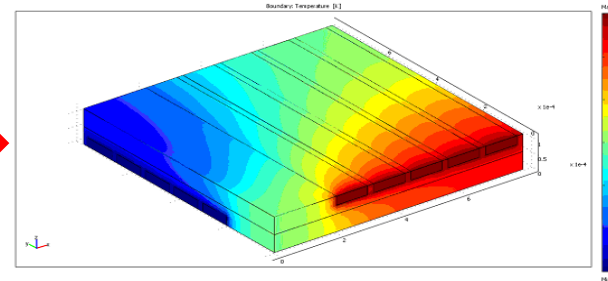
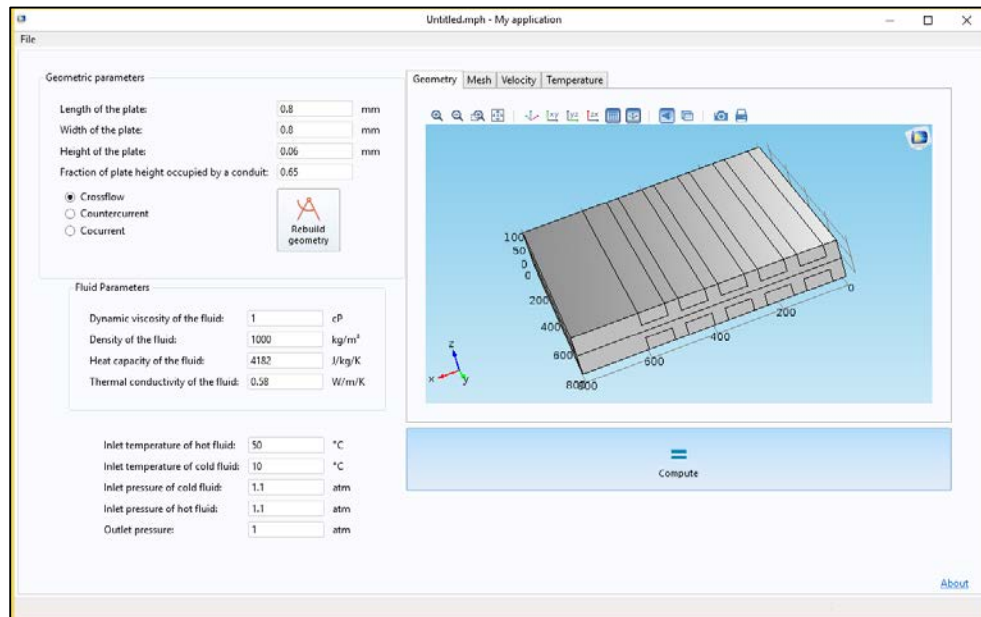


Session Chair: Jeffrey Fong, National Institute of Standards & Technology

October 8, 2015

1:00 PM – 2:30 PM

# Application of COMSOL Multiphysics™ Software in Transport Phenomena Educational Processes



Mikhail Vasilev  
Pranav Sharma  
Patrick L. Mills\*

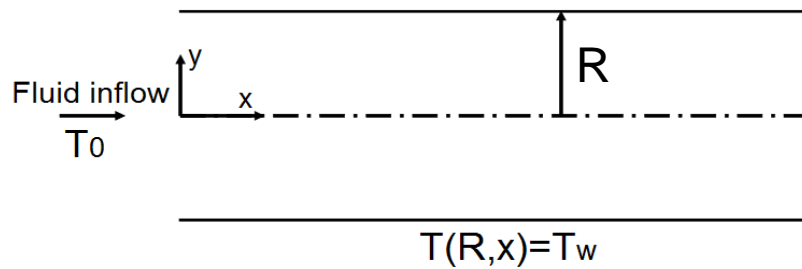
Department of Chemical and Natural Gas Engineering  
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Micro Heat Exchanger (MHE) Application

Anuradha Nagaraj  
Department of Environmental Engineering

# Transport Phenomena: Connecting Theory to Practical Problems

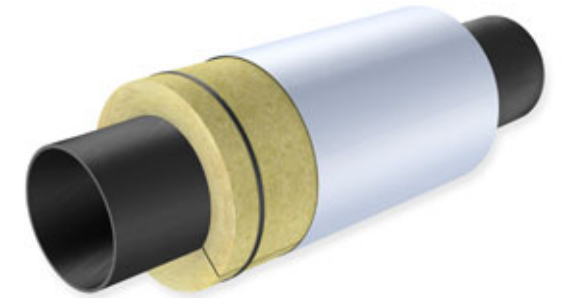
## Graetz-Nusselt Problem



Not constant boundary conditions?  
Flux specified only for some region of the pipe?  
Imperfect thermal insulation?



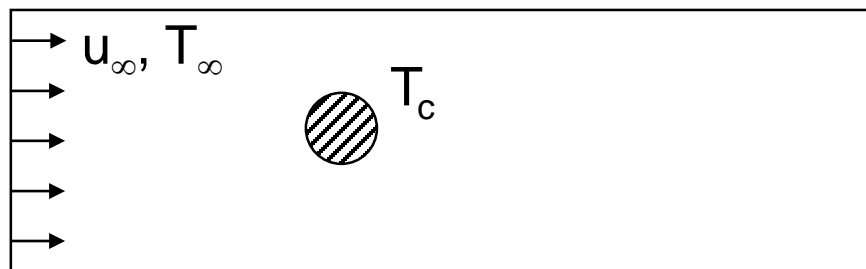
## Electrically Heated Pipe



## Subsea Pipeline



## Nonisothermal Flow Over a Cylinder



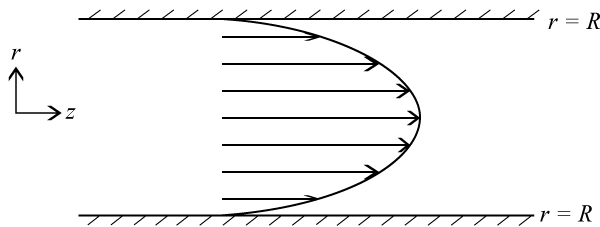
Complex arrangement of multiple pipes?  
Viscous flow?  
Higher Reynolds number?

# Examples of Typical Transport Phenomena Course Problems

## Momentum transport

1-D fluid flow through a circular pipe

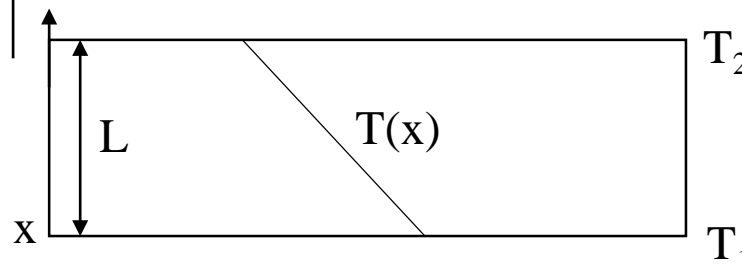
$$u(r) = u_{max} \left[ 1 - \left( \frac{r}{R} \right)^2 \right]$$



## Energy transport

Linear heat conduction through a solid wall

$$T(x) = \frac{(T_2 - T_1)}{L} x + T_1$$

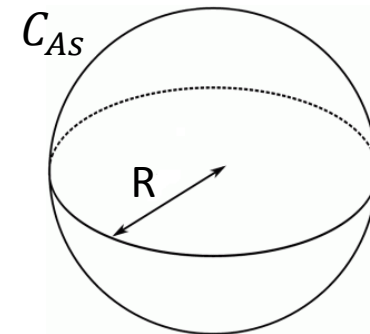


## Mass transport

Fickian diffusion in isothermal spherical catalyst particle followed by a 1<sup>st</sup> order reaction.

