

TEACHING NONIDEAL REACTORS WITH CFD TOOLS

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Behavior of nonideal reactors and their flow pattern characterization are issues taught in a majority of chemical reaction engineering (CRE) courses^[1-4] (depending on the curriculum structure, usually at the undergraduate level) and therefore they are addressed in most CRE textbooks.^[6,8-8] In this respect, the classical stimulus-response tracer experiments^[9] are essential to obtain theoretical functions such as the residence time distribution (RTD), which are crucial for diagnosis of equipment operation, reactor modeling, and prediction of conversion. Comprehension of the involved concepts, which are not easily grasped by students, can be improved with laboratory sessions—but this is not always feasible. This disadvantage can be overcome, however, by implementing computer simulation of tracer experiments,^[10] particularly with a commercial computational fluid dynamics (CFD) tool.^[11-13]

CFD codes have been widely used for simulating flow pattern in real systems, and their use in a chemical engineering undergraduate course has several advantages, as pointed out by Sinclair.^[14] Among those advantages are: first, the use of color in CFD plots allows students to visualize flow behavior, and this visualization of the flow phenomenon can significantly facilitate and enhance the learning process. Second, students can explore the effects of change in the system geometry, system properties, or operation conditions. All these advantages, apart from the fact that students *like* to experience software tools used in industry (which are usually user-friendly), justify implementation of CFD codes in CRE courses, particularly when teaching RTD theory.

Such tools have some disadvantages and/or limitations, however. Commercially available codes may be extremely powerful, but their operation requires a high level of skill and understanding to obtain meaningful results. In addition, CFD cannot be adequately used without continued reference to experimental and/or analytical validation of numerical results.^[13]

The case study described here can be implemented as homework for students taking a CRE course dealing with nonideal reactors. Simulations can be performed using a commercial

package such as Fluent, but it is advisable that a brief tutorial be provided so students can quickly familiarize themselves with the program. In this tutorial, the essential steps that must be followed for any simulation should be outlined. Different reservoir/reactor geometries can be provided for different groups of two-to-three students, but each group should perform its own parametric study (*e.g.*, evaluate the effect of space-time, or Reynolds number, in flow pattern characterization, or Damköhler number in reaction simulations). Finally, the students should compile the results obtained by other colleagues and discuss them in a final written report.

Using 2-D reservoirs/reactors with laminar flow (described in detail in the next section), students should perform the following tasks, which are also the objectives of this paper:

1. Characterize the hydrodynamics in the vessel(s).
2. Determine the RTD from tracer experiments, which includes diagnosis of reservoir/reactor operation.
3. Predict the conversion in a continuous-flow system.

CASE STUDY FORMULATION AND SIMULATION WITH FLUENT

It is well known that the mean residence time (\bar{t}_r) has an important effect on the performance of some large natural

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conversion systems, such as biological lagoons, since it affects the biological conversion of biodegradable matter. Moreover, the geometry of the reservoirs seems to affect the RTD, and thus \bar{t}_r . It is therefore very important to perform tracer experiments in these systems (or try to estimate the RTD function) in order to better design such wastewater treatment plants. The mean residence times in these large reservoirs or lagoons are extremely high (ranging from one day up to several months^[15,16]), however, so tracer experiments are impractical.

Possible strategies to overcome this problem involve obtaining the RTD on pilot-scale setups with various geometries, where tracer experiments are easily conducted, and performing a scale-up analysis, or deriving the RTD by solving the Navier-Stokes and diffusion-convection equations that students learned in the fluid mechanics curricula.^[e.g.,16] Commercially available CFD packages (*e.g.*, Fluent, CFX, Fidap, Phoenix, STAR-CD, FLOW3D, etc.) can readily solve the balance equations for reactor operation coupled with the Navier-Stokes equations. Thus, we adopted the second approach.

