COMSOL Day
Orange County

Thursday
May 17, 2018
8:30AM–4:00PM

Microfluidics and Chemical Reaction Engineering

COMSOL Day Orange County, May 17 2018

Mina Sierou

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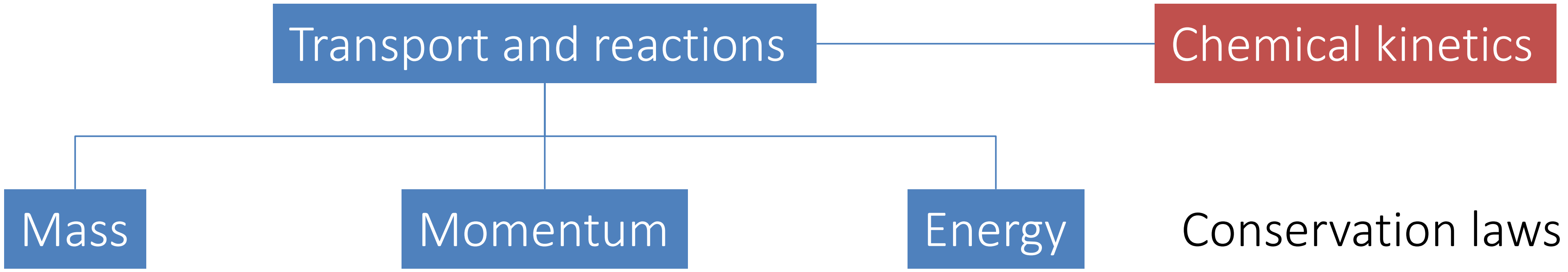
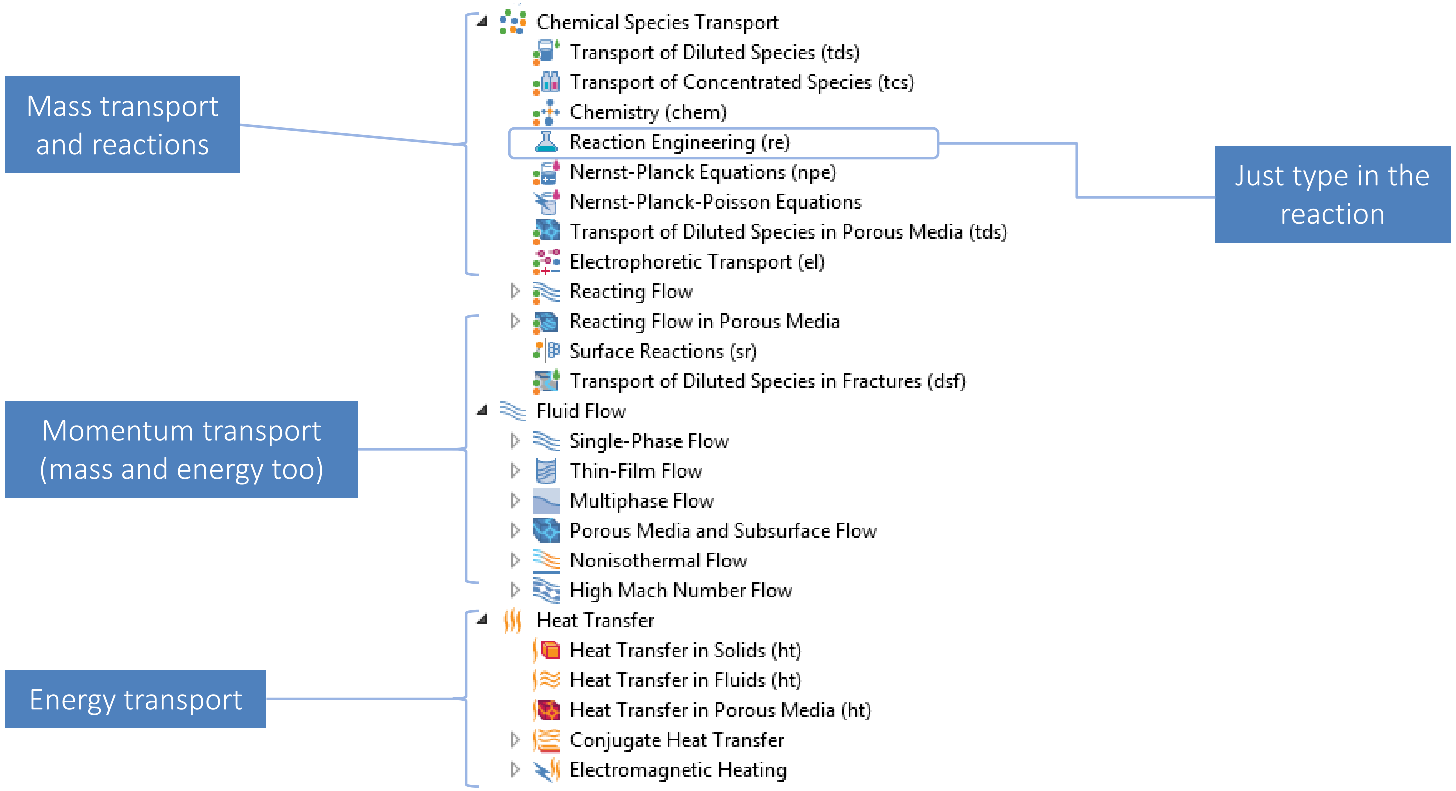
Mass, Energy, Momentum, and Reactions