$$\Psi(\lambda) = \frac{1}{\lambda} \left( \frac{\sinh(\phi\lambda)}{\sinh(\phi)} \right),$$

where  $\Psi = \frac{C_A}{C_{As}}$  and  $\lambda = \frac{r}{R}$



## Pros:

- Not very complicated – Straightforward to understand
- Existence of analytical solutions
- Provides initial insight into more complex problems

## Cons:

- Lack of model response visualization
- Limited applicability to real-world problems
- Transient solutions for 1-D problems are not simple to compute, e.g., infinite series of complex Eigenfunctions and Eigenvalues

# Motivation for Creating COMSOL Applications

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## Desired Problem Attributes

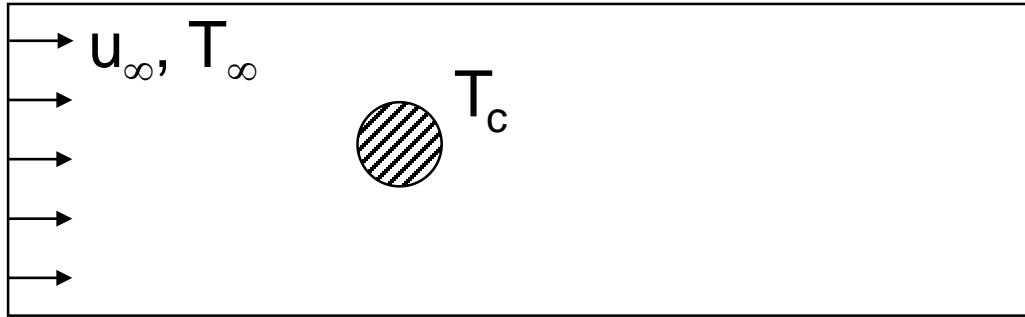
- Reinforce 1-D problems by extension to multi-dimensions (2-D or 3-D) and multi-physics.
- Contains various physico-chemical parameters that can be varied by the user.
- Solution can be generated within seconds to minutes with modern computing hardware.
- Ability to readily modify the application to account for problem variations and other derived quantities.

## Applications Developed

- Non-isothermal Flow Over a Cylinder
- Graetz-Nusselt Problem
- Flow Through a Duct
- Micro Heat Exchanger
- Rotating Cone Pump
- Catalytic Wall Microreactor
- T-Micromixer

# Example 1: Nonisothermal Flow Over a Heated Cylinder

## Problem Statement



## Model Equations

- Equation of Continuity

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

- Navier-Stokes Equations

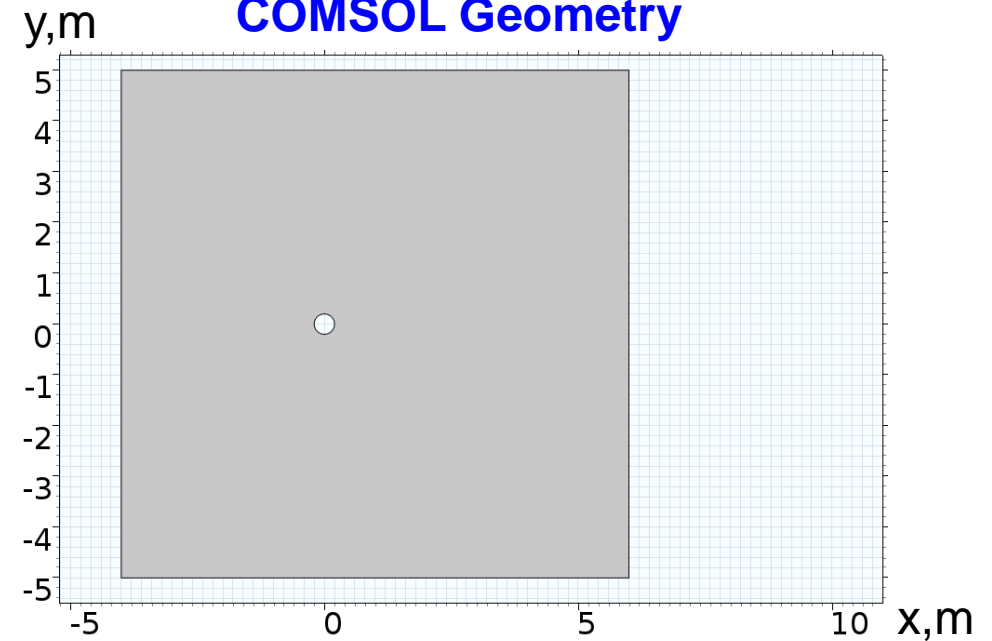
$$\rho(\mathbf{u} \cdot \nabla) \mathbf{u} = \nabla \cdot [p\mathbf{I} + \mu(\nabla \mathbf{u} + (\nabla \mathbf{u})^T)] + \mathbf{F}$$

- Energy Transport Equations

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

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

## COMSOL Geometry



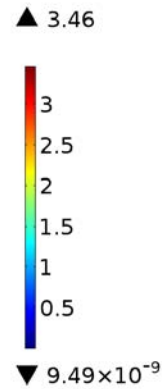
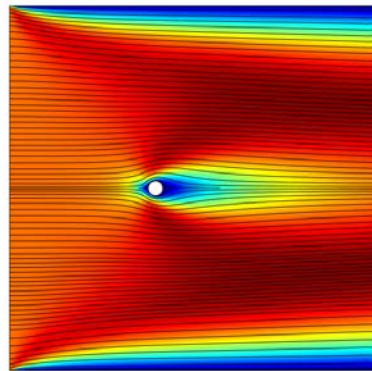
## Model Parameters

Name	Expression	Value	Description
Vinf	0.0002[m/s]	2E-4 m/s	Far-field velocity
T0	300[K]	300 K	Temperature of the cylinder
T1	293.15[K]	293.15 K	Temperature of the fluid at the inlet
D	0.2[m]	0.2 m	Diameter of the cylinder
H	10[m]	10 m	Height of the fluid domain

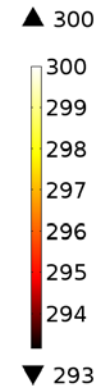
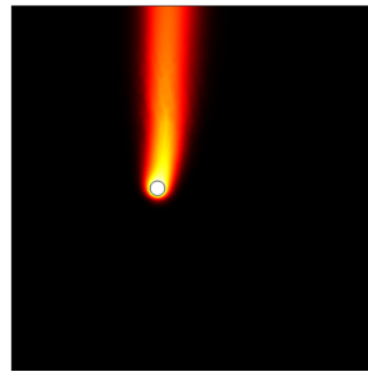
# Velocity, Temperature and Pressure Profiles at Various Reynolds Numbers

$Gr = 10^8$

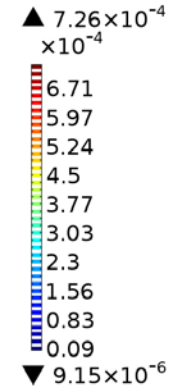
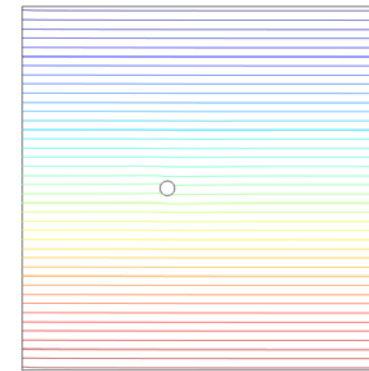
## Velocity Profiles (Re)



