Application of COMSOL Multiphysics in Transport Phenomena Educational Processes

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Abstract: Use of simulation software for solving realistic engineering problems has grown significantly in recent years due to the availability of less expensive but more powerful computers and the development of user-friendly yet robust modeling codes. From an educational perspective, students in STEM disciplines can now solve complex problems in a relatively short period of time, which provides new opportunities for strengthening their knowledge of fundamentals and gaining better insight into the interaction between realistic system design geometries, problem parameters, and the role of various multiphysics. One key result is an acceleration of their development as technologists, which allows them to ultimately provide greater business impact and leadership in their chosen career. In chemical engineering, teaching of transport phenomena, which is a subject that provides the underpinning of the discipline, is often restricted to problems where analytical solutions can be developed, such as one-dimensional fluid flow in a duct or pipe, linear heat conduction in a solid, or Fickian diffusion and first-order reaction in an isothermal porous catalyst. COMSOL Multiphysics™ provides a powerful platform for enhancing student knowledge by first confirming the analytical solutions based upon simplifying assumptions using numerical solutions, and then extending the problem to multi-dimensions with the addition of one or more multiphysics. Although this approach is gaining momentum among some chemical engineering educators, the experiences are not well-known or documented.

The primary objective of this paper is to illustrate how COMSOL Multiphysics has been used as an instrument for enhancing teaching the principles of transport phenomena to first-year chemical engineering graduate students. Another objective is to summarize the techniques used to incorporate it into the course material.

Keywords: Non-isothermal flow over a cylinder, Graetz-Nusselt problem, Micro heat exchanger, Application builder.

1. Introduction

Even though heat, mass and momentum transfer were independently developed as branches of classical physics, their combined study is one of the most important engineering sciences in modern engineering. The subject of *Transport Phenomena* is taught in a variety of ways at several different student levels. The essence of this subject is to understand the interaction between various multiphysics by the application of conservation principles, flux expressions, constitutive equations, initial conditions, and boundary conditions to a particular engineering system geometry.

COMSOL Multiphysics™ provides a robust platform to solve complicated transport phenomena problems and to generate results that lead to a better understanding of the physical significance and their real-world applications. This paper discusses various methods to implement some of the tools in COMSOL Multiphysics™ to enhance the teaching process of transport phenomena. For example, the Application Builder can simplify the explanation of complex problems in a time-conserving manner. Additionally, textbooks tend to illustrate limited results, whereas a COMSOL Multiphysics™ application can generate a broad range of results needed for a better fundamental understanding of the problem being studied.

2. Governing Equations

The equation of continuity, the Navier-Stokes equation, and convective energy transport equation were solved for each problem outlined below in two-space dimensions.

Equation of Continuity
$$\rho \nabla \cdot (\boldsymbol{u}) = 0$$
Navier-Stokes Equation
$$\rho(\boldsymbol{u} \cdot \nabla)\boldsymbol{u} = \nabla \cdot [p\boldsymbol{I} + \mu(\nabla\boldsymbol{u} + (\nabla\boldsymbol{u})^T)] + F$$
Energy Transport Equation
$$\rho C_p \boldsymbol{u} \cdot \nabla T + \nabla \cdot \boldsymbol{q} = Q + Q_p + Q_{vd}$$
$$\boldsymbol{q} = -k\nabla T$$

2. Nonisothermal Flow Over a Cylinder

An incompressible Newtonian fluid enters a duct at a prescribed constant upstream velocity and flows over a heated cylinder of known radius and infinite length (Fig. 1).

This problem includes coupled fluid-flow and heat transfer, and does not have a closed-form solution. However, some experimental data are available for comparison [3].

To discretize the domain with a finite number of elements, the duct dimensions (height and width) are chosen so that the walls have a negligible effect on the fluid flow patterns.
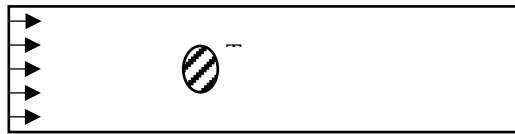
Figure 1. Nonisothermal flow over a cylinder.