Transport Phenomena interfaces



Chemical Reaction Engineering Module
and CFD Module

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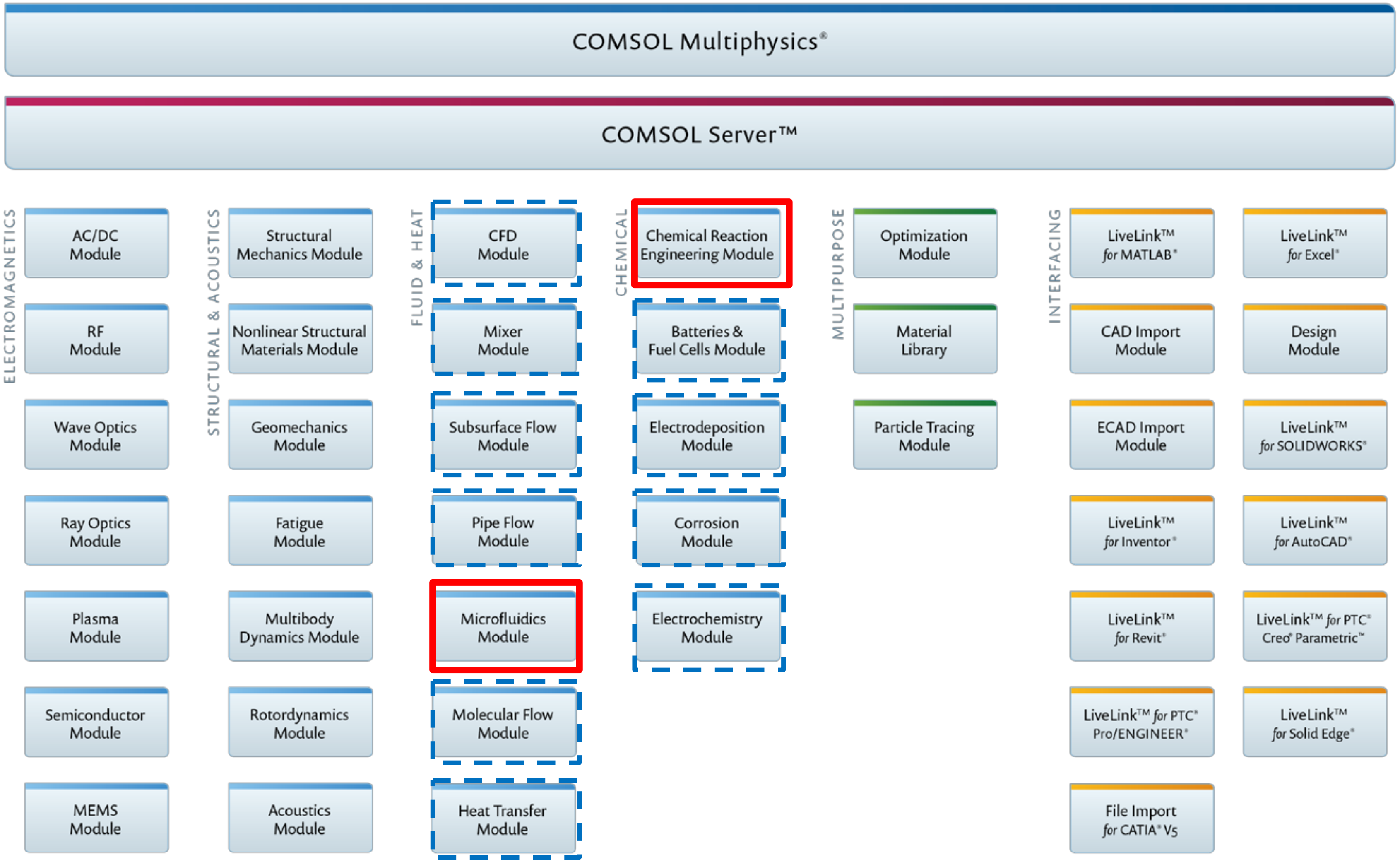
Transport related Modules in the COMSOL® Product Suite