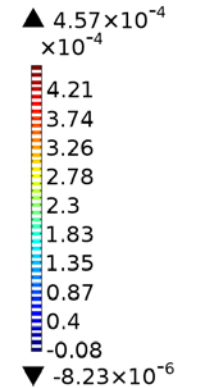
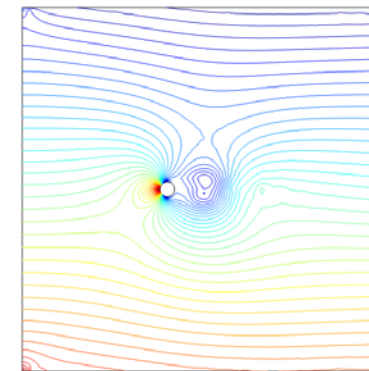
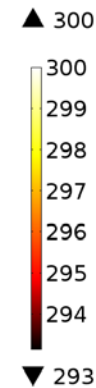
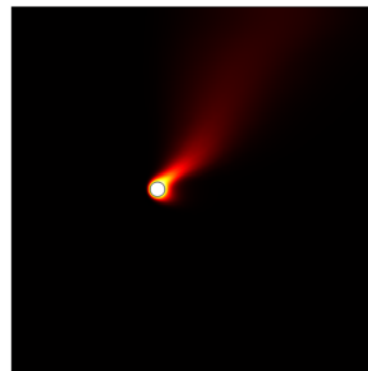
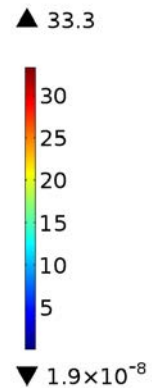
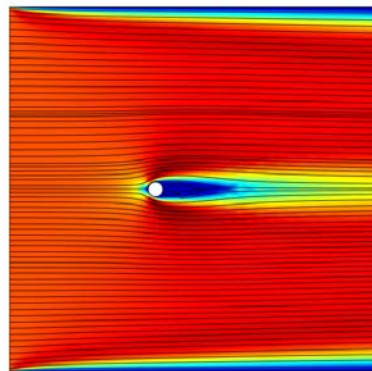
## Temperature Profiles (K)



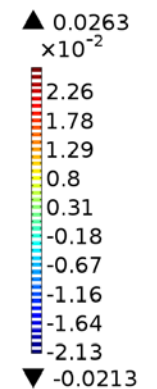
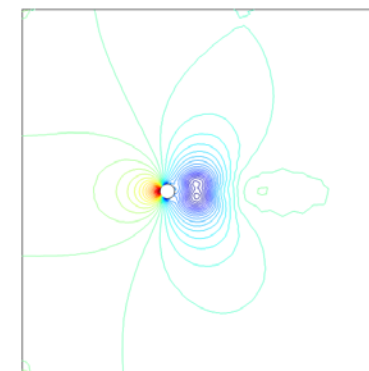
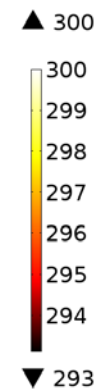
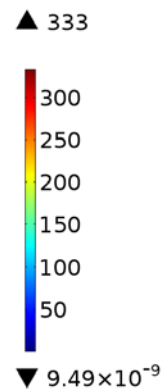
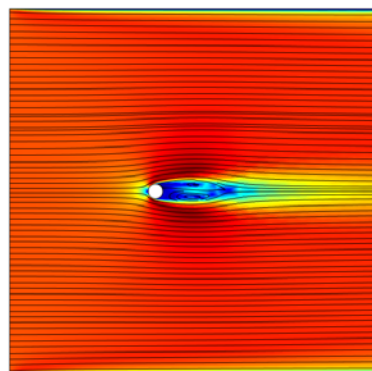
## Pressure Profiles (Pa)



