the hydrodynamics, RTD and reaction experiments, using experimental conditions chosen by themselves (for instance, similar to those used in the previous lab course). Some groups also perform nice CFD animations, particularly for other systems/geometries.

To simulate the flow pattern in the experimental tubular reactor, a laminar 2D model was adopted, this being the system geometry (mesh) previously constructed with a pre-processing software (Gambit, in our case). For better accuracy, a computational grid containing 10,000 elements was adopted in the results presented below. Although this involves a somewhat long simulation time (several hours with a 2.00 GHz Pentium IV processor), this can easily be decreased to about 15–20 minutes if students use less elaborate meshes, without significantly affecting the precision of their results. Such less refined meshes are provided for students, who use them in the simulations performed in the class. Refining of the meshes is only advisable if students wish to obtain a higher precision in their simulations, and this can be performed outside class time.

It is noteworthy that, since the problem under study is axis-symmetric, only one half of the tube has to be considered in the geometric domain ($L = 1.01$ m, $ID = 1.1 \times 10^{-2}$ m). One face (upper, in the figures shown below) is defined in the boundary conditions as a wall (no-slip conditions and null fluxes), while the other is an axis (the symmetry axis, which corresponds to the center line of the cylindrical reactor). At the inlet, a perfectly developed parabolic profile was imposed, computed using the Hagen-Poiseuille equation (equation (2)).

The components considered were water and a tracer solution, both having identical properties, so that there is no interference with the reactor hydrodynamics. Mixture properties were computed based on fluid characteristics, using mixing-law (mass-weighted or volume-weighted) formulations.

To simulate the tracer experiments, the system is initialized imposing a null tracer concentration throughout the domain. At time $t = 0$ a step change is introduced at the reactor inlet, with uniform tracer concentration. The tracer concentration history at the reactor outlet (obtained from a mass-weighted average formulation) is then computed and saved in an ASCII file, allowing subsequent manipulation with any spreadsheet software, such as Microsoft Excel^{TM}.

For simulation of the reaction process, Fluent's steady scheme was adopted. In addition, the volumetric reaction menu was activated, requiring introduction of the reaction rate parameters (reaction order, stoichiometric coefficients, frequency factor and activation energy). The new compounds (reactants and products) and their properties were also included in the materials database, as well as the operating temperature (but an isothermal process was considered). Obviously, the mass fraction of each compound was introduced in the inlet boundary conditions.

Finally, it should be noted that all the simulation results presented here required a preliminary analysis in order to choose the best conditions and numerical algorithms to adopt, so that higher accuracy could be achieved. Students are warned about this, and to obtain smaller computational times the numerical algorithms that should be adopted are explained in their CFD tutorial. The simulations discussed below were run using the QUICK scheme, convergence criterion of 1×10^{-4} (although residuals were frequently much smaller). In the specific case of unsteady state simulations, the second order-implicit

formulation was adopted with a time step of 1 s. In this manner, the results are independent of the time-step size. The same criterion was used for the selection of the mesh size (grid with 10,000 elements).

RESULTS AND DISCUSSION

Flow pattern characterization in the tubular reactor

The data shown in Fig. 2 illustrate the history of the normalized absorbance data at the reactor outlet after performing a step change in the tracer concentration at the feed. That is, it represents the experimentally recorded Danckwerts' F curve $(F(t) = C_{out}(t)/C_{in})$, which shows the expected shape, only reaching the asymptotic value of 1 for very long times. In addition, the tracer reaches the reactor outlet at about $t = 216$ s, which is practically half the space-time, as is to be expected for a laminar velocity profile (fluid elements in the centre of the pipe have the highest velocity, $u_{max} = 2u_{mean}$, thus reaching the exit at $t = \tau/2$). While recording the data, students should pay particular attention to the parabolic velocity profile that can be seen travelling along the reactor, since its wall is transparent and the tracer solution coloured.