2.1. Boundary conditions

The following Dirichlet boundary conditions are applied to this system:
1. A uniform velocity profile is specified at the duct inlet;
2. The no slip condition is used at the duct walls and on the cylinder surface;
3. The fluid pressure is specified at the duct outlet.
4. The surface of the cylinder is assumed to exist as a prescribed temperature.

2.2 Results

The following results were obtained for the temperature and velocity profiles for different flow regimes with a Grashof number of 1.1×10^8.
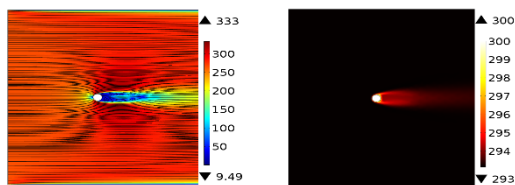- Forced convection with Reynolds numbers from 200 to 300.

Figure 2. Reynolds number and temperature field for the regime where forced convection is controlling.

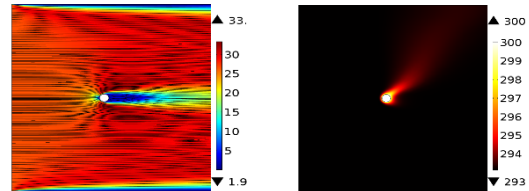- Mixed regime with Reynolds numbers from 20 to 30.

Figure 3. Reynolds number and temperature field for the mixed regime where both forced convection and buoyancy are affecting the fluid velocity and fluid temperature.

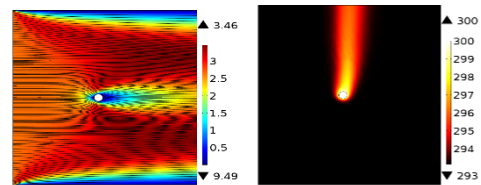- Buoyancy-dominated regime with Reynolds number from 2 to 3.

Figure 4. Reynolds number and temperature field for the regime where buoyancy is controlling.
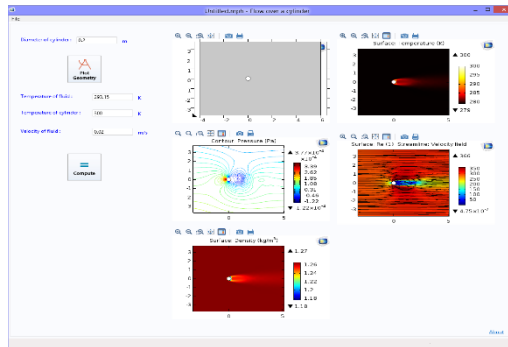
2.3 Application builder

Figure 5. COMSOL Application for non-isothermal flow over a cylinder.

The COMSOL Application for this problem (Fig. 5) is capable of illustrating the effect of variation of any problem parameter on the fluid velocity, pressure and temperature fields. The user can track transitional flow effects, *e.g.*, vortex shedding, by varying primitive parameters, which specifies values for the dimensionless groups (Re and Gr).
The adjustable parameters are:
- Approaching velocity of the fluid (u_∞)
- Bulk temperature of the fluid (T_∞).

- Temperature of the cylinder.(T_c)
- Radius of the cylinder.(R)

3. Graetz-Nusselt Problem

An incompressible, Newtonian fluid is introduced into a circular tube (z = 0) at a constant temperature (T_{in} = 280 K) under laminar-flow conditions. The tube wall is maintained at a constant temperature of T_w = 350 K. A simpler version of this problem was first analyzed by Graetz in 1883. The objective of this problem is to obtain steady-state temperature distribution in the fluid as it flows down the tube.
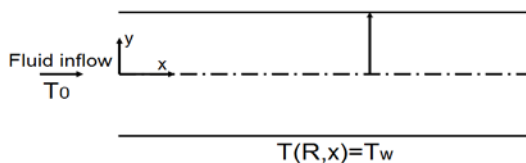

Figure 6. The Graetz –Nusselt problem [4].

