Application of COMSOL Multiphysics® in Transport Phenomena Educational Processes

M. Vasilev, P. Sharma and P. L. Mills

Texas A & M University – Kingsville

Department of Chemical & Natural Gas Engineering

Kingsville, TX, USA

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Introduction

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 development of user-friendly yet robust 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, gaining better insight into the interactions between realistic 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 cases where analytical solutions can be developed, such as a single space dimension and time. 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. Examples of using COMSOL for this purpose are illustrated.

Objectives

- Illustrate how COMSOL Multiphysics has been used for enhancing teaching the principles of transport phenomena to first-year chemical engineering graduate students.
- Summarize the techniques used to incorporate it into the course material.

Governing Multiphysics Equations

The following physics were used either separately or as in combination with each other.

Laminar Fluid Flow

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

$$\rho(\mathbf{u}\cdot\nabla)\mathbf{u} = \nabla\cdot\left[-p\mathbf{I}+\mu\left(\nabla\mathbf{u}+(\nabla\mathbf{u})^T\right)\right]$$

Convective Energy Transport

$$\rho C_p\mathbf{u}\cdot\nabla T+\nabla\cdot\mathbf{q}=Q$$

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

Convective Species Transport

$$\nabla\cdot(-D_i\nabla c_i)+\mathbf{u}\cdot\nabla c_i=R_i$$

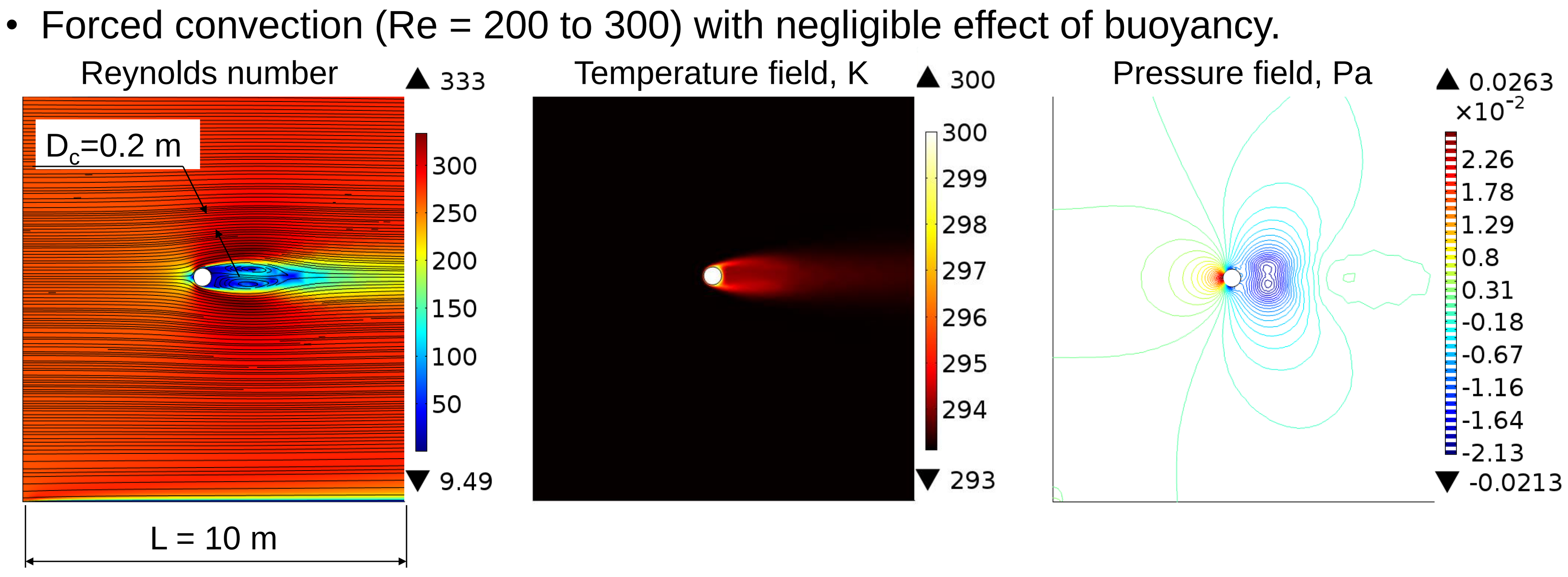
$$\mathbf{N}_i=-D_i\nabla c_i+\mathbf{u}c_i$$