$Re = 2.5$

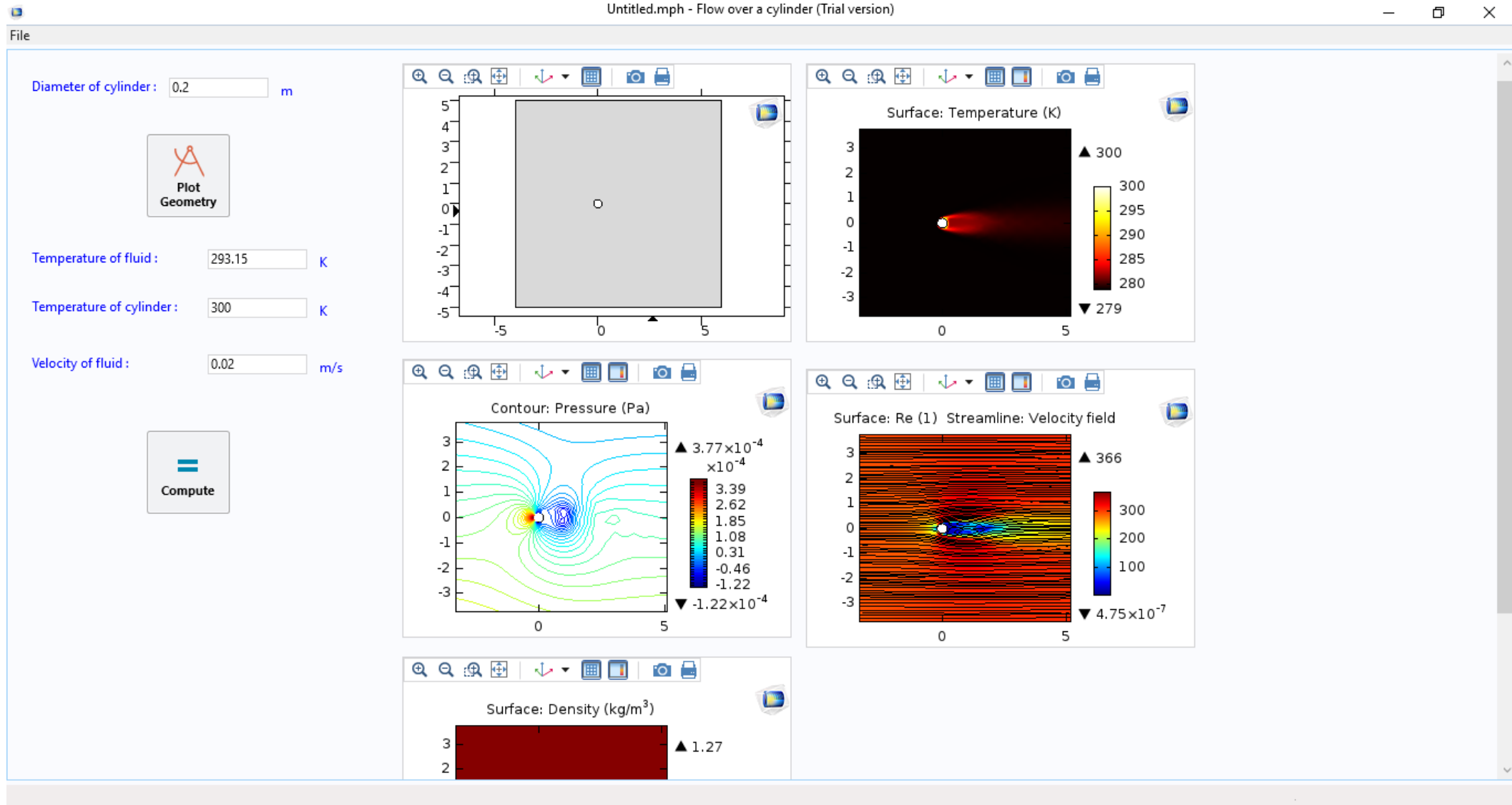


$Re = 25$



$Re = 250$

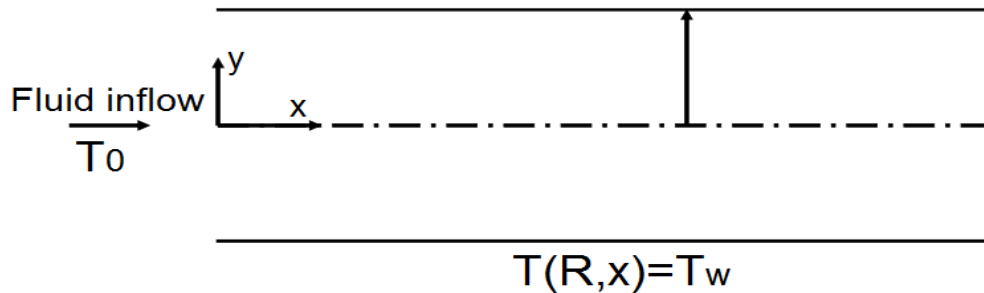
# COMSOL Application: Non-isothermal Flow over a Heated Cylinder





# Example 2: Graetz-Nusselt Problem (Constant Wall Temperature)

## Problem Statement



## Model Equations

- **Equation of Continuity**

$$\nabla \cdot \mathbf{u} = 0$$

- **Navier-Stokes Equations**

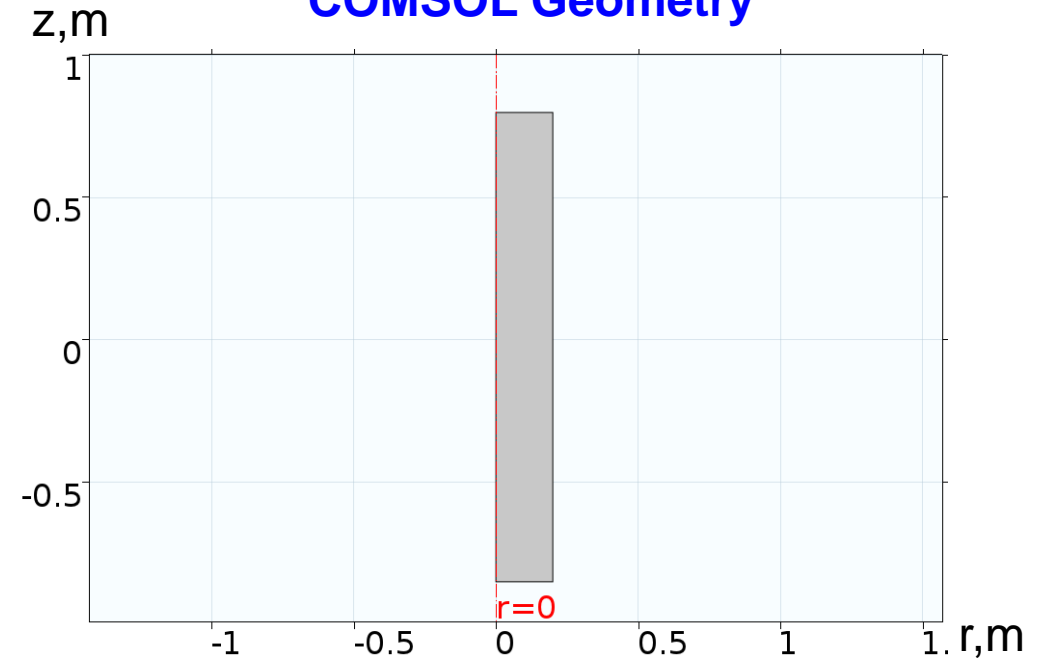
$$\rho(\mathbf{u} \cdot \nabla)\mathbf{u} = \nabla \cdot [p\mathbf{I} + \mu(\nabla\mathbf{u} + (\nabla\mathbf{u})^T)] + \mathbf{F}$$

- **Energy Transport Equations**

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

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

## COMSOL Geometry

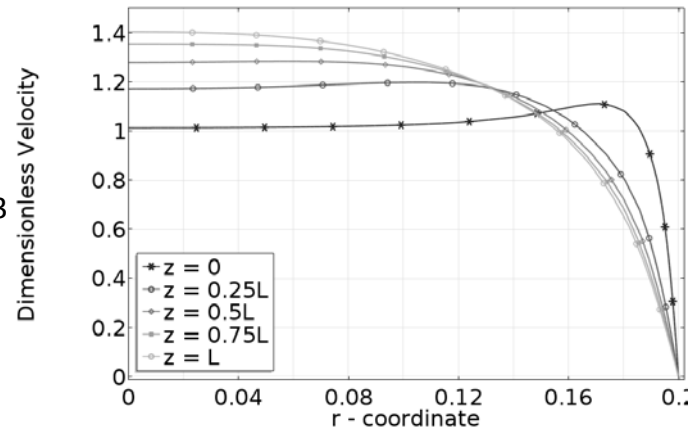


Name	Expression	Value	Description
R	0.2[m]	0.2 m	Radius of pipe
L	1.65[m]	1.65 m	Length of pipe
T <sub>in</sub>	280[K]	280 K	Temperature of fluid
T <sub>w</sub>	350[K]	350 K	Temperature of pipe wall
V <sub>in</sub>	0.001[m/s]	0.001 m/s	Inlet fluid velocity

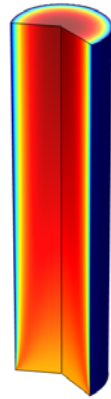


# Velocity and Temperature Profiles

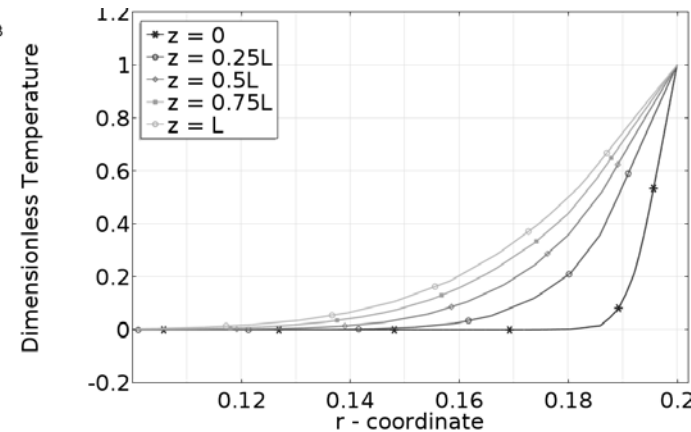
Dimensionless Velocity for Various Axial Positions