The case study considers a 2-D reservoir with dimensions L (length) and H (height) in laminar flow and isothermal conditions (see Figure 1). Reservoirs with different aspect ratios (L/H) were considered, varying between 0.5 and 20 (with $H = 0.1$ m). Both the inlet and the outlet boundaries of the reservoirs have a height of 0.01 m, with distances from the bottom of the reservoir of 0 and 0.02 m, respectively. A fully developed parabolic velocity profile is imposed at the inlet boundary

$$u_x = U_{\max} \left[1 - \left(\frac{y - H/20}{H/20} \right)^2 \right] \quad (1)$$

where U_{\max} is the fluid velocity at the center of the inlet boundary, $U_{\max} = 1.5 U_{\text{mean}}$. A constant species concentration profile is assumed at the inlet boundary. On the walls (see Figure 1), no-slip conditions are assumed ($u_x = u_y = 0$) and a null flux (zero gradient) of species concentration is imposed. At the outflow boundary condition, the CFD code extrapolates the required information from the interior cells (a zero diffusion flux is assumed for all flow variables in the direction normal to the exit plane). In the simulations, the Reynolds number,

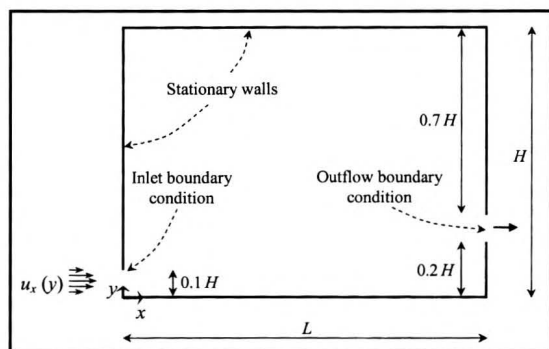


Figure 1. Sketch of reservoir geometry.

here defined based on inlet conditions, ranged from 1 to 100. Changing Re for a given fluid and reservoir is equivalent to changing the fluid velocity (and thus the residence time).

The governing equations to be solved are (for an incompressible fluid)

Continuity

$$\frac{\partial u_x}{\partial x} + \frac{\partial u_y}{\partial y} = 0 \quad (2)$$

Momentum

$$\rho \frac{\partial u_x}{\partial t} + \rho \left[\frac{\partial(u_x^2)}{\partial x} + \frac{\partial(u_x u_y)}{\partial y} \right] = -\frac{\partial P}{\partial x} + \mu \left(\frac{\partial^2 u_x}{\partial x^2} + \frac{\partial^2 u_x}{\partial y^2} \right) \quad (3)$$

$$\rho \frac{\partial u_y}{\partial t} + \rho \left[\frac{\partial(u_x u_y)}{\partial x} + \frac{\partial(u_y^2)}{\partial y} \right] = -\frac{\partial P}{\partial y} + \mu \left(\frac{\partial^2 u_y}{\partial x^2} + \frac{\partial^2 u_y}{\partial y^2} \right) \quad (4)$$

Species Transport

$$\frac{\partial C}{\partial t} + \frac{\partial(u_x C)}{\partial x} + \frac{\partial(u_y C)}{\partial y} = D \left(\frac{\partial^2 C}{\partial x^2} + \frac{\partial^2 C}{\partial y^2} \right) + S(C) \quad (5)$$

In Eq. (5), $S(C)$ is a source term. For the transport of an inert tracer, by convection-diffusion, $S(C) = 0$, while for the transport of a reagent species, $S(C) = -kC$ (assuming a first-order irreversible reaction).

Simulations were run with the commercial package Fluent 6.0. The fluid considered is water ($\nu = \mu/\rho = 10^{-6} \text{ m}^2\text{s}^{-1}$), and a tracer solution was created in Fluent's database with identical properties of water, so that it does not affect reactor hydrodynamics. A molecular diffusivity of $5 \times 10^{-10} \text{ m}^2\text{s}^{-1}$ was considered, which is a typical value for liquids.^[17] A tracer step input was used, with uniform concentration across the entrance section, together with the parabolic velocity profile defined in Eq. (1).

Fluent can simulate both the hydrodynamics and chemical reaction processes, and therefore the reservoirs previously considered can be used for modeling continuous-flow reactors (*e.g.*, biological lagoons). In this case, simulations were run by defining a reactant and a product, both with properties identical to water. The reactor is initially full of water (inert), the laminar flow is established; after that (time $t = 0$) the reactant is fed to the reactor, similarly to the tracer step input. Conversion of reactant is calculated based on the time evolution of species concentration at the reactor exit, obtained from a mass-weighted average formulation.