Results

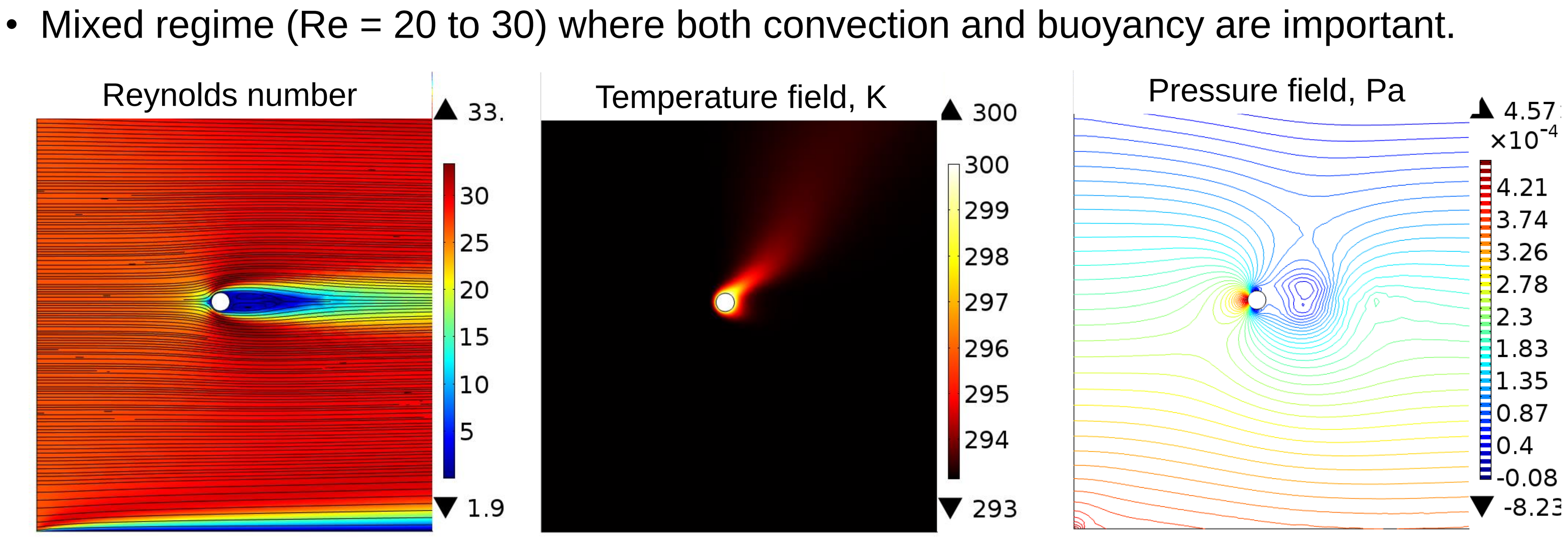
Nonisothermal Flow Over a Cylinder [1]

Fluid approaches a stationary, heated cylinder of infinite length with different velocities. Grashof number = 1.1 x 10^8

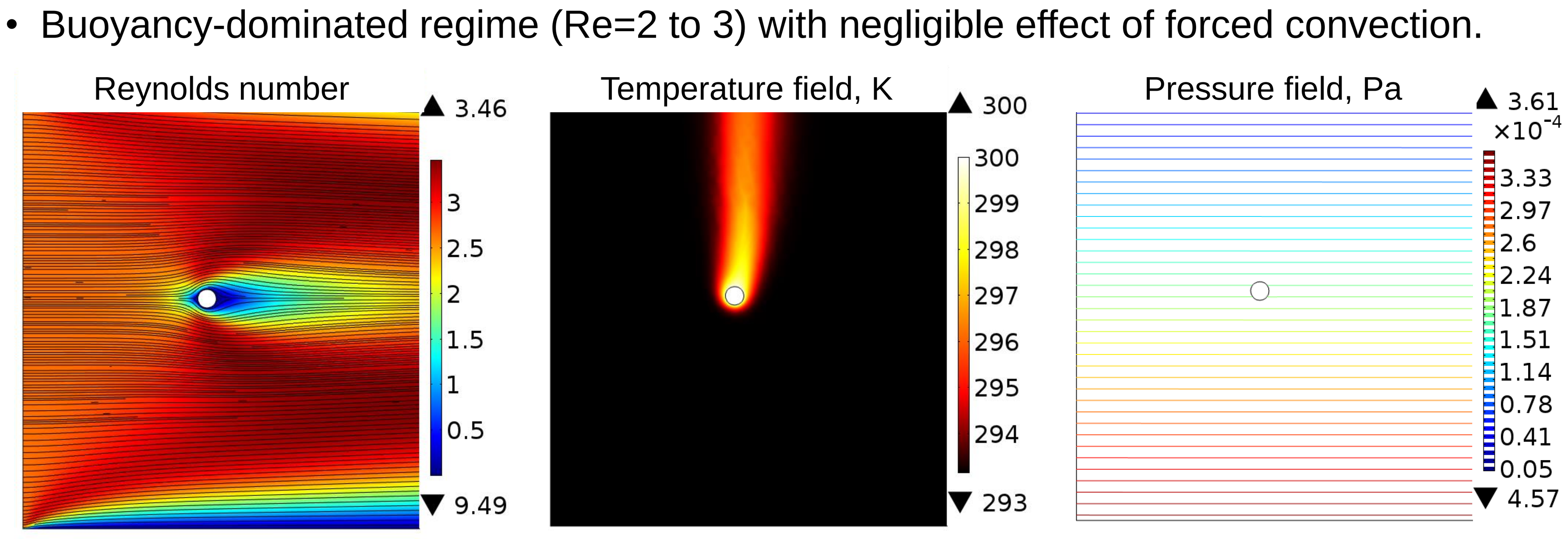
- Forced convection (Re = 200 to 300) with negligible effect of buoyancy.