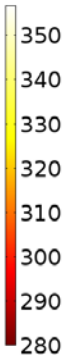
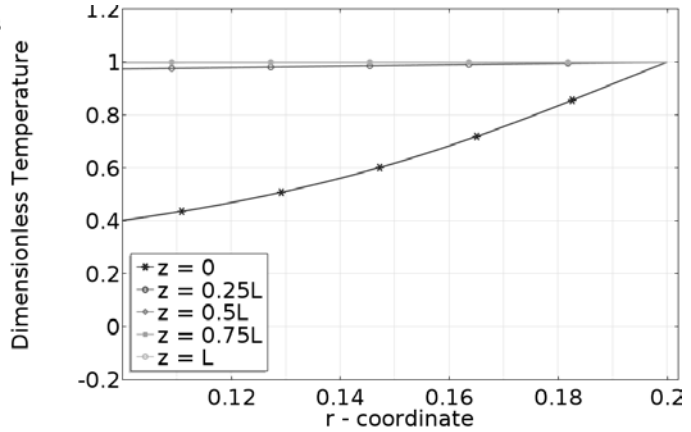
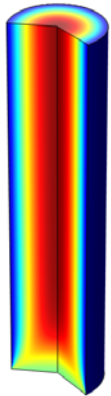
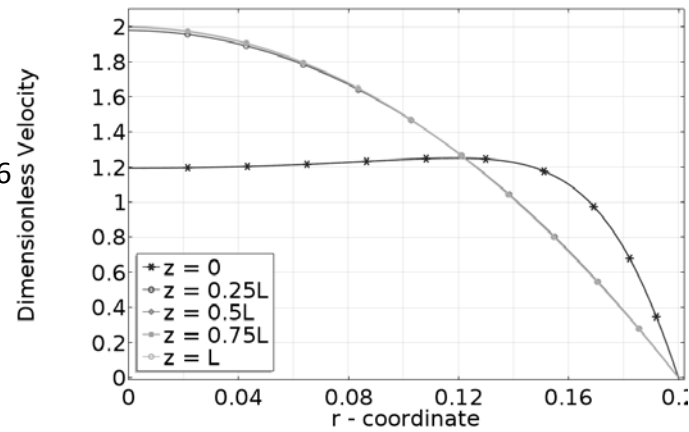
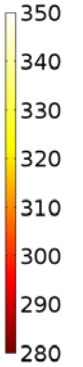
3-D Representation of Velocity Profiles



Dimensionless Temperature for Various Axial Positions



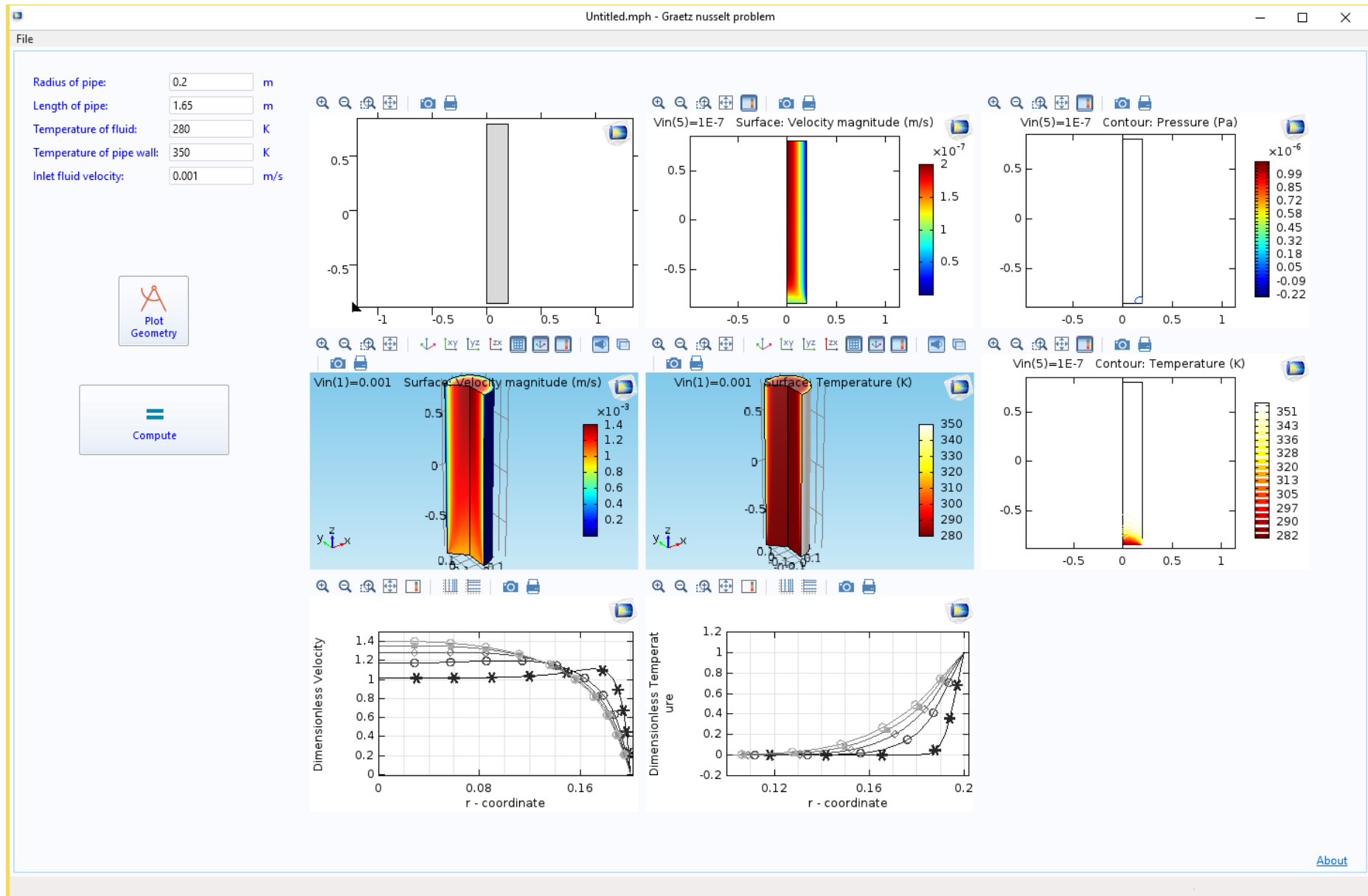
3-D Representation of Temperature Profiles



$$\psi(r, z) = \frac{V(r, z)}{V_{in}}$$

$$\theta(r, z) = \frac{T(r, z) - T_{in}}{T_w - T_{in}}$$

# COMSOL Application: Graetz-Nusselt Problem



# Example 3: Micro Heat Exchanger

## Objectives:

- Compare the heat exchanger effectiveness factor by changing the fluid flow.
- Predict temperature profiles by solving the coupled momentum-energy transport equations for a 3-D geometry.