We must point out that to achieve a high level of accuracy, all the simulation results presented in this paper involved a detailed analysis of the numerical algorithms, the mesh employed, and the time step adopted (in transient simulations). For instance, the QUICK scheme of Leonard^[18] was selected for discretization of the convective terms, a second-order

implicit formulation was used during unsteady stimulation, and the computational grid contained typically 100x100 elements (note that for reservoirs with $L/H \gg 1$, it is convenient to use a larger number of cells in the x-direction). It is always a good practice to perform the calculations on several meshes with different levels of refinement in order to obtain mesh-independent results. A similar procedure should be adopted regarding the time step used in transient calculations. A control-volume approach is used by Fluent to numerically solve the governing equations.^[11]

RESULTS AND DISCUSSION

► *Hydrodynamic Characterization*

Figure 2 shows contour plots of the stream function within the reservoir, with $L/H = 1$, which illustrates the trajectories of the fluid elements (streamlines). For a given inlet velocity (or more broadly speaking, a given Reynolds number), the formation of a recirculation zone above the entrance of the reservoir, where velocity is small, is evident, thus suggesting formation of a stagnant region. It is noteworthy that the importance of such a region increases with Re , becoming particularly large for Re values around 100 where fluid trajectories are almost linear. Lower Re numbers lead to a smaller stagnant region and more curved streamlines. For $Re < 1$, inertia is negligible and the trajectories obtained are equivalent to creeping-flow conditions.

For longer reservoirs, the conclusions are similar, but now the importance of the recirculation zone decreases (for the same fluid inlet velocity). Indeed, the steady state streamlines shown in Figure 3, obtained for a reservoir with $L/H = 5$, show formation of a stagnant zone above the entrance, where the size increases with the Reynolds number. Comparison with the stream function contours of Figure 2, however, shows that for the same Re , the fraction of dead volume decreases when the geometric ratio L/H increases.

► *RTD Determination from Tracer Experiments*

After performing steady state simulations, students can proceed to transient runs, but they must first define a tracer step input at the inlet boundary condition. They must also be aware that for $t = 0$, no tracer exists within the reservoir and that the laminar flow is already established. They must first initialize the entire domain with a null tracer concentration and wait until the laminar regime is established before introducing the tracer step change at the inlet. After that, the CFD code solves the convection-diffusion equation that describes the tracer transport in the reservoir and the concentration field of tracer under transient regime is obtained. Particularly interesting is its concentration at the outflow boundary, $C_{out}(t)$. The contours of tracer concentration throughout the reservoir along time are also very interesting because they provide a good perspective on the evolution of concentration fronts. For a reservoir with $L/H = 1$, some frames were recorded at different times and are shown in Figure 4. They

show that only for $\theta = t/\tau$ around 0.22 can one start to 'see' tracer at the reservoir exit. In addition, even for a very long time of operation (about five times the residence time), the reservoir is not completely full of tracer, due to the stagnant zone previously identified. To better illustrate this transient behavior, it is possible to create an animation sequence with Fluent, using several frames obtained from the previous simulation. This was done and is available at <http://www.fe.up.pt/~mmalves/cfd/reactor/index.htm>.

With the data of transient tracer concentration at the outlet of the reservoir, which can be exported to an ASCII file, students can then compute the so-called Danckwerts' F curve, the normalized response of the reactor to a step input,

$$F(t) = \frac{C_{out}(t)}{C_{in}} \quad (6)$$

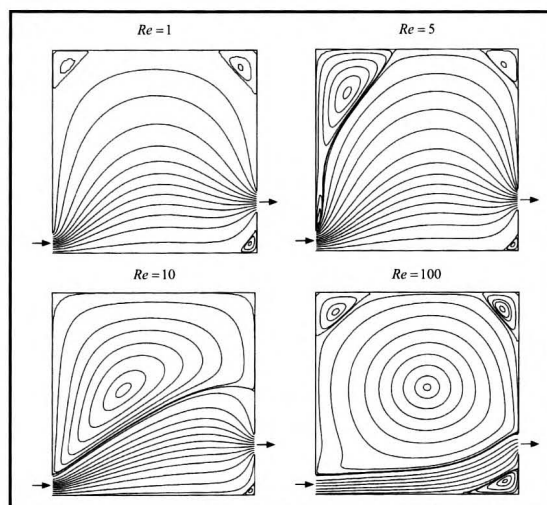


Figure 2. Steady state contours of the stream function for the reservoir with $L/H = 1$ as a function of the Reynolds number.