- Mixed regime (Re = 20 to 30) where both convection and buoyancy are important.

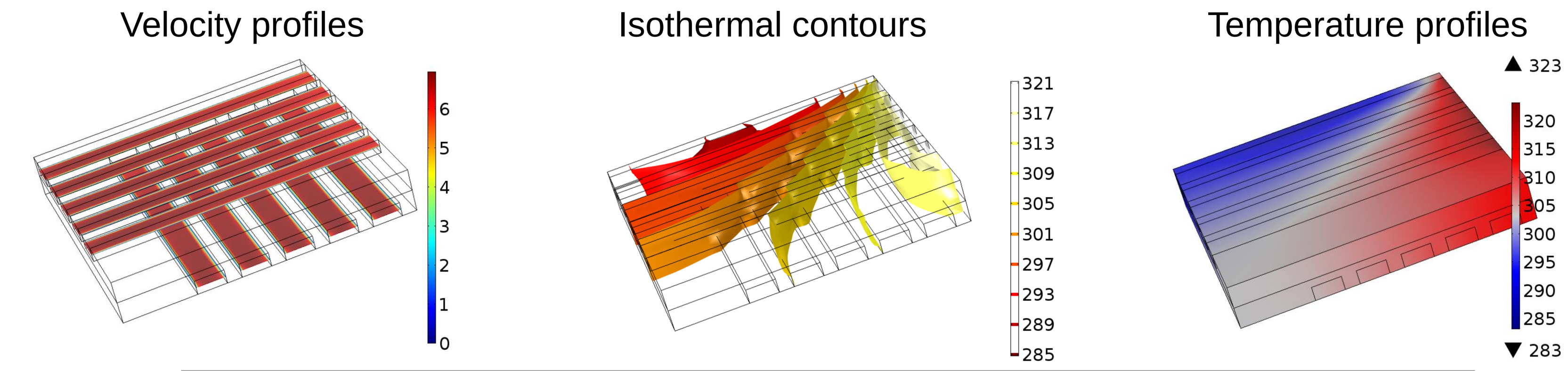


- Buoyancy-dominated regime (Re=2 to 3) with negligible effect of forced convection.



Micro Heat Exchanger (MHE) [2]