Because one is dealing with laminar flow in a tube, an analytical solution exists for both the residence time distribution and the Danckwerts' F curve, as shown above (equations (3–4)). In order to fit the theoretical model to their experiment results and therefore determine the value of the single model parameter (τ), students can use the 'Solver' add-in available in Microsoft Excel™ and perform a nonlinear fitting. In this case, optimization of the least-squares provided the following value: $\tau = 483.3$ s. The corresponding fitting curve is also shown in Fig. 2. Although some discrepancy exists between the experimental space-time value $(\tau = V/Q = 436.8$ s, where V is the total volume of the reactor and Q the volumetric flow rate) and that obtained from the fitting process, this is certainly not due to irregularities in the reactor's operation, like stagnant regions or by-passes. This difference is most probably a consequence of experimental errors, particularly those associated with V and Q determination. Students are asked to analyze and discuss this in more detail.

When using the CFD software to characterize the hydrodynamics in the reactor, students can start by analyzing the steady-state contours of the stream function, which illustrate the trajectories of the fluid elements. The streamlines obtained must be absolutely parallel, as expected for laminar flow, so that no intermixing occurs with neighbouring elements.

The simulated velocity profiles at any axial position are also interesting to observe. Fig. 3 illustrates a typical profile, after the convergence criteria are satisfied. In this case the tube's outlet boundary was chosen to build the velocity plot, although any other position may be created for that purpose. Data obtained show the expected parabolic profile, with the higher velocities at the centre of the tube and with null velocities near the wall. The simulated data are very well described by the Hagen-Poiseuille law (equation (2)).

After performing steady-state simulations, students may proceed to transient runs. After defining the tracer step input at the inlet boundary, the software code solves the convection-diffusion equation that describes the tracer transport and the student obtains the concentration field of tracer under transient regime. The contours of tracer concentration throughout the reactor along time are quite interesting to observe because they provide a good perspective of how the concentration front evolves. The frames recorded and shown in Fig. 4 show that it is only for $t = \tau/2$ that one starts 'seeing' tracer at the reactor outlet, as expected for laminar flow in pipes (see equation (4)). In addition, even for very long times (about five times the space-time) the tube is not completely full of tracer, due to the very low velocities near the walls.