3.1. Boundary conditions

The following boundary conditions are specified for this system:
1. A uniform velocity of 0.01 m/s is assumed at the tube inlet. This particular inlet velocity was selected to maintain a laminar flow regime.
2. The fluid pressure at the outlet of the pipe is zero.
3. The no slip condition is used at the tube walls.

The fluid velocity at the inlet and fluid pressure at the exit could be set to other user-specified values.

3.2 Results and discussion

Figure 7 shows the dimensionless velocity profiles $v^* = v(r,z)/v_0$ where v_0 is the inlet velocity at different locations along the length of the pipe. The particular axial locations correspond to z = 0 (inlet), 0.25L, 0.50L, 0.75L, and L (outlet)) where L = 1.65 m. It is evident that the velocity approaches a fully-developed profile with increasing pipe length, which is equivalent to increasing fluid residence time $\tau = L/\langle v \rangle$ where $\langle v \rangle$ is the average velocity. The increased residence time allows fluid momentum

and thermal energy to be transferred across the pipe radius and approach a fully-developed state. The magnitude of the velocity in the middle of the pipe eventually approaches the maximum centerline value only after z > 0.75L.
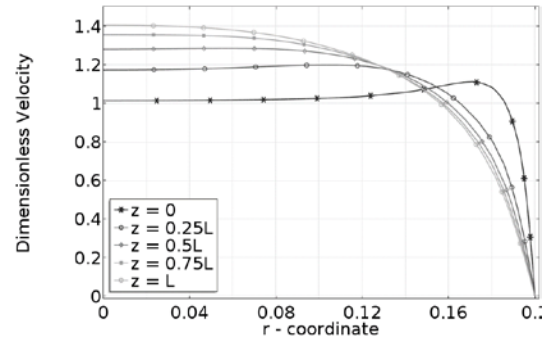

Figure 7. Velocity profiles at various axial positions.

Figure 8 shows the dimensionless temperature profiles $\theta(r,z) = (T(r,z) - T_{in})/(T_w - T_{in})$ at the same pipe locations used in Figure 7. Defining the dimensionless temperature variable in this fashion will define limits between zero and unity corresponding to the inlet condition T_{in} or if the fluid temperature reaches the wall temperature T_W.

The profiles show that at the entrance of the pipe, the difference between the fluid temperature in the interior of the pipe and the wall temperature is significant. However, as the fluid travels down the pipe, the temperature gradually increases due to combined convective and conduction heat transfer processes so that the difference between the bulk and wall temperature is reduced. A fully developed temperature profile is not achieved for the assumed pipe length since the profile is still increasing between 0.75 L and L.
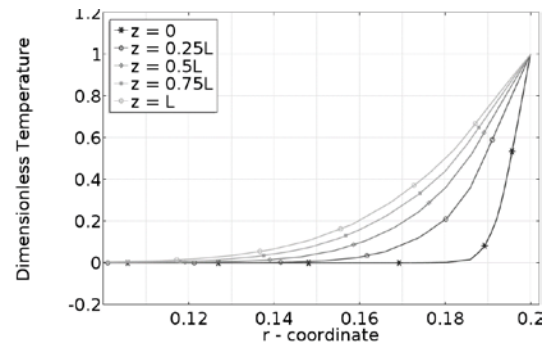

Figure 8. Temperature profiles at different positions throughout the pipe for Re = 400.

If the inlet velocity is reduced low enough, so that convective flow of energy out of the system becomes lower, than conductive flux through the walls, then thermal equilibrium is achieved within the length of the pipe, raising outlet temperature to the wall temperature.