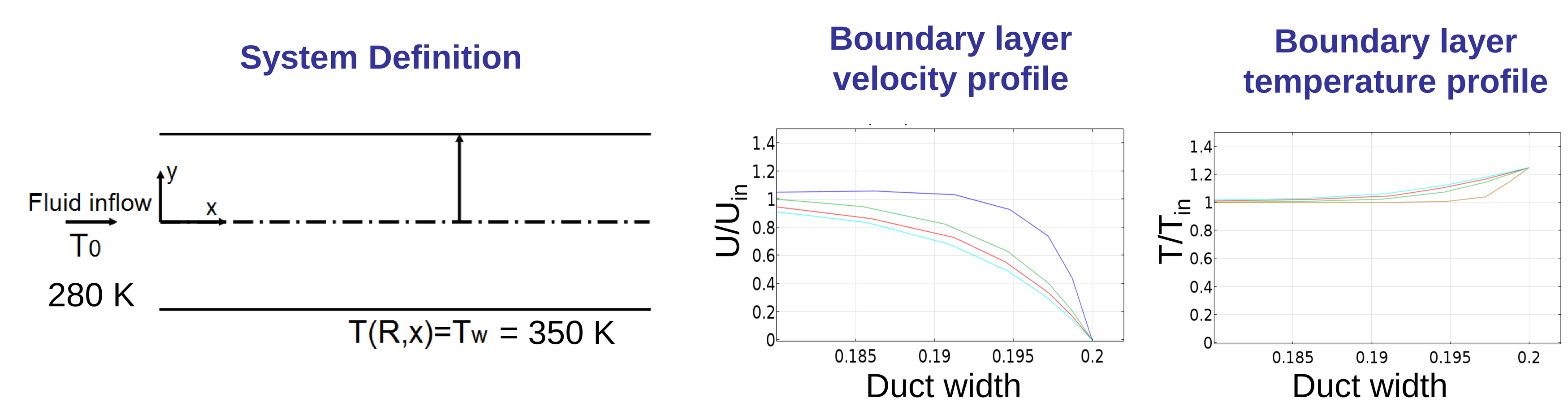
- MHE's are used in micro-process systems, semiconductor systems and MEMS.
- COMSOL readily solves the multiphysics and allows the system to be optimized.