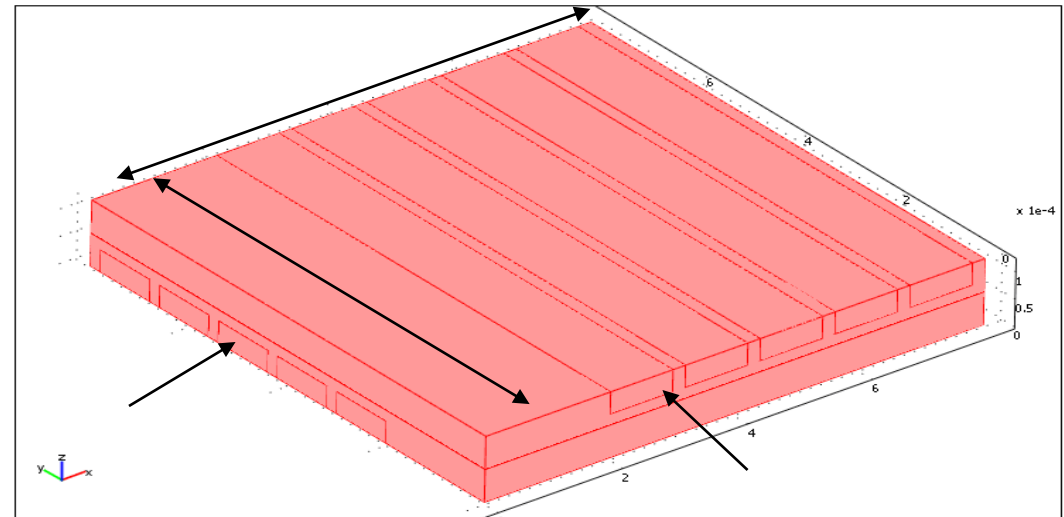
## Model Geometry:

5 rectangular ducts

Cross-flow orientation

## Dimensions:

Length of each slab	800 $\mu\text{m}$
Width of each slab	800 $\mu\text{m}$
Height of each slab	60 $\mu\text{m}$
No. of Microchannels	5
Microchannel width	100 $\mu\text{m}$
Microchannel height	30 $\mu\text{m}$
Mat'l of Construction	Copper



# Micro Heat Exchanger Model Equations & Effectiveness Factor

## Model Equations:

### Momentum Transport Equations

$$\text{x- direction: } \rho \left[ \frac{\partial u_x}{\partial t} \right] - \mu \left[ \frac{\partial^2 u_x}{\partial x^2} + \frac{\partial^2 u_x}{\partial y^2} + \frac{\partial^2 u_x}{\partial z^2} \right] + \rho \left[ u_x \frac{\partial u_x}{\partial x} + u_y \frac{\partial u_x}{\partial y} + u_z \frac{\partial u_x}{\partial z} \right] + \frac{\partial p}{\partial x} = 0$$

$$\text{y-direction: } \rho \left[ \frac{\partial u_y}{\partial t} \right] - \mu \left[ \frac{\partial^2 u_y}{\partial x^2} + \frac{\partial^2 u_y}{\partial y^2} + \frac{\partial^2 u_y}{\partial z^2} \right] + \rho \left[ u_x \frac{\partial u_y}{\partial x} + u_y \frac{\partial u_y}{\partial y} + u_z \frac{\partial u_y}{\partial z} \right] + \frac{\partial p}{\partial y} = 0$$

$$\text{z-direction: } \rho \left[ \frac{\partial u_z}{\partial t} \right] - \mu \left[ \frac{\partial^2 u_z}{\partial x^2} + \frac{\partial^2 u_z}{\partial y^2} + \frac{\partial^2 u_z}{\partial z^2} \right] + \rho \left[ u_x \frac{\partial u_z}{\partial x} + u_y \frac{\partial u_z}{\partial y} + u_z \frac{\partial u_z}{\partial z} \right] + \frac{\partial p}{\partial z} = 0$$

### Conduction-Convection Equation:

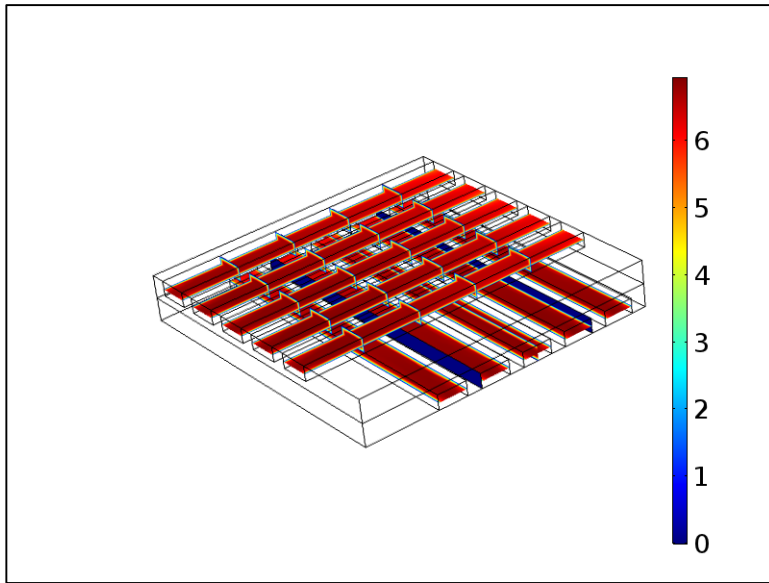
$$\rho C_p \left( \frac{\partial T}{\partial t} + u_x \frac{\partial T}{\partial x} + u_y \frac{\partial T}{\partial y} + u_z \frac{\partial T}{\partial z} \right) = \left( k_x \frac{\partial^2 T}{\partial x^2} + k_y \frac{\partial^2 T}{\partial y^2} + k_z \frac{\partial^2 T}{\partial z^2} \right) + Q$$

### Parameter Estimation:

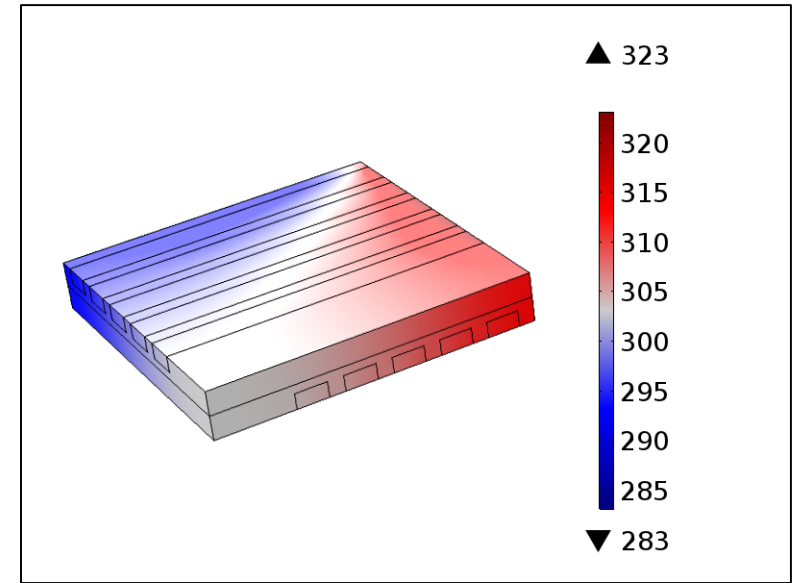
$$\text{Effectiveness factor } \varepsilon = \frac{q}{q_{\max}} = \frac{m^\circ C_p (T_{\text{hot-in}} - T_{\text{hot-out}})}{m^\circ C_p (T_{\text{hot-in}} - T_{\text{cold-in}})} = \frac{(T_{\text{hot-in}} - T_{\text{hot-out}})}{(T_{\text{hot-in}} - T_{\text{cold-in}})}$$

$\rho$  is the fluid density,  $\eta$  is the fluid viscosity,  $p$  is the fluid pressure,  $K$  is fluid conductivity,  $T$  is temperature,  $m^\circ$  mass flow rate, and  $C_p$  is the Specific heat capacity

