Novel Approach for Teaching Microchemical Systems Analysis to Chemical Engineering Students Using Interactive Graphical User Interfaces (GUIs)

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Abstract: Microchemical process technology is a key emerging technology having applications from research to small-scale commercial production of high value-added, highly energetic, or highly reactive materials, such as pharmaceuticals, explosives, and free-radical reaction initiators. To introduce this new technology to chemical engineering undergraduate students, Graphical User Interfaces (GUI's) have been created to facilitate understanding of the conservation principles associated with microchemical systems and the role of various system parameters on device performance. The ability to account for 2-D and 3-D geometries and to combine multiphysics for microchemical systems is normally not within the reach of most undergraduate education programs. The prototype versions of the GUI's were created in 2012 using *MATLAB Guide* with COMSOL Vers 3.5a as the numerical engine. The availability of the *COMSOL Application Builder* provides an alternate approach for creating the GUI's that is more straightforward to implement. This paper describes the creation of selected GUI's using *COMSOL Application Builder* for comparison to previous efforts based on *MATLAB Guide*. The examples selected here include solute mixing effects in a 2-D tee-micro mixer and a performance analysis of a catalytic wall microreactor. The use of *MATLAB Guide* although more tedious, allows more flexibility in creating the GUI's when compared to the current version of *COMSOL Application Builder*.

Keywords: microchemical process, GUI, multiphysics, tee-micro mixer, catalytic wall reactor

1. Introduction

Materials derived from chemical and biological reactions are an integrated part of daily life. Sound management of material production using advanced manufacturing processes is essential for safe, environmentally-friendly operation while achieving required business metrics for profitability. Next-generation technologies must be developed that replace outdated manufacturing processes and empirical process engineering methods to create safe, compact, flexible, eco-friendly, energy efficient processes and plants[1]. Though these changes are rather obvious in the industry, the same is not true for the academia. Hence, there is a need for the students to be exposed to these new emerging technologies and design techniques.

Microchemical systems are one such key emerging technology with applications ranging from discovery research through commercial processes. To introduce this technology to students the Department of Chemical Engineering at Texas A&M-Kingsville (TAMUK), a learning module was developed called an *Interlinked Curriculum Component* (ICC) on *Microchemical Systems* as a part of the undergraduate curriculum reform project that was initially funded by NSF in 2008 [1]. An ICC connects the organizing principles of molecular transformations, multi-scale analysis, and a systems approach. This is accomplished by first providing a qualitative overview of specific microprocess systems and then focusing on quantitative aspects of key microprocess components. An ICC module utilizes the latest tools for 2-D and 3-D imaging, animation, and modeling so the concepts and processes being studied are represented using both numerical and graphical form. The module enables students to work through a series of exercises that start from basic principles and concepts to more complex situations where opportunities exist for both critical thinking and creativity.

COMSOL Multiphysics was selected as the numerical engine to simulate various microprocess system components involving fluid flow, heat transfer, and species transport, such as fluid micromixers and micro reactors. A library

of various models was also created so that students could readily explore the effect of various model parameters on the physical system without worrying about numerical solution details. This approach allows them to focus on developing better insight and understanding of the system physics, which helps to reinforce the fundamentals that are taught in required courses on fluid mechanics, heat transfer, and mass transfer. To provide a more direct connection between the model equations and the calculated results, a Graphical User Interface (GUI) was created using COMSOL that provides either a 2-D and 3-D visualization of the model simulations where the effect of various model parameters can be explored [1-6]. The original GUIs were created using MATLAB Guide with COMSOL 3.5a, which was very tedious and required notable effort. A simpler, more robust approach that facilitates creation of the GUI's is preferred.

The primary objective of this study is to use *COMSOL Application Builder* to create the user interface so students can change selected input parameters. The application created will be then compared with the user interfaces using *MATLAB Guide* so that conclusions can be developed on the advantages and limitations of *Application Builder*.

2. Catalytic Wall Reactor

2.1 Problem description

In this model, a continuous flow of gas is introduced into a microchannel reactor as shown in Figure 1. The reactor geometry is a 2-D duct with a specified length and width. The top surface is coated with a thin layer of heterogeneous catalyst where a first-order reaction occurs. In this particular case, no homogeneous gas or liquid-phase reactions occur in the microchannel sub-domain, but only at the top surface boundary of the microchannel. The flow rate and other conditions are selected so the flow is well within the laminar flow regime.