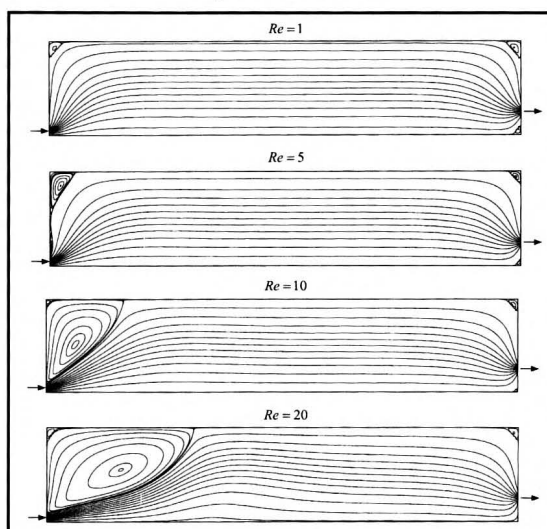


Figure 3. Steady state contours of the stream function for the reservoir with $L/H = 5$ as a function of the Reynolds number.

Data can then be manipulated with a spreadsheet program such as Microsoft Excel. Results shown in Figure 5 show the expected F curve, which only reaches the asymptotic value of 1 for very long times. It is worth mentioning the use of a logarithmic time scale, showing that tracer starts to exit the reservoir at around $\theta = t/\tau = 0.22$ due to its transport by convection, while fluid elements that enter the stagnant region only come out (by diffusion) much later (see detail of Figure 5).

With the response to a step input, the RTD function can now be computed by

$$E(t) = \frac{dF(t)}{dt} \quad (7)$$

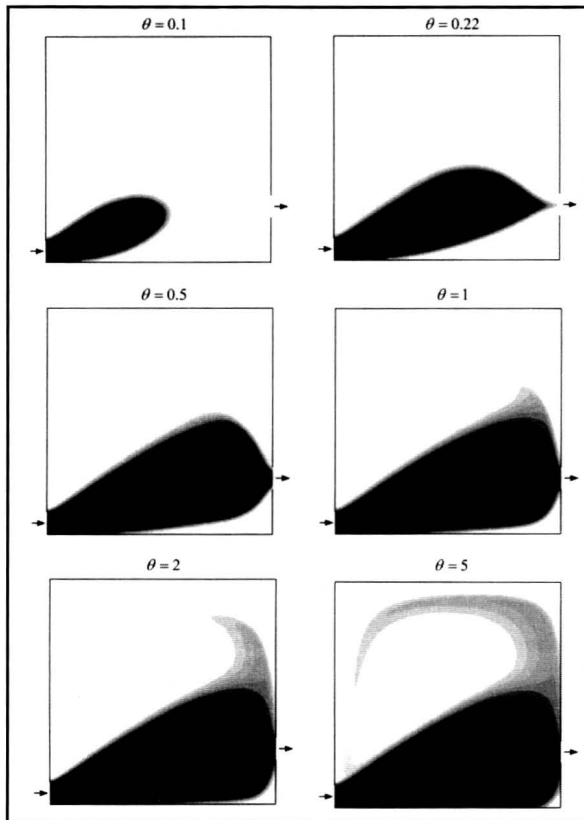


Figure 4. Transient tracer concentration contours for the reservoir with $L/H = 1$ ($Re = 10$).