Example of this case is shown in Figure 9. It is apparent, that after fluid travels around 25% of the length of the pipe, it heats up to the wall temperature. 3-D representation of this result can be found in Figure 11
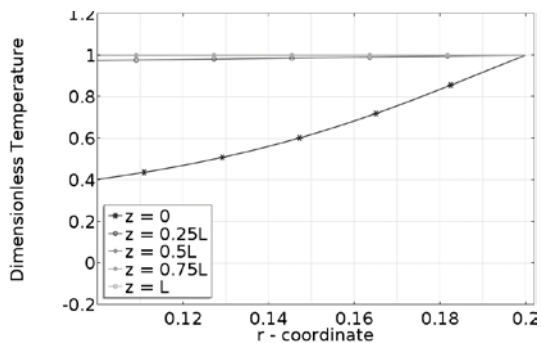

Figure 9. Temperature profiles at different positions throughout the pipe for Re = 0.4

3.3 Application builder

The COMSOL Application for this problem is shown in Figure 10.
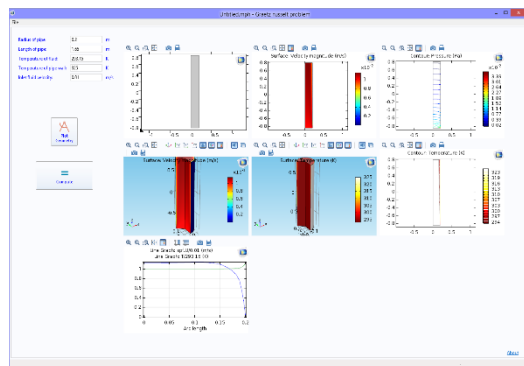

Figure 10. Graetz –Nusselt application.

The purpose of this application is to allow the student to observe changes in fluid velocity and temperature profiles that occur with variations in the problem parameters. In this particular case, the student user can change the radius and height of the cylinder as well as the inlet fluid temperature and the wall temperature. The magnitude of the fluid temperature difference will clearly affect the degree of variation in the fluid temperature profile as it travels down the tube. This will also affect the behavior of temperature profile in the boundary region along the walls.

The user can also change the value of the inlet velocity, which will result in a fully-developed laminar velocity profile at lower flows (Fig 11), or an obscured profile if the velocity is set as too high (Fig 12).
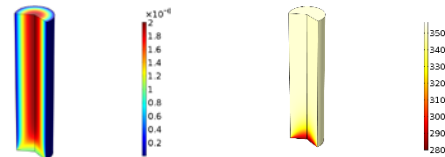

Figure 11. Velocity and temperature profiles for a very low velocity of 1×10^{-6} m/s

The temperature profile in Fig 11 shows that the fluid temperature increases as soon as it enters the pipe. This is because the conductive heat flux is notably higher than the convective flux through the pipe for very low velocities. The magnitude of these two fluxes could be calculated and compared as part of the App.
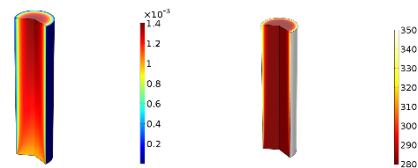

Figure 12. Velocity and temperature profiles for a very low velocity of 0.001 m/s

All of the results are compiled by the application so the student user only has to modify the parameter values as desired. Limits can also be imposed on the parameters to avoid the use of unrealistic values.

4. Flow Through a Duct

This particular COMSOL application, which is shown in Figure 13, describes laminar fluid flow through a duct. This problem has axial symmetry so the 3-D system of equations can be solved in 2-D coordinate space. This application provides the student user with the option of re-building the geometry by changing the dimensions of the duct. It also gives an option to re-mesh the geometry once the changes in the spatial dimensions are made. A choice also exists to change fluid properties, such as density

and viscosity, so their effect can be investigated.. Additionally, problem parameters, such as inlet and outlet pressure, can also be manipulated by the student user.
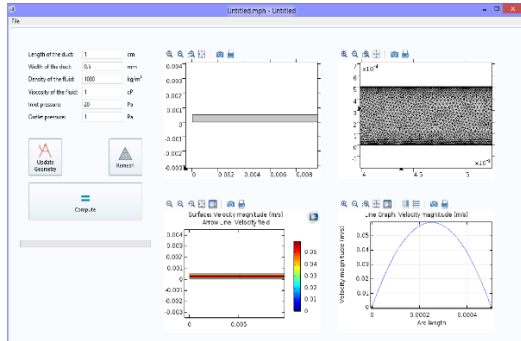

Figure 13. Laminar flow of a fluid through a duct**.**

The application computes the velocity profile of the fluid through the entire length of the duct as well as at the mid-point of the duct. Hence, the students would be able to observe the changes in the velocity along the duct length that are caused by adjusting individual or multiple parameters.