As mentioned above, during unsteady simulations the student may save the tracer concentration at the outflow boundary in an ASCII file, so that the Danckwerts' F curve can be subsequently computed. Figure 5a shows the $F(t)$ curve
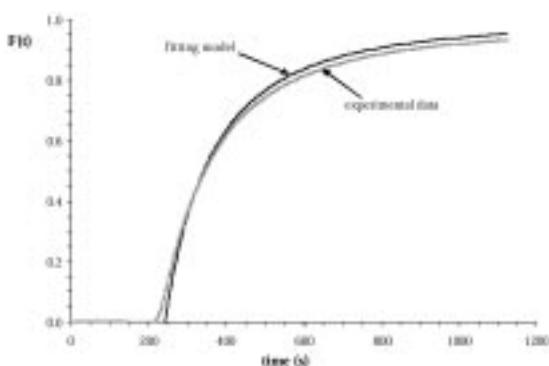
Fig. 2. Experimental Danckwerts' F curve $(\tau = V/Q = 436.8$ s) and theoretical fitting using equation (4) $(\tau = 483.3$ s).
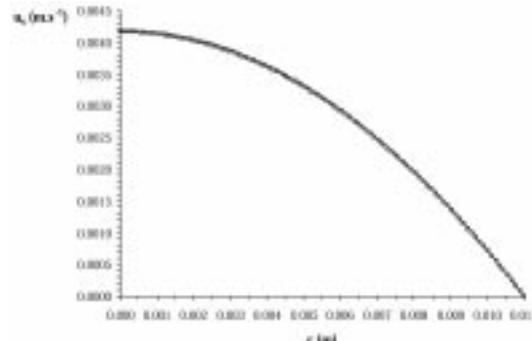
Fig. 3. Axial velocities at the reactor outlet as a function of the radial position, obtained from Fluent simulation (points) and from the Hagen-Poiseuille equation (solid line) $(\tau = 483.3$ s).
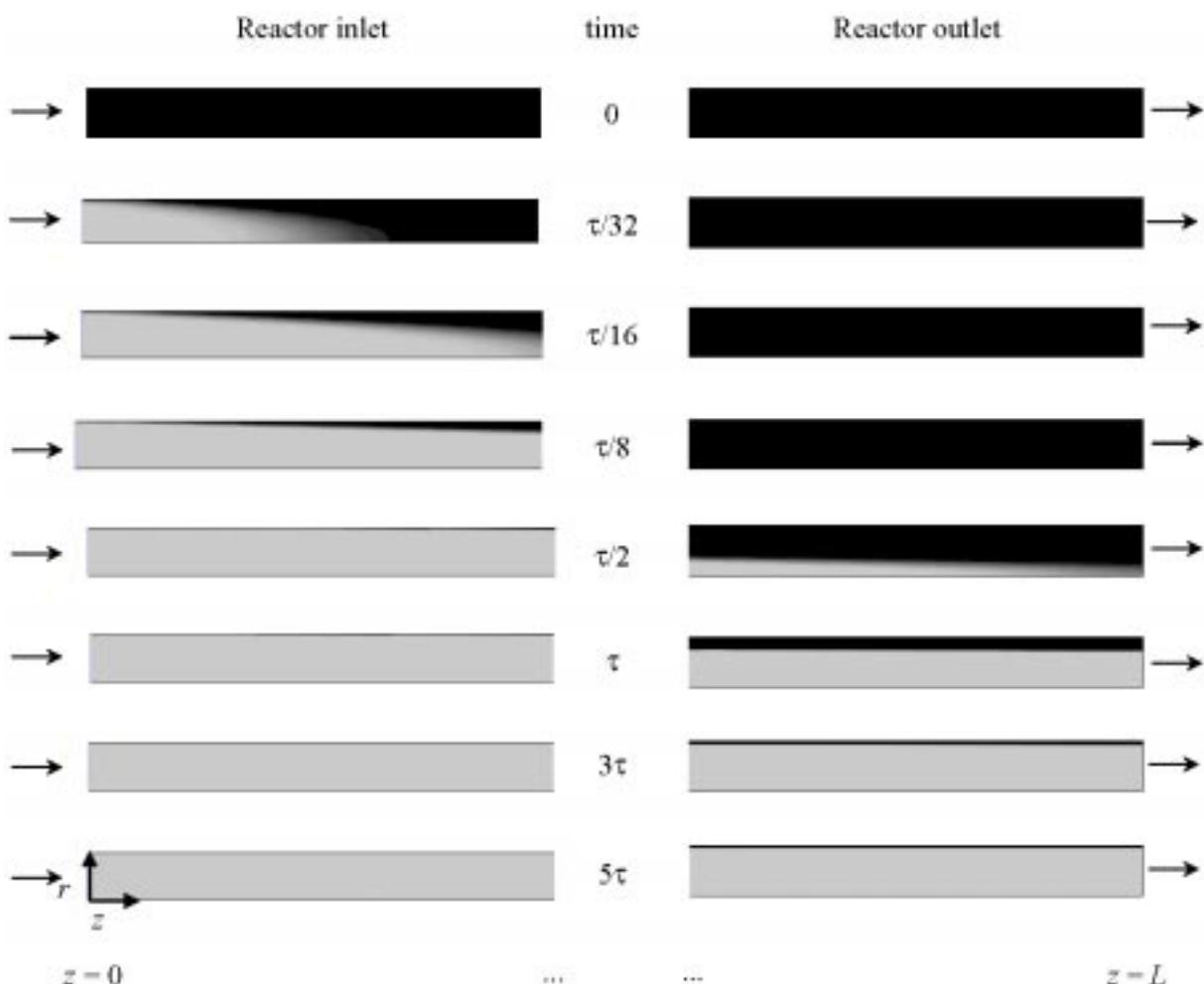
Fig. 4. Transient tracer concentration contours at the inlet and outlet sections of the tubular reactor ($\tau = 483.3$ s). The entire reactor length cannot be shown because of the high L/D ratio.

obtained from Fluent simulation. It is noteworthy that the simulated data practically coincide with the analytical solution (equation (4)), the difference being more evident at times around 240 s (see detail of Fig. 5a); i.e., when the tracer concentration front reaches the reactor outlet. Figure 5b shows the $E(t)$ curve, obtained by derivation of the $F(t)$ data, which exhibits the typical very long tail.