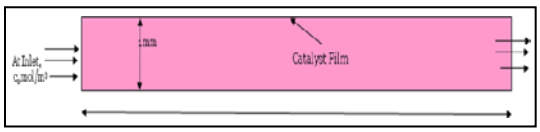

Figure 1. Model Geometry for the Wall-Catalyzed Microchannel Reactor.

The reaction is assumed to follow the stoichiometry where specie A is converted to specie B.

$$A \rightarrow B$$

An example of this type of reaction would be the isomerization of hydrocarbons. More complex single and multiple reaction networks can be considered and these will be the subject of future work.

The reaction rate for the disappearance of specie A is assumed to follow first-order kinetics so that

$$-R_A = kC_A$$

where k is the first-order rate constant, and C_A is the concentration of specie A on the surface of the catalytic film.

2.2 Fluid & Species Transport-Kinetics Model

The specie mass and momentum balance equations are summarized below.

Species convection-diffusion equation

$$\nabla \cdot \left(-D_i \nabla c_i\right) + \boldsymbol{u} \cdot \nabla c_i = R_i$$

Here, c_i denotes the concentration of specie i in the reaction mixture, D_i denotes the diffusion coefficient for specie i in the flowing stream, u denotes the velocity vector, and R_i is the rate of generation of specie. For the case considered here, the specie indices are i = A and B.

Continuity, momentum and energy equations

The remaining balances include the microscopic forms of the continuity equation, the Navier-Stokes equations for laminar flow, and the energy equation.

Continuity equation

$$\nabla \cdot (\rho \boldsymbol{u}) = 0$$

Momentum (Navier-Stokes) equation

$$\frac{\partial}{\partial t}\rho \boldsymbol{u} = -\left[\nabla \cdot \rho \boldsymbol{u}\boldsymbol{u}\right] - \nabla p - \left[\nabla \cdot \overline{\overline{\boldsymbol{\tau}}}\right] + \rho \mathrm{g} = 0$$

Energy equation

$$\rho C_P \frac{DT}{Dt}\boldsymbol{u}\nabla T = -(\nabla \cdot \boldsymbol{q}) - \left(\frac{\partial \ln P}{\partial \ln T}\right)\frac{Dp}{Dt} - (\overline{\overline{\boldsymbol{\tau}}} : \nabla \boldsymbol{u})$$

The quantity $\boldsymbol{q}$ is energy flux due to heat conduction

$$\boldsymbol{q} = -k\nabla T$$

2.3 Boundary conditions

At the reactor inlet, the fluid velocity, the species concentration, and fluid temperature are usually specified.

$$\boldsymbol{u} = -U_0 \cdot \boldsymbol{n}$$

$$c_i = c_{i0}$$

$$T = T_{i0}$$

The parameter U_0 denotes a uniform velocity whereas **n** denotes the unit normal vector.

At the walls, no-slip boundary conditions are used.

At y = 0 and at y = h,

$$\boldsymbol{u} = \begin{bmatrix} u_x \\ u_y \end{bmatrix} = 0$$

At the reactor outlet, the fluid pressure is specified

$$p = p_{i0}$$

The closed form of the Danckwerts boundary conditions are often used for both species and temperature

$$\boldsymbol{n} \cdot (D_i \nabla c_i) = 0$$

$$\boldsymbol{n} \cdot (k\nabla T) = 0$$

2.4 Results and discussion

The user interface developed using *MATLAB Guide* with COMSOL Vers 3.5a as the numerical engine is shown in Figure 2. It contains three different sub-panels for accepting user input.

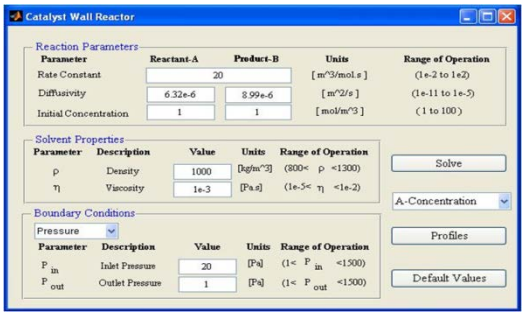

Figure 2. GUI Showing Parameter Entry for the Catalytic Wall Reactor.