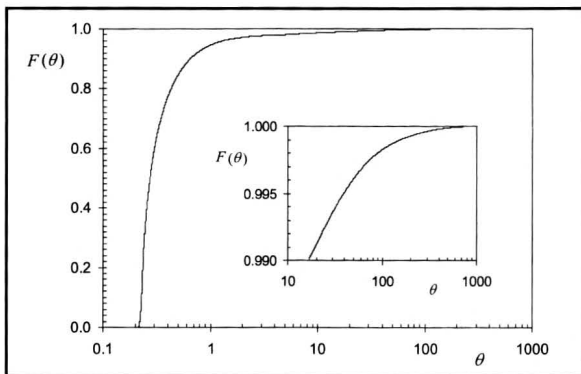


Figure 5. Danckwerts' F curve for the reservoir, with $L/H = 1$ ($Re = 10$).

or, in terms of reduced time θ ,

$$E(\theta) = \frac{dF(\theta)}{d\theta} = \tau E(t) \quad (8)$$

Figure 6 shows the RTD curves as a function of the Reynolds number, which gives an idea (for a given fluid) how space-time affects the RTD function. In all cases, the RTD curves evidence a very long tail and that a large fraction of fluid elements exits the reservoir with ages younger than the space-time, τ . Both features are indicative of the existence of large stagnant regions, together with slow recirculating flows near the inlet, as can be seen in Figure 2. The fact that Re affects the RTD curve is also visible in Figure 6. Higher Reynolds numbers imply that the fluid elements start to leave the reactor sooner and a higher fraction of fluid elements has a smaller residence time.

The effect of the reservoir geometry on the RTD is shown in Figure 7. It can be seen that when L/H increases, the curves are shifted to the right, *i.e.*, the mean residence time seems to increase because the importance of the recirculating zone decreases. This was previously found in the steady state streamlines shown in Figures 2 and 3. It is particularly noteworthy that for very long reservoirs, one tends toward an asymptotic $E(\theta)$ curve, also shown in Figure 7. This curve corresponds to the case of laminar flow between parallel plates, given by^[19]

$$E(\theta) = \begin{cases} \frac{1}{3\theta^3} & \theta \geq \frac{2}{3} \\ \sqrt{1 - \frac{2}{3\theta}} & \theta < \frac{2}{3} \\ 0 & \theta < \frac{2}{3} \end{cases} \quad (9)$$

It must be stressed that for this situation, *i.e.*, laminar flow between parallel plates, the parabolic profile is characterized by a maximum velocity at the center that is 1.5 times the average velocity, while for flow in pipes this ratio is 2.

The RTD functions can then be used to calculate the mean residence time, defined as

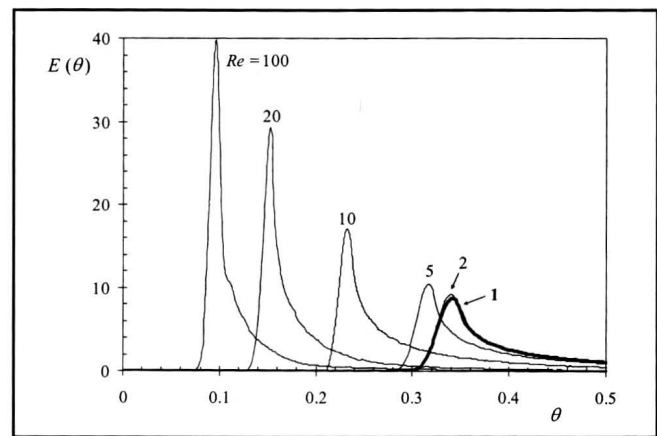


Figure 6. Effect of the Reynolds number on the residence time distribution (reservoir with $L/H = 1$).

$$\bar{t}_r = \int_0^{\infty} tE(t)dt \quad (10)$$

or

$$\bar{\theta}_r = \frac{\bar{t}_r}{\tau} = \int_0^{\infty} \theta E(\theta)d\theta \quad (11)$$

For a closed-closed system (*i.e.*, with no dispersion) and if no bypass or stagnant regions exist, it is well known that the mean residence time and space-time are equal.^[7,20] Due to the very long tail of the RTD function, however, this is only verified if simulations are run up to very high times, typically θ of $0(10^3)$. Otherwise, the normalization condition

$$\int_0^{\infty} E(t)dt = \int_0^{\infty} E(\theta)d\theta = 1$$

is not satisfied and the computed mean residence time is smaller than the real space-time.