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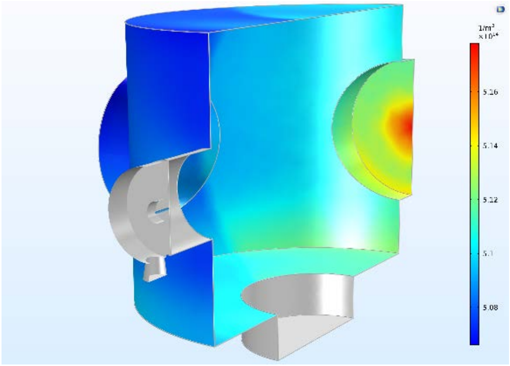
The Microfluidics Module

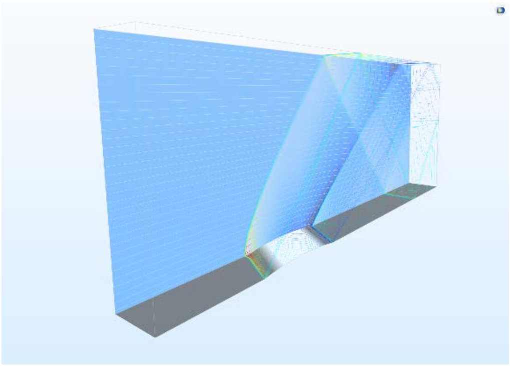
Flow Regime Approximations

- Molecular flow
- Rarified flow
- Stokes flow
- Steady laminar flow

- Unsteady laminar flow
- Turbulent flow
- Compressible turbulent flow
- Inviscid flow



Gas flow through a narrow tube into a high vacuum chamber



Compressible turbulent flow in a benchmark model for high Ma flow

Fluid Flow Equations

- Navier-Stokes, continuity, and equation of state

$$\rho\left(\frac{\partial \boldsymbol{u}}{\partial t}+(\boldsymbol{u}\cdot\boldsymbol{\nabla})\boldsymbol{u}\right)=-\boldsymbol{\nabla}p+\boldsymbol{\nabla}\cdot\left[\mu\left(\boldsymbol{\nabla}\boldsymbol{u}+(\boldsymbol{\nabla}\boldsymbol{u})^{\mathrm{T}}-\frac{2}{3}(\boldsymbol{\nabla}\cdot\boldsymbol{u})\mathbf{I}\right)\right]+\boldsymbol{F}$$

$$\frac{\partial\rho}{\partial t}+\boldsymbol{\nabla}\cdot(\rho\boldsymbol{u})=0$$

$$\rho=\rho(p,T)$$

- Estimate the Reynolds number using characteristic scales: L, U, ρ, μ

$$\mathrm{Re}=\frac{\rho UL}{\mu}=\frac{UL}{\nu}\sim\frac{inertial\ forces}{viscous\ forces}$$

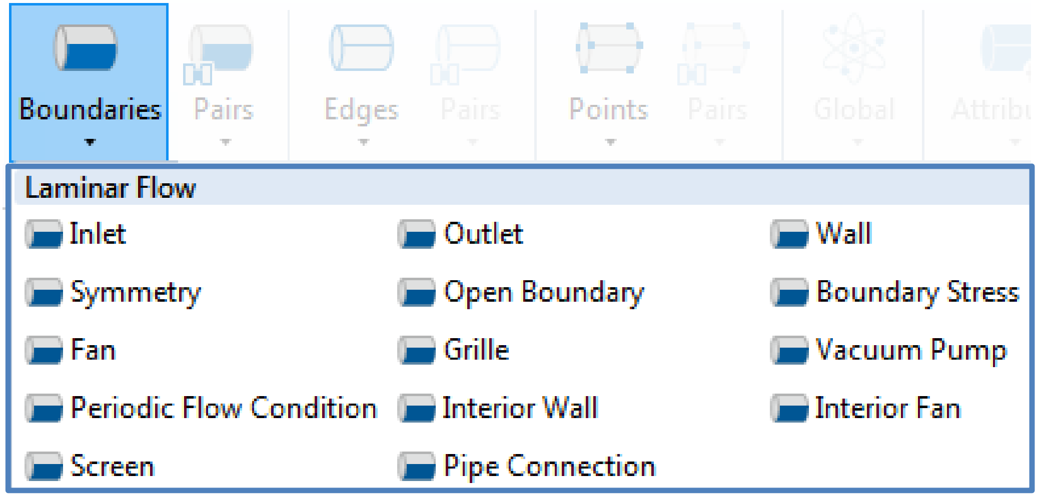
Flow Regimes covered by