In the upper section of the input screen, the user can vary the *reaction parameters*, which includes the reaction rate constant, diffusion coefficients, and the initial concentrations of species A and B. The middle section of the input screen allows the user to vary the reaction *solvent parameters*, which includes the fluid density and viscosity. In the lower portion of the input screen, the desired momentum equation *boundary conditions* can also be selected, *i.e.*, specified inlet and outlet pressures or specified inlet velocity and exit pressure.

After selecting the 'Solve' button, MATLAB passes these variables, along with the COMSOL modeling equation commands, to the COMSOL engine. The COMSOL engine then solves the Naiver-Stokes equations and the species convection-diffusion equations for the fluid velocity profiles, pressure profiles, and the species concentration profiles. These various results are then passed back to MATLAB, which can be observed as surface plots by pressing the 'Profiles' button.

The velocity profiles and concentration profiles are shown in Figures 3 - 5.

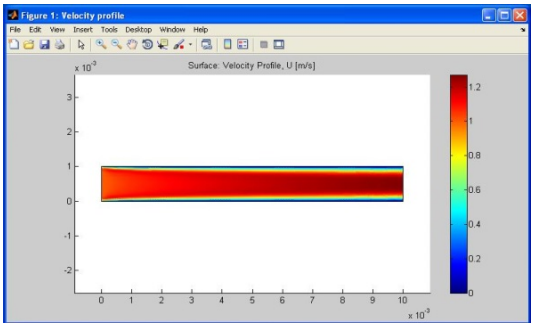

Figure 3. Velocity Profiles for the Catalytic Wall Reactor; Parameters: U_{in}= 1 m/s, μ = 1.0 x 10^{-3} Pa-s, ρ = 1000 kg/m^3.

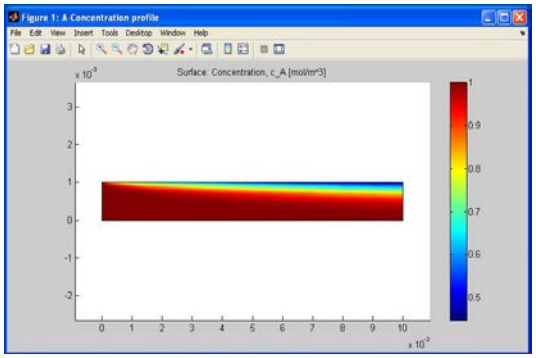

Figure 4. Concentration Profiles for Reactant A; Parameters: C_{A0} = 1 mol/m^3, k = 20 1/s, D_A = 6.32 x 10^{-6} m^2/s, D_B = 8.99 x 10^{-6} m^2/s.

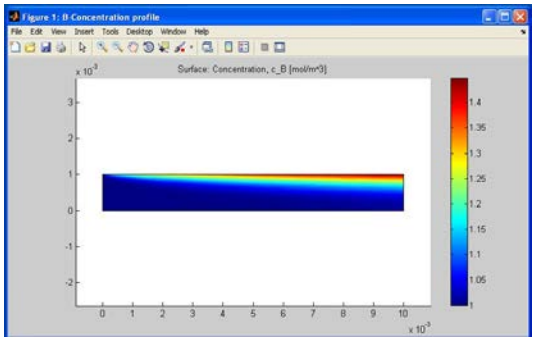

Figure 5. Concentration Profiles for Product B; Parameters: C_{A0} = 1 mol/m^3, k = 20 1/s, D_A = 6.32 x 10^{-6} m^2/s, D_B = 8.99 x 10^{-6} m^2/s.

The pedagogical aspects of this example include: (1) coupling of single phase, isothermal fluid momentum transport with dilute solute transport and chemical reaction (2) developing insight into various parameters that are used to characterize chemical reaction; and (3) ability to examine the effect of fluid properties, solute properties, and reaction rate constant for a catalytic reaction

The user interface developed for this same problem using *COMSOL Application Builder* is shown in Figure 6. Comparison of the overall arrangement of the user input screen to the one created using *MATLAB Guide* is quite different in appearance, although the functionality is very similar. A key difference is the time and effort required to develop the simulation and create the input screen using *COMSOL Application Builder* compared to *MATLAB Guide*. The latter required several months of effort to become familiar with the coding, create the screen, and perform debugging. Conversely, the former required less than a few days of effort once the simulation had been developed. The advantage of using the current application builder is obvious, although one is somewhat constrained to the formatting of the input screen layout.