Calculation of the mean residence time is very important for evaluation of malfunctions during the reactor's operation. Indeed, a straightforward way to diagnose the reactor's flow performance consists of comparing the computed value of the mean residence time from Eq. (10) with the space-time ($\tau = V/Q$, where V is the total volume of the reactor and Q is the volumetric flow rate), which is equivalent to comparing $\bar{\theta}_r$ with 1. Disagreement between these two values may indicate the existence of bypasses, dead volumes, etc. For instance, as indicated by Froment,^[5] if a region of the vessel retains a portion of the fluid for an order of magnitude greater than the mean residence time of the total fluid, then for all practical purposes, that portion is essentially at rest and the region is wasted space in the vessel.

The values obtained for the mean residence time shown in Tables 1 and 2 were calculated by integration of the RTD curves up to $\theta = 10$. It is evident that they strongly depend on both the Reynolds number and the geometry of the reservoir. As Re decreases, the mean residence time increases (Table 1). As expected, when L/H increases, the mean residence time approaches the space-time value (Table 2).

Because in all cases, $\bar{t}_r < \tau$ or $\bar{\theta}_r < 1$, we can conclude that a stagnant region exists, which in practice would be a dead volume, leading to a lower reactor performance. The fraction of the reactor volume occupied by the dead region is given by^[6,20]

$$\frac{V_d}{V} = 1 - \frac{\bar{t}_r}{\tau} \quad (12)$$

The dead volume fractions obtained, shown in Tables 1 and 2, indicate that for high Re

values (or high fluid velocities) and for geometries where L/H approaches 1, or even smaller, a large fraction of the reservoir will not be efficiently used for reaction purposes.

► Prediction of Conversion in the Continuous-Flow Reactor

In a real reactor, the RTD function can be used to predict the limiting values of conversion under the two extremes of micromixing, using the well-known total segregation or maximum mixedness models.^[21] For first-order reactions (linear systems), however, the state of mixing does not affect conversion,^[20] and therefore the easy-to-use segregation approach can be applied to predict reactor performance. The total segregation model assumes that all 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.^[7] Because there is no interchange of matter between fluid elements, each one acts as a batch reactor, so the mean steady-state conversion (\bar{X}) in the real reactor is given by

$$\bar{X} \int_0^{\infty} X_{\text{batch}}(t) = E(t)dt = \int_0^{\infty} X_{\text{batch}}(\theta) E(\theta)d\theta \quad (13)$$

where $X_{\text{batch}}(t)$, for a first-order reaction, is given by

$$X_{\text{batch}} = 1 - e^{-kt} = 1 - e^{-Da\theta} \quad (14)$$

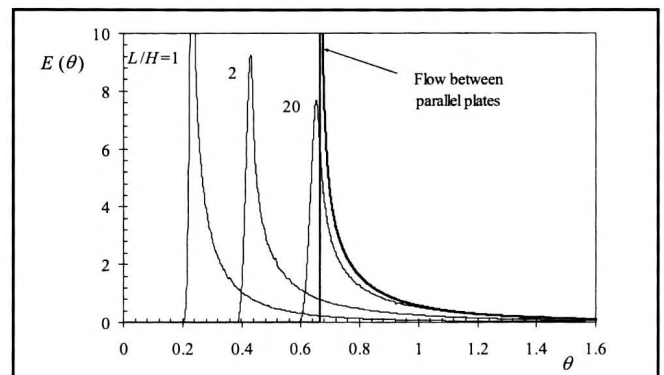


Figure 7. Effect of the geometric ratio L/H on the residence time distribution ($Re = 10$).

TABLE 1
Influence of the Reynolds Number on the Mean Residence Time and Fraction of Dead Volume (Reservoir with $L/H = 1$)

Values calculated from RTD curves up to $\theta = 10$.

Re	Mean Residence Time	Fraction of Dead Volume
	$\bar{\theta}_r = \bar{t}_r / \tau$	V_d / V
1	0.778	0.222
5	0.724	0.276
10	0.412	0.588
20	0.318	0.682
100	0.261	0.739

TABLE 2
Influence of Reservoir Geometry on the Mean Residence Time and Fraction of Dead Volume (for $Re = 10$)

Values calculated from RTD curves up to $\theta = 10$.