5.   Micro Heat Exchanger.

This particular COMSOL application allows the student user to examine the performance of a micro-scale heat exchanger. The geometry consists of two identical plates with conduits in contact with each other. The dimensions of the heat exchanger are: 800 μm x 800 μm x 60 μm. Conduits occupy a fixed fraction of the width of the plate whose height that can be adjusted. One plate can be rotated while the other remains stationary, which creates either co-current, counter-current, or cross-current flow contacting patterns and hence different driving forces for heat transfer.

It is worth noting that this problem is fairly complex and cannot be solved with the techniques normally taught in a typical undergraduate course on heat transfer or transport phenomena.

5.1 Boundary conditions

The following boundary conditions are specified for this problem:
1.   The inlet and outlet fluid pressures for both the cold and hot fluids.
2.   No-slip condition on all solid walls.
3.   The inlet temperatures of both the hot and cold fluids.

All values can be changed to evaluate how the temperature and velocity fields are affected by these parameters.

Since the fluid pressures are specified at the inlet and outlet, the inlet velocities are then calculated as part of the solution. Another option would be to specify the inlet flow rates for the hot and hot streams and the outlet pressures.

5.2 Results and discussion

Examples of the velocity profiles and temperature distribution are shown in Figure 14 and Figure 15. The following parameters and boundary conditions have been used:
–   The fraction of conduit height to total height of the plate = 0.65
–   Cross-current flow contacting pattern
–   Inlet temperature of cold fluid = 323K
–   Inlet temperature of hot fluid = 283K
–   Pressure on both inlets = 1.1 atm.
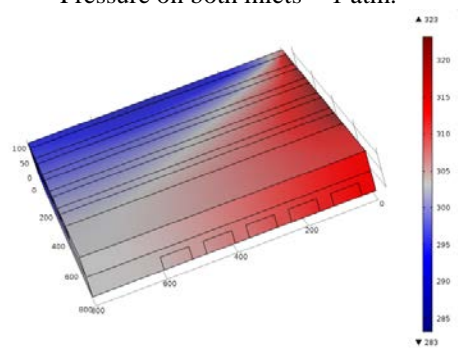–   Pressure on both inlets = 1 atm.

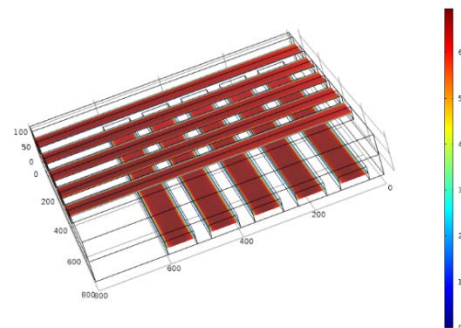**Figure 14.** Temperature profiles for cross-current flow contacting pattern.

Figure 15. Velocity profiles for cross-current flow contacting pattern.

5.3 Application Builder.

The COMSOL application for this problem (Figure 16) allows students to fully adjust problem parameters so any case can be studied. Students can set different parameters, such as geometric (dimensions of plates, fraction of plate height occupied by conduits, type of flow), fluid physical properties (viscosity, density, heat capacity, thermal conductivity) and operating conditions (pressure, inlet temperature).
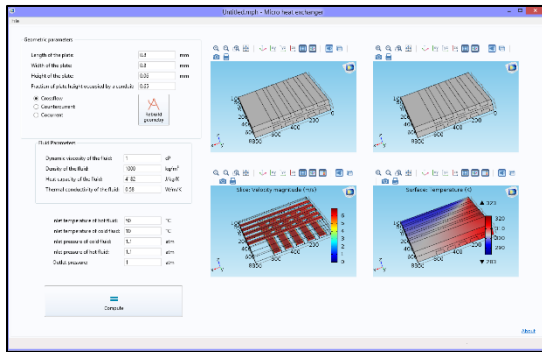

Figure 16. Micro heat exchanger application.