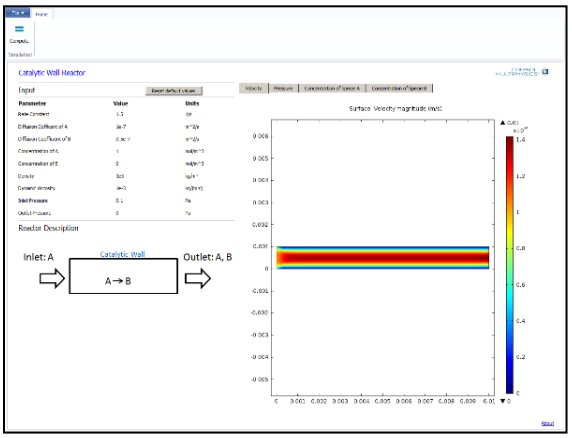

Figure 6. Catalytic wall reactor GUI at the Parameter Entry Stage.

3. Tee-Micromixer

3.1 Problem description

This example consists of a tee-micro mixer. It consists of two inlets and an outlet. Liquid to be mixed enter from the two inlets and the degree of mixing will be controlled by the relative ratio of the fluid residence time to the solute diffusion time. The two fluid streams considered here have the same density and viscosity. To reduce the complexity, a 2-D model geometry was used for this exercise. The velocities of the streams are determined using the Navier-Stokes equations and then the convection-diffusion equations are solved to determine the solute concentration profiles. Variation of mixing by adding various obstacles, such as rectangular and circular obstacles, was also studied.

The equations used to describe the solute transport and mixing are similar to those used for the previous example for the catalytic wall reactor so they are omitted here for brevity. The boundary conditions are also nearly identical except that the specie concentrations are specified at each inlet.

A diagram of system geometry is shown in Figure 7. It consists of two inlets that converge into a single duct. The dimensions are shown in Table 1.

Table 1. Dimensions of T-Micromixer

Parameter	Size, mm
Length	12
Inlet width	0.5
Outlet width	1
Height	0.5
Circular baffles diameter	0.3

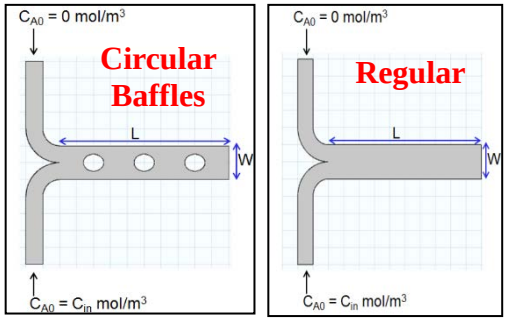

Figure 7. Geometry of the Tee Micro-Mixer.

3.4 Results and Discussions

The user interface developed using *MATLAB Guide* with COMSOL Vers 3.5a as the numerical engine is shown in Figure 8. Three versions of the Tee-Micromixer are defined: (1) without baffles; (2) with circular baffles; and (3) with rectangular baffles. The user can input different values of problem parameters, such as the fluid density and fluid viscosity, and also select the desired boundary conditions, *i.e.*, either specified pressures at the duct inlets and outlet, or specified duct inlet velocity with a specified outlet pressure. After specifying all these parameters, the 'Solve' button is clicked. MATLAB then passes these variables, along with the COMSOL modeling equation commands and parameters, to the COMSOL engine. COMSOL then solves the Navier-Stokes and convection-diffusion equations simultaneously and passes the values of the velocity field back to MATLAB.

The solute concentration profiles, velocity profiles and the variations of the mixing parameters are shown as graphs. The computer output results are shown in Figures 9 to 11. The 'Plot' button generates the graphs while the 'Default value' button sets the base set of values for the parameters.

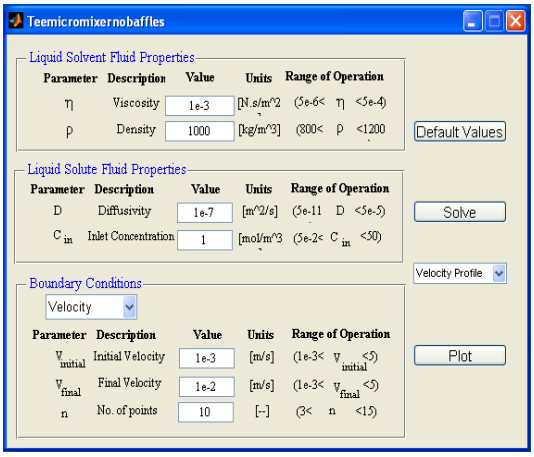

Figure 8. GUI for the 2-D Tee-Micromixer.