L/H	Mean Residence Time	Fraction of Dead Volume
	$\bar{\theta}_r = \bar{t}_r / \tau$	V_d / V
0.5	0.300	0.700
1	0.412	0.588
2	0.752	0.248
5	0.935	0.065
10	0.992	0.008
20	0.997	0.003

and $Da = k\tau$ is the Damköhler number.

Steady-state conversion is then computed by using Eq. (13), with the RTD function previously determined. It is important to remark that the segregation model can also be used for prediction of the reactor transient behavior. In this case, the upper integration limit in Eq. (13) must be set to t (or θ). This was done for our case study and the results, shown in Figure 8, illustrate the reactant conversion in transient conditions, up to steady state, for different Damköhler values. One must take care that the RTD used for prediction of reactor performance depends on its geometry and on the Reynolds number. In addition, because of the very long tail of the RTD function (as shown in Figure 5 for the $F(\theta)$ curve), prediction of steady-state conversion requires RTD data up to very large times (note the logarithmic time scale). This interesting feature is also evident in Figure 8—a non-negligible contribution to the overall reactor performance (in terms of fractional conversion), which is noticed at very long times. Such behavior can be attributed to the stagnant region and to the different time scales for the involved phenomena: reaction, convection, and molecular diffusion.

As mentioned above, Fluent can also be used to simulate the system in the presence of a reaction, and so the data shown in Figure 8 can be obtained either through the total segrega-

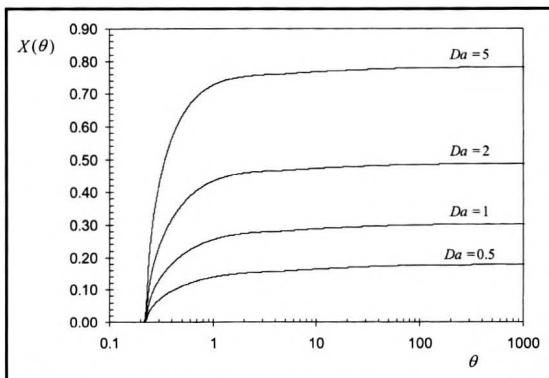


Figure 8. Unsteady-state conversion obtained for the reactor with $L/H = 1$, predicted from the segregation model ($Re = 10$).

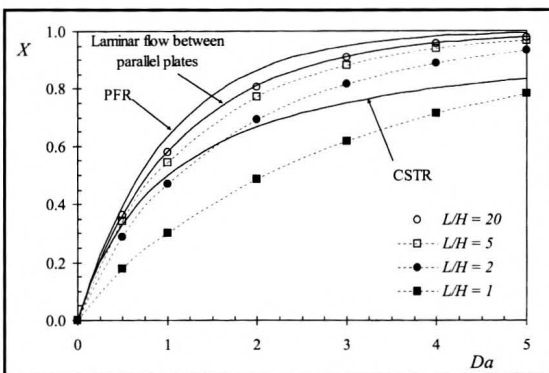


Figure 9. Steady-state conversion versus Damköhler number for reactors with different geometries ($Re = 10$).

tion model or directly from CFD simulations (obtained curves coincide). Asking students to compare results from both approaches is important because they feel more confident about the simulation results and calculations.

Simulation of the continuous-flow reactor via CFD can also be used to evidence the contours of species concentration throughout the reactor, for instance at steady state. Some color pictures can be seen on our web site at <http://www.fe.up.pt/~mmalves/cfd/reactor/index.htm>. The color gradient inside the reactor is particularly interesting to observe.

Finally, it is convenient to ask students to compare the steady-state conversion attained in the real reactor with those achieved with the ideal reactors that they learned in previous CRE courses: continuous stirred tank and plug flow reactors. For a first-order reaction, performance achieved by these reactors is given by^[e.g.,7,8]

$$X_{\text{CSTR}} = \frac{Da}{1 + Da} \quad (15)$$

$$X_{\text{PFR}} = 1 - e^{-Da} \quad (16)$$

Data shown in Figure 9 indicate that when dead regions or stagnant zones are negligible, *i.e.*, for geometries where L/H is higher than about 5 (for $Re = 10$), the performance of the real reactor lies between that of the CSTR and PFR. When L/H is close to 1, or even smaller, such anomaly (dead volume) leads to a much lower performance of the nonideal reactor—even lower than that achieved with a perfectly mixed reactor. It is also noteworthy that for very long reactors (*i.e.*, high L/H ratios), one approaches the theoretical behavior of a laminar flow reactor (flow between parallel plates) computed using the RTD function given in Eq. (9) and the segregation model.