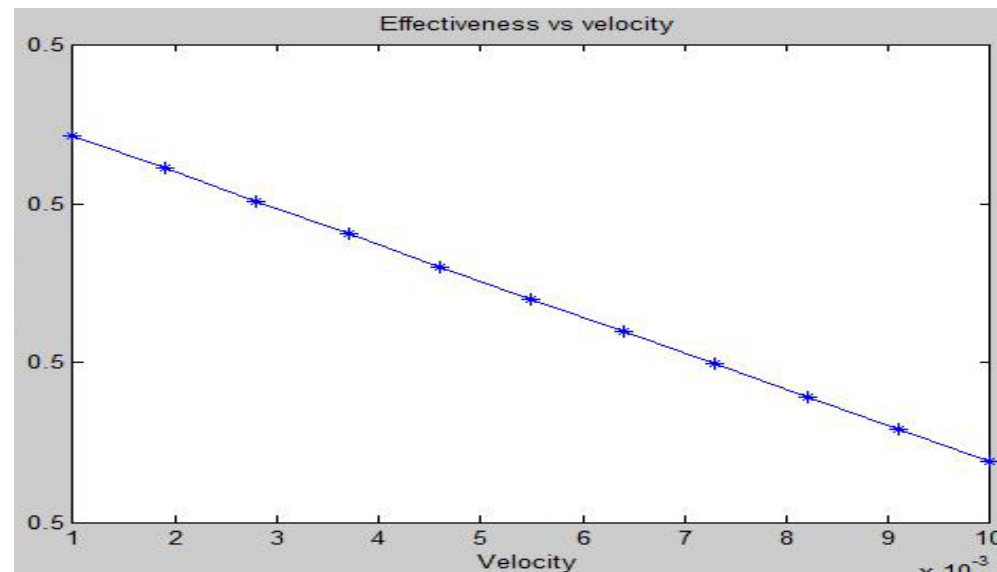
# Micro Heat Exchanger Velocity & Temperature Profiles



**Velocity Profile  
Slice Plot**



**Temperature Profile  
Isosurface Plot**



**Effectiveness  
Factor vs Fluid Velocity**

# COMSOL Application: Micro Heat Exchanger

Untitled.mph - My application

File

Geometric parameters


Length of the plate:  mm

Width of the plate:  mm

Height of the plate:  mm

Fraction of plate height occupied by a conduit:

Crossflow  
 Countercurrent  
 Cocurrent

 Rebuild geometry

Fluid Parameters

Dynamic viscosity of the fluid:  cP

Density of the fluid:  kg/m<sup>3</sup>

Heat capacity of the fluid:  J/kg/K

Thermal conductivity of the fluid:  W/m/K

Inlet temperature of hot fluid:  °C

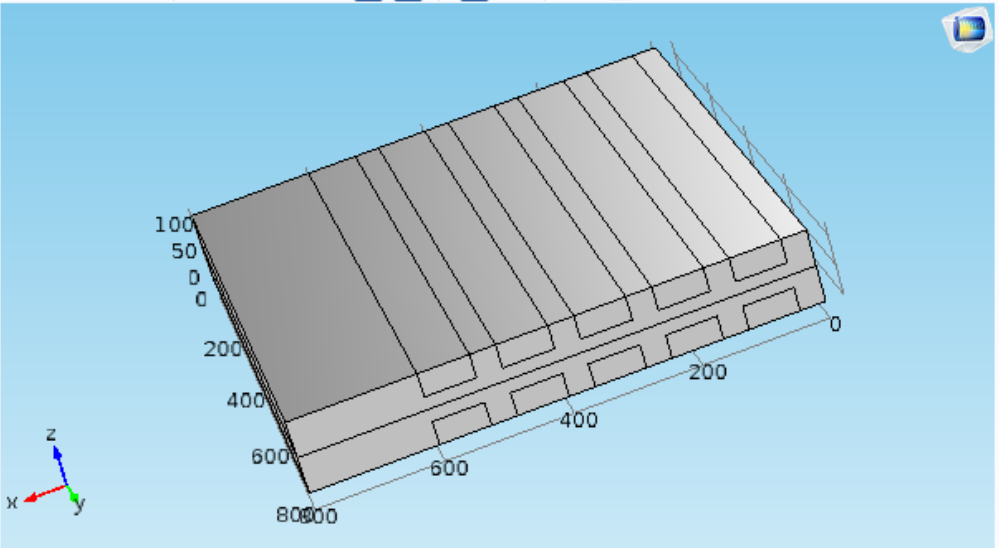
Inlet temperature of cold fluid:  °C

Inlet pressure of cold fluid:  atm

Inlet pressure of hot fluid:  atm

Outlet pressure:  atm

Geometry Mesh Velocity Temperature



Compute

[About](#)

# COMSOL Application: Catalytic Wall Microreactor

**Catalytic Wall Reactor**

Input

Parameter	Value	Units
Rate Constant	1.5	1/s
Diffusion Coefficient of A	1e-7	m <sup>2</sup> /s
Diffusion Coefficient of B	0.5e-7	m <sup>2</sup> /s
Concentration of A	1	mol/m <sup>3</sup>
Concentration of B	0	mol/m <sup>3</sup>
Density	1e3	kg/m <sup>3</sup>
Dynamic Viscosity	1e-3	kg/(m·s)
Inlet Pressure	0.1	Pa
Outlet Pressure	0	Pa