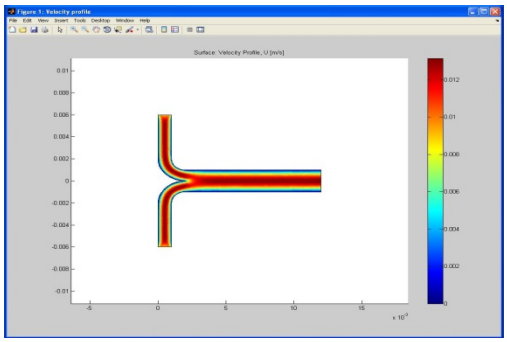

Figure 9. GUI for the Tee-Micromixer Displaying the Velocity Profiles.

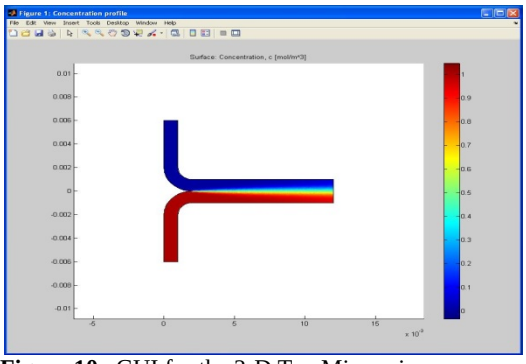

Figure 10. GUI for the 2-D Tee-Micromixer Displaying the Concentration Profiles.

The user interface developed for the above problem using *COMSOL Application Builder* is shown in Figure 12. As in the previous example, the overall arrangement of the user input screen compared to the one created using *MATLAB Guide* is quite different in appearance, although the functionality is very similar.

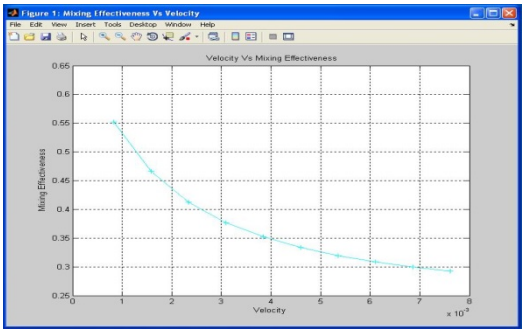

Figure 11. GUI for the 2-D Tee-Micromixer Displaying Mixing Effectiveness versus Velocity.

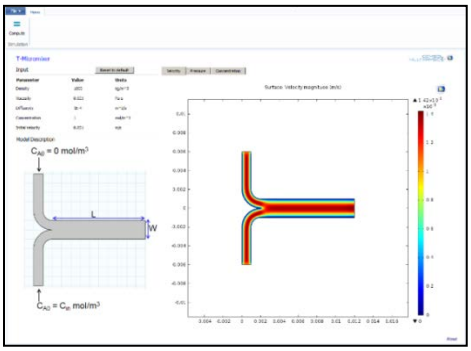

Figure 12. GUI for the 2-D Regular Tee-Micromixer created using *COMSOL Application Builder*.

Figure 13 shows the steady-state fluid velocity profiles for the case of specified inlet and outlet fluid pressures using the above *App*.

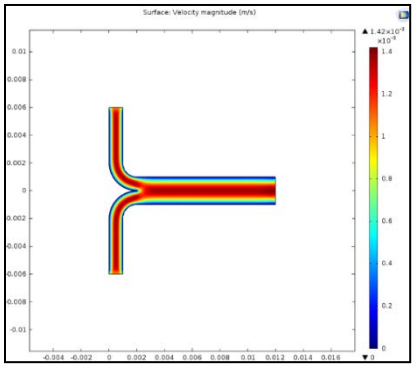

Figure 13. Velocity Profiles Obtained for a Tee-Micromixer at Steady State.

Typical solute concentration profiles, which are shown in Figure 14, are solved sequentially after solving for the velocity profiles to obtain faster convergence. The effect of the solute diffusivity can also be easily studied. The concentration profiles for different solute diffusivities can also be determined using parametric linear or non-linear solvers.