CONCLUDING REMARKS

Concepts dealing with the RTD theory and nonideal reactors are not very familiar to undergraduate students, and thus it is not an easy task to teach these matters in CRE courses. Explanation of how stimulus-response tracer experiments provide the theoretical functions that are crucial for a reactor's diagnosis, prediction of conversion, etc., becomes clearer through experimentation, which is not always feasible. For such purposes, the use of CFD packages has been particularly advantageous. Besides, CFD tools provide a graphical portrait of flow throughout the reservoir/reactor, thus allowing going beyond simply predicting what will come out of the reactor to predicting all of the properties of interest within the reactor. Some of the concepts involved are more easily understood, such as the progression of the tracer concentration front, the formation of dead volumes, or the existence of a concentration profile along the reactor. Therefore, implementation of a CFD code has a considerable pedagogical content.

The case study we have described, a 2-D lagoon with laminar flow, was solved with the commercial package Fluent.

Using reservoirs/reactors with different geometries and/or different operating conditions, students may be asked to

- Characterize the hydrodynamics
- Determine the residence time distribution from tracer experiments, which provides diagnosis of reactor operation
- Predict conversion in a continuous-flow reactor (both steady state and transient behavior)

Our experience shows that use of the CFD code allows students to more easily understand some of the basic concepts taught in CRE curricula. Finally, comparison of numerical with analytical solutions known for laminar flow between parallel plates (*i.e.*, for geometries with high L/H ratios) improves their self-reliance regarding CFD results.

In a survey sent a few years ago to chemical engineering departments spread all over the world, two of the main points addressed by the departments to a question relating to the future of CRE courses were:^[2] the increasing importance of computer applications and software packages, and putting more emphasis on nonideal reactors. With the case study herein proposed, both issues are dealt with. In addition, students learn the potential of CFD codes, which have been successfully used in practice to design commercial-size reactors, usually with complex flow processes.^[22]

NOMENCLATURE

C	concentration of tracer, reactant, or product (mol.m ⁻³ or kg.m ⁻³)
D	diffusivity (m ² s)
Da	Damköhler number, dimensionless
E(t)	resident-time distribution function (s ⁻¹)
E(θ)	normalized RTD function, dimensionless
F(t)	Danckwerts' F curve, dimensionless
H	height of the reservoir/reactor (m)
k	reaction rate constant of the first-order reaction (s ⁻¹)
L	length of the reservoir/reactor (m)
P	pressure (Pa)
S	source term (mol m ⁻³ s ⁻¹ or kg m ⁻³ s ⁻¹)
Q	volumetric flow rate (m ³ s ⁻¹)
Re	Reynolds number, dimensionless
t	time (s)
\bar{t}_r	mean residence time (s)
U_{\max}	fluid velocity at the center of the inlet boundary (ms ⁻¹)
U_{mean}	mean fluid velocity at the inlet boundary (ms ⁻¹)
u_x	x-velocity (ms ⁻¹)
u_y	y-velocity (ms ⁻¹)
\bar{V}	volume of reservoir/reactor (m ³)
V_d	dead volume in the reservoir/reactor (m ³)
X	conversion, dimensionless
x	horizontal coordinate (m)
y	vertical coordinate (m)

Subscripts

batch	refers to batch reactor
CSTR	continuous stirred tank reactor
in	inlet conditions
PFR	plug flow reactor

out outflow conditions

Greek Symbols

$\theta = t/\tau$	reduced time, dimensionless
$\bar{\theta}_r = \bar{t}_r / \tau$	reduced mean residence time, dimensionless
μ	viscosity of the fluid (kg m ⁻¹ s ⁻¹)
ν	kinematic viscosity of the fluid (m ² s ⁻¹)
ρ	density of the fluid (kg m ⁻³)
τ	space-time (s)

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