It should be pointed out that, although more accurate data could be obtained with CFD simulation (for instance with a more refined mesh), this is completely unnecessary. Indeed, with the numerical algorithms used and the time-step and grid adopted, the steady-state conversion prediction leads to a relative error below 1%, when comparing the Fluent simulation with the analytical solution (as mentioned below).

Students are also warned that the $E(t)$ curve does not need to be obtained from their experiment data. First, one introduces too much numerical noise when computing the derivative of the $F(t)$ curve. Second, to accurately predict the steady-state conversion directly from the RTD data, tracer experiments should be performed for very long times. Otherwise, the area under the $E(t)$ curve is not duly taken into account in the total

segregation model (compare equation (5)). Indeed, due to the very long tail of the $E(t)$ curve, the normalization condition ($\int_0^\infty E(t)dt = 1$) is only satisfied if experiments/simulations are performed for very protracted times (typically about five times the space-time, such that relative errors are below 1–2%). Therefore, conversion is predicted using the analytical RTD equation, since the flow pattern corresponds to that of an LFTR.

Determination of steady-state conversion in the laminar-flow tubular reactor

Although it is beyond the scope of the present paper, it should be noted that in a previous lab session students determined the rate constant for the reaction between crystal violet and sodium hydroxide. This is done in a batch reactor, at three different temperatures, so that the activation energy can also be obtained. Experiments performed in the range 15–25°C provided the following results for the frequency factor and activation energy: $k_o = 1.193 \times 10^7 \, \text{m}^3 \, \text{mol}^{-1} \text{s}^{-1}$ and $E_a = 6.195 \times 10^4 \, \text{J} \, \text{mol}^{-1}$ [14]. These values will subsequently be used for prediction of the theoretical conversion.
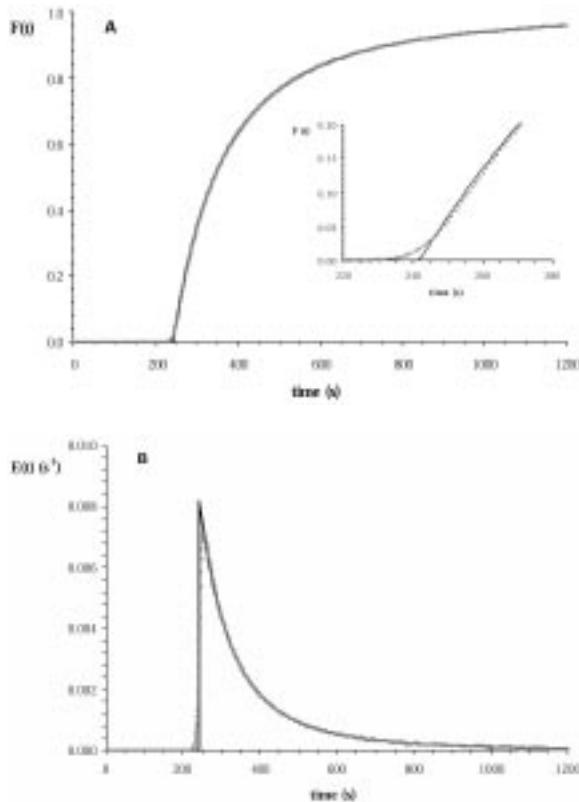
Fig. 5. Fluent simulation data (grey points) versus analytical solutions (black solid lines) for: (a) Danckwerts' F curve and (b) residence time distribution function ($\tau = 483.3$ s).

Table 1. Crystal violet conversion obtained experimentally by CFD simulation and theoretical values*.

Calculation procedure	X_{CV} (%)
Experimental value	60.9
Fluent simulation	62.6
Segregation model—equation (5)	63.0
Mass balance—equation (8)	63.0

* $\tau = 452.2$ s, $T = 19.45$°C.