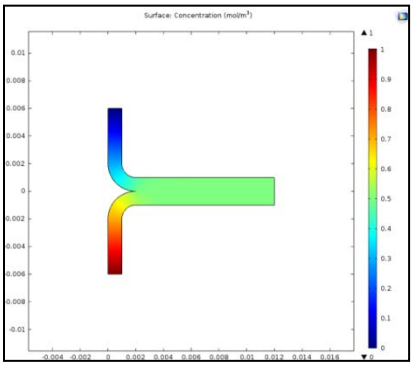

Figure 14. Concentration Profiles Obtained for the Tee-Micromixer at Steady State.

The user interface developed for a Tee-Micro mixer containing three circular baffles using *COMSOL Application Builder* is shown in Figure 15. The development of a separate App for each different arrangement of baffles resulted in simplification of the development, although it would have been possible to create a single App that could handle various different baffles or other mixer internals.

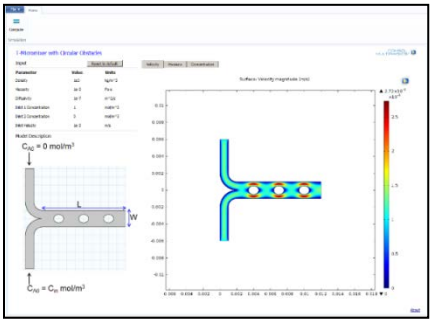

Figure 15. GUI for Velocity Profiles in 2-D Tee-Micromixer with Circular Baffles Using *COMSOL Application Builder*.

The velocity profiles and solute concentration profiles for the above geometry are shown in Figures 16 and 17, respectively. Additional baffles create a mixture that is similar to the one shown above in Figure 14 corresponding to an empty mixer. This can be attributed to the magnitudes of the molecular diffusivity for both species A and B, respectively (not shown for brevity).

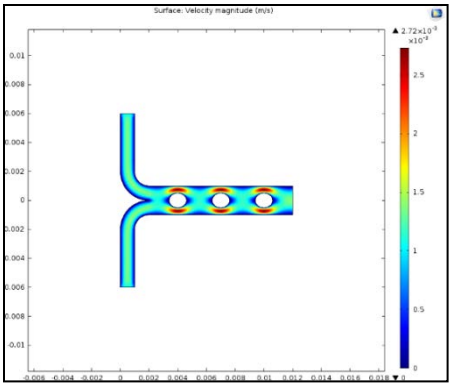

Figure 17. Velocity Profiles Obtained for a Tee-Micromixer with Circular Baffles.

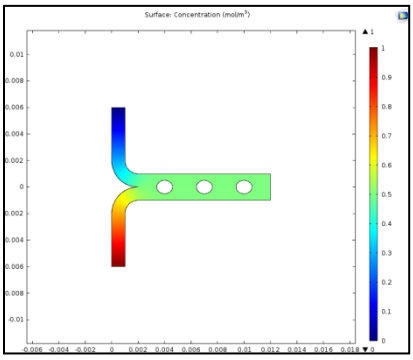

Figure 18. Concentration Profiles Obtained for a Tee-Micromixer with Circular Baffles.

4. Conclusions

COMSOL Multiphysics provides a powerful numerical platform where various models for microchemical process technology components can be readily created for both education and research. This modeling tool allows chemical engineering students to focus on understanding the effects of various microchemical system component design and operational parameters versus coding and debugging of the numerical methods. The GUIs enable students to readily study the effect of various design parameters. These applications not only reduce the complexity of model setup and computational time, but also emphasize understanding of multiphysics in multi-dimensions that is otherwise not possible with simple 1-D models. This approach helps students to understand complex chemical systems using an interactive approach versus laborious manual calculations or using other software tools.

5. Notation

U	velocity [m/s]
P	pressure [Pa]
V	average velocity [m/s]
ρ	density [kg/m^3]
η	viscosity [Pa.s]
c	concentration of specie [mol/m^3]
D	diffusivity [m^2/s]
ϑ	stoichiometric ratio [moles of specie i / mole of the reference specie]
r	rate of reaction [moles/m^{3}s]
N	molar flux of species [moles/(m^2.s)]
C_0	initial concentration of the component [moles/m^3]
T	temperature [K]
T_0	initial temperature [K]
C_p	specific heat constant [J/(kg.K]
k	reaction rate constant [1/s]
Q	external heat supplied [W/m^3]
q	heat flux [W/m^2]

6. References

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