Reactor Description

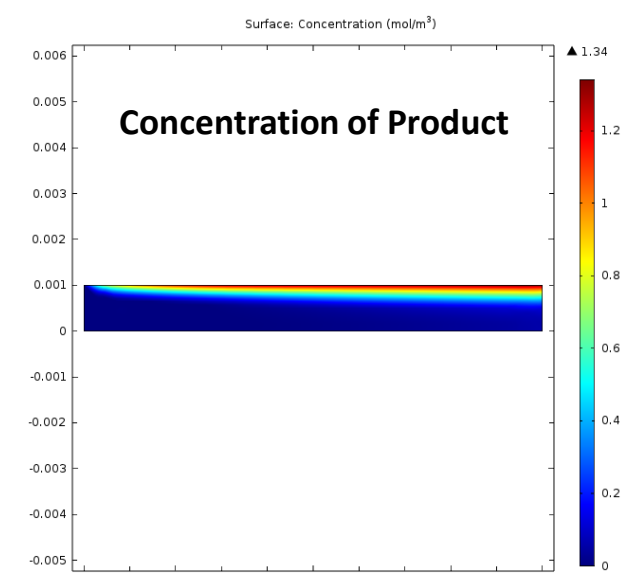
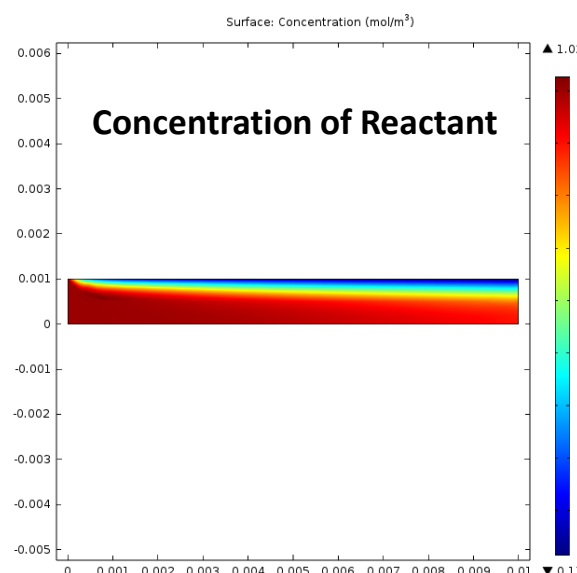
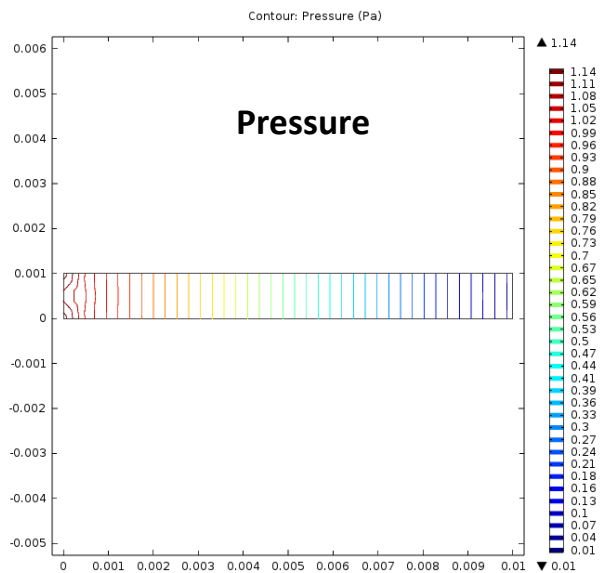
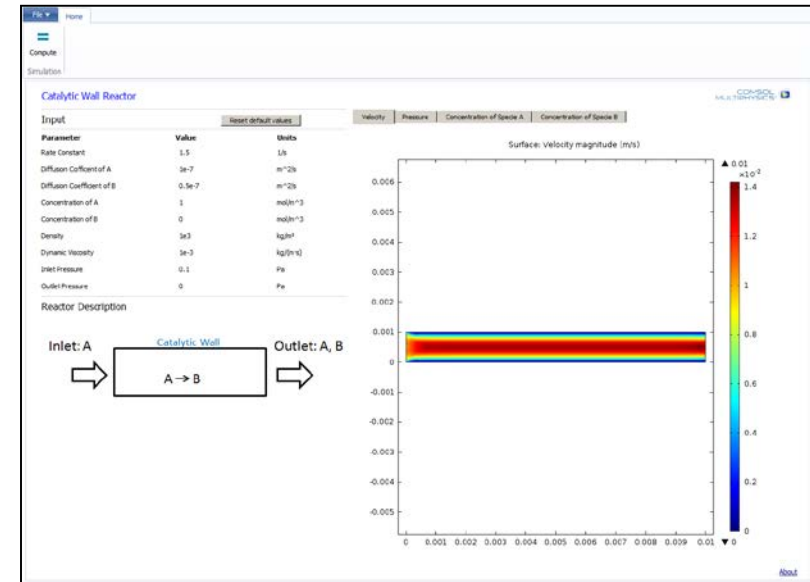
Inlet: A → Catalytic Wall (A → B) → Outlet: A, B

**Model Description**

**Results Panel**

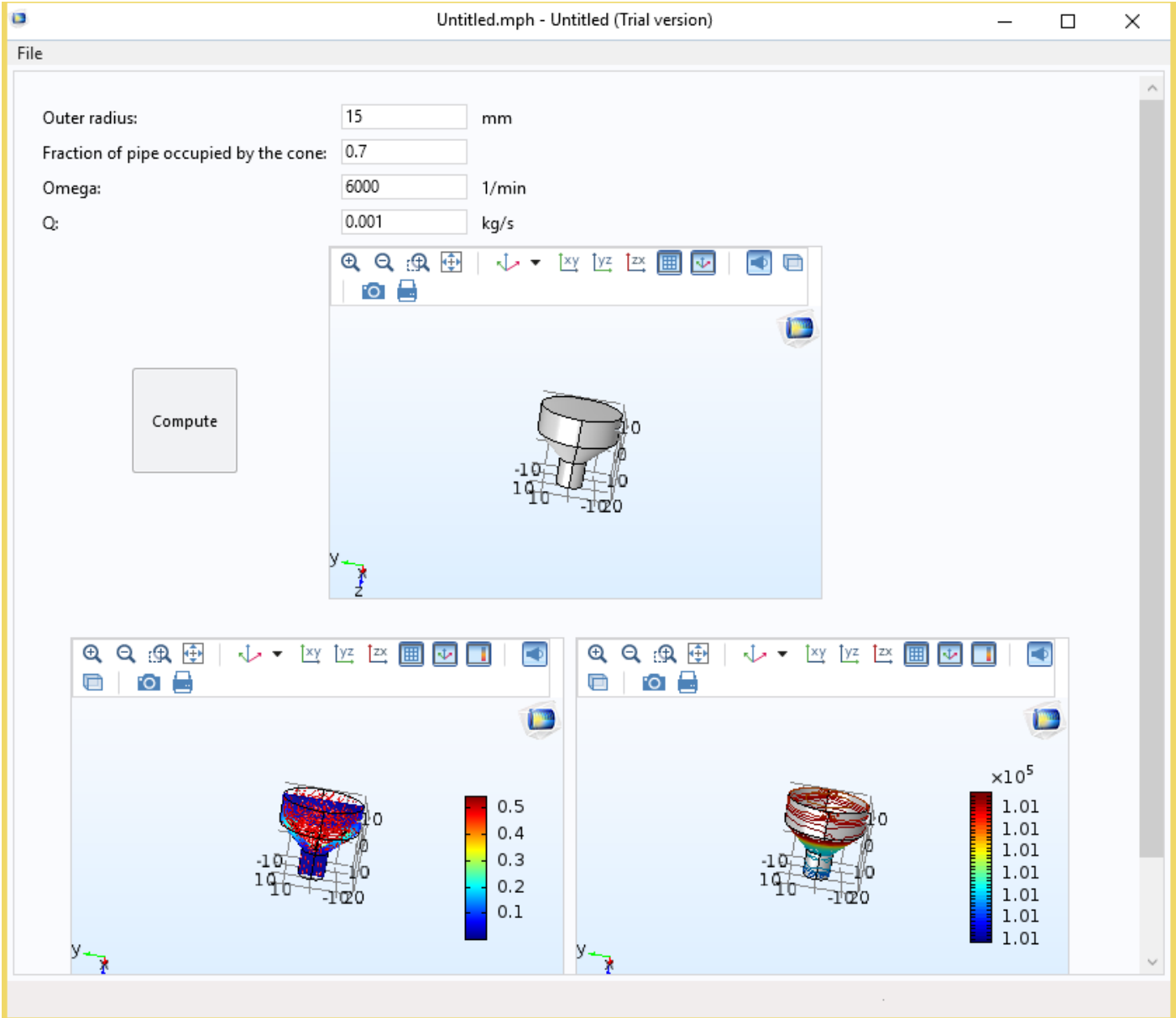
**Input**

**Tabs**





# COMSOL Application: Rotating Cone Pump



# Conclusions

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## COMSOL Multiphysics™ :

- Provides robust representation of different multiphysics problems that can be used as a tool for teaching transport phenomena principles.
- Can be used as an intermediate learning instrument between university education and real-world applications.
- Allows different cases of the same problem to be combined into a single application for parametric studies.
- Allows more realistic simulation of real world problems for improved insight.

The student can observe the effect of input parameters on any output variable.

Thank you for your attention.