In the lab, students operate the continuous-flow reactor until a constant absorbance is recorded at the reactor outlet. At this stage, a strong change in colour may be observed along the axial position, due to the crystal violet concentration gradient. From such steady-state value and the absorbance at the reactor inlet (which must be corrected taking into account the flow rate ratio of both reactant streams), a first estimate for the crystal violet conversion ($X_{overall}$) is obtained. However, since the reaction continues in the exit line before reaching the spectrophotometer cell, that value must be corrected. For reasons of simplicity, plug flow behaviour can be assumed in the tube ($X_{tube} = 1 - e^{-k'\tau_{tube}}$), and so the experiment conversion is obtained from the following equation:

$$X_{CV} = \frac{X_{overall} - X_{tube}}{1 - X_{tube}} \quad (7)$$

which can easily be deduced by students, assuming a series-association of two reactors with space-times τ and τ_{tube}. The value obtained in the experiment was $X_{CV} = 0.609$ (see Table 1).

As mentioned above, Fluent also simulates the flow system with a chemical reaction present, which simply requires the introduction of a reactive feed stream (with specification of reaction parameters, as explained). Simulation of the continuous-flow reactor via CFD can also be used to evidence the contours of species concentration along the reactor, which are particularly interesting to observe. To obtain the steady-state conversion, the surface integral for the limiting reactant (crystal violet) must be evaluated at the outer interface, using a mass-weighted average formulation. The result obtained is shown in Table 1, being less than 3% higher than the experimentally recorded value.

Once again, it is very important that students may compare their experiment and/or simulated results with those predicted from theory, because in this way they will feel more confident about their own work. First, they can use the above-described total segregation model. Once the tracer experiments have shown that the tubular reactor can be modelled as an LFTR, the $E(t)$ expression given in equation (3) can be used and equation (5) can be easily integrated. This was done with the Maple 7.00 software, and the result obtained is shown in Table 1 ($X_{CV} = 63.0\%$). It is worth noting that there is very good agreement between this value and both the experiment one and, particularly, that achieved by CFD simulation.

Finally, students can still use another approach to predict the theoretical conversion. Indeed, the mass balance for first-order irreversible kinetics in a laminar-flow reactor has an analytical solution given by [12, 13]:

$$\frac{\overline{C_{out}}}{C_{in}} = 1 - X = e^{-\lambda}(1 - \lambda) + \lambda^2 \int_\lambda^\infty \frac{e^{-z}}{z} \, dz$$

$$= e^{-\lambda}(1 - \lambda) + \lambda^2 ei(\lambda) \quad (8)$$

where $\overline{C_{out}}$ is the reactant average exit concentration, $\lambda = k'L/u_{\max} = k'\tau/2$ and $ei(\lambda)$ the exponential integral (which is tabulated in most mathematical handbooks or can be obtained from Maple software, for instance). As expected, the value obtained for the crystal violet conversion is identical to that predicted by the segregation model (*cf.* Table 1). Although application of equation (8) is also simple, the use of the segregation model has the advantage of also allowing students to predict the transient behaviour of the LFTR. For that, they should simply replace the superior limit of integration in equation (5) by t. Such a dynamic response can also be easily compared with either experiment or CFD-simulated data, although they have not been shown here.

CONCLUSIONS

The lab experiment described here is simple to operate and inexpensive. Moreover, it has been well received by students. The very nice parabolic velocity profile that can be seen during the tracer experiments and the change in colour of the reactants along the laminar-flow tubular reactor (LFTR) help to reinforce what students have learned from theory. Besides, theoretical prediction of the steady-state conversion requires that students use data from previous lab sessions, namely the RTD function and the kinetic data, thus giving a concept-integration character to the experiments.

After performing the lab classes, a CFD code is proposed for use by students (although in a subsequent course), and then they are asked to: (i) characterize the hydrodynamics in the LFTR; (ii) determine the residence time distribution (or simply the $F(t)$ curve) from a tracer experiment; and (iii) predict the steady-state conversion in the continuous-flow reactor. Finally, comparison of the numerical simulations with their experiment results and analytical solutions improves their self-reliance, since the differences obtained are typically small.

Our experience shows that the use of computer-aided simulation, particularly with the help of a CFD code, allows students to more easily explore and understand some of the basic concepts taught. The use of colour in the graphical representations allows for easy visualization of the flow phenomenon, which can significantly facilitate and enhance the learning process. Also, students can easily explore the effects of changing the operating conditions without requiring additional lab experiments. Finally, the use of other reactor dimensions or configurations or even other reactions can easily be investigated.

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