6. Rotating cone pump

This complex flow problem describes a rotating cone pump, which is a type of micropump. The typical student problem only considers the 1-D case so interesting features of the realistic 3-D problem are not accessible.

A typical rotating cone pump geometry is shown Figure 17. It consists of a vertical, rotating inner cone with an upper radius $R_0 = 15$ mm, a rotating inner solid cone with a radius that is 70 to 90% of R_0, and a stationary outer cone.
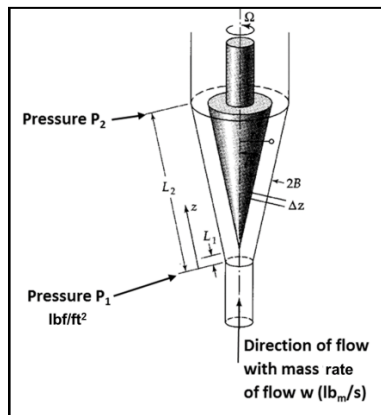

Figure 17. Rotating cone pump geometry

The current model is based upon homogeneous single-phase turbulent fluid flow. To solve the RANS equations, the k-ε model has been used. This model belongs to the two equation turbulent model family and imposes two additional variables, namely, the turbulent kinetic energy (k) and turbulent dissipation (ε).

6.1 Boundary conditions

To calculate the pressure and velocity profiles and, ultimately, estimate pump performance, the following boundary conditions are specified:
- Inlet pressure.
- Outlet mass flow rate.
- No-slip condition on the walls
- Moving wall condition for the rotating domain (inner cone).

6.2

6.3 Results and discussion

Figure 18 shows an example of the model application output for the following parameters: semi angle of the cone, α = 12°; angular velocity, Ω = 6000 RPM.   The velocity profiles change from being mainly in the axial direction at the inlet to the angular direction in the angled region. After exiting the angled region of the cone, the velocity undergoes a transition from an angular-controlled pattern to a combination of angular and axial behavior.
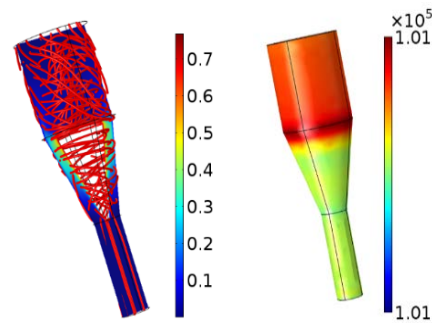

Figure 18. Example of the velocity and pressure profiles from the rotating cone pump application.

Although this problem can be approximated as a 1-D laminar flow problem [1], the relative error in calculated pressure drop can reach 100% for micro-scale geometries. One of possible sources of error may be omitting curvature and end effects which are accounted for in the 3-D model.

6.4 Application builder.

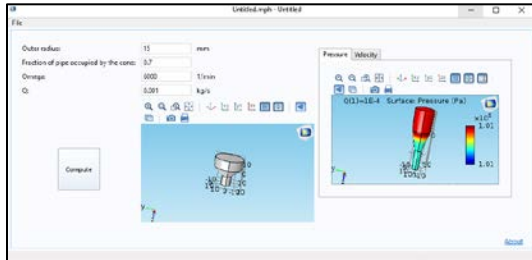The main window of the application is shown in Figure 19.

Figure 19. Rotating cone pump application.

One of the most important pump efficiency parameters is the amount of head pressure that can be generated for a fixed mass flow rate and angular velocity of the rotor. This parameter can be estimated either from experimental data or from a detailed CFD simulation. The COMSOL application for this problem allows the student to generate solutions for the velocity and pressure fields from which the head pressure pump can be evaluated for a given set of input parameters.

7. Conclusions

- COMSOL Multiphysics™ provides robust representation of different multiphysics problems that can be used as a tool for teaching key principles

- COMSOL Application Builder allows more realistic simulation of complex problems.

- The student can readily observe the effect of change in any input parameter on any desirable output variable.

8. References

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