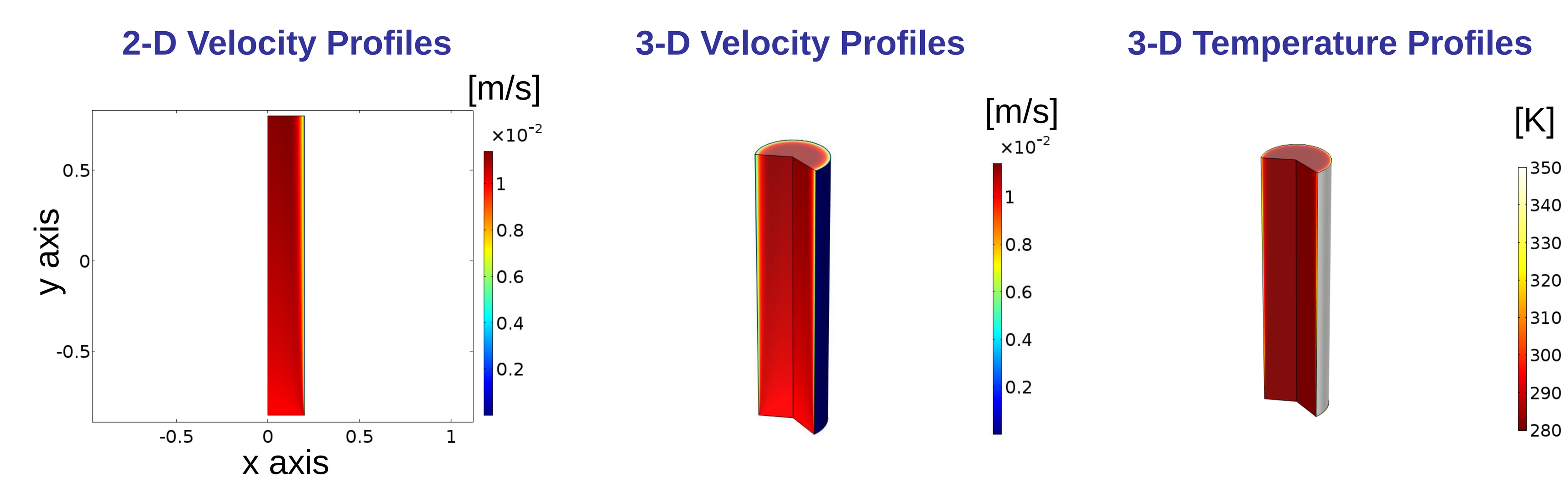


	Length (μm)	Width (μm)	Height(μm)
Plate	800	800	60
Channel	800	80	40

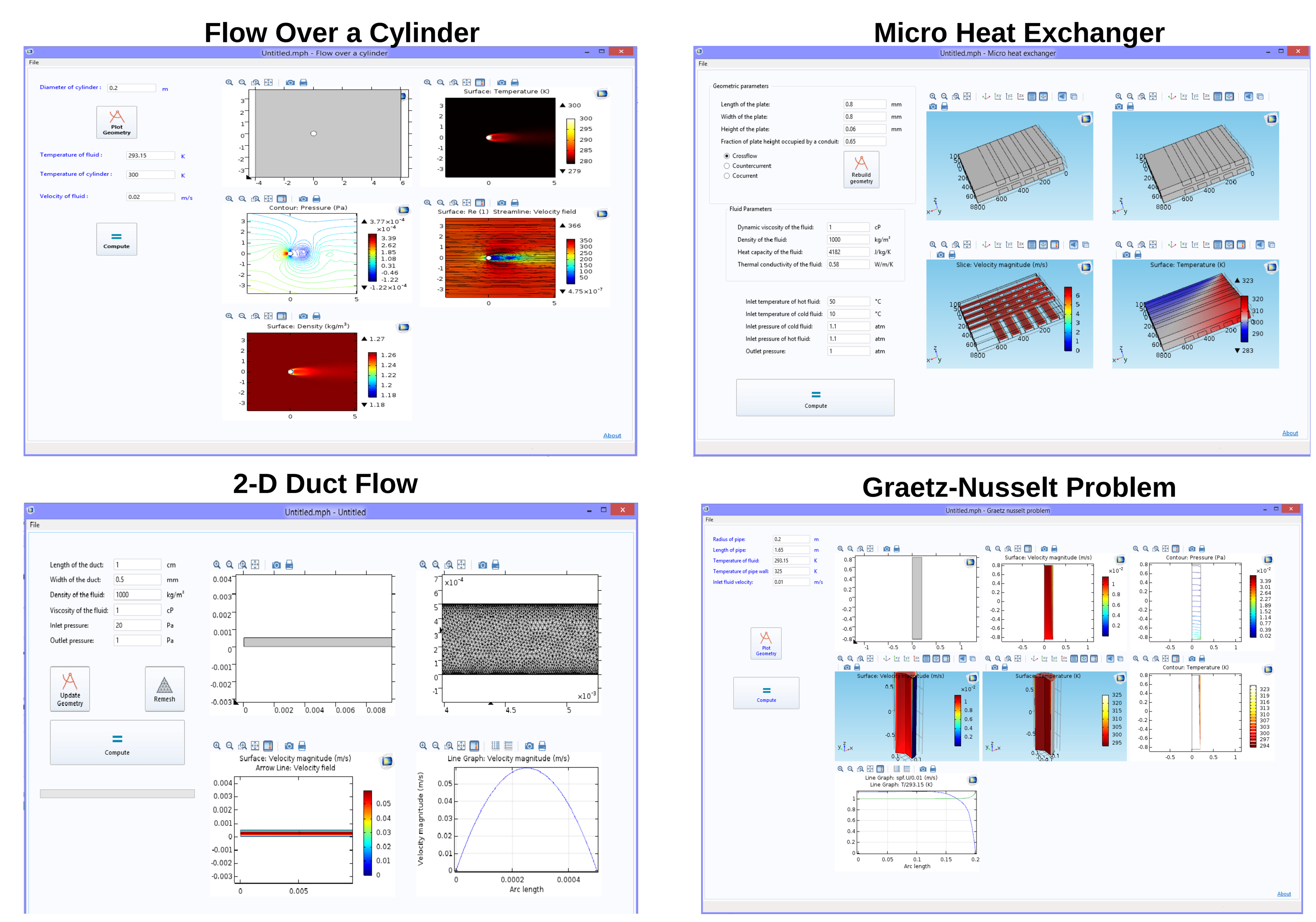
Graetz-Nusselt problem [1]

Steady-state heat transfer to a fluid flowing through a duct. The fluid enters the duct at constant temperature and encounters a wall at a constant but different temperature. The systems has axial symmetry so it can be solved in two spatial dimensions.





Selected Example Applications from Transport Phenomena



Conclusions

- COMSOL Multiphysics™ provides a robust representation of different multiphysics problems that is useful for enhancing educational experiences in chemical engineering.
- COMSOL Application Builder allows more realistic simulation of more complex problems.
- COMSOL Apps allow students to readily study the effect of input parameters on output variables, which is useful for strengthening their understanding of multiphysics interactions.

References

1. Bird, R.B, Stewart, W.E & Lightfoot, E.N. (2007). **Transport Phenomena**. (2nd ed.). New York: John Wiley & Sons, Inc.
2. Seelam S. (2009). "Design of Graphical User Interface for Interlinked Curriculum Component Modules for Microchemical Systems and Modeling of T-shaped Microchemical Reactor," MS Thesis, Texas A&M University-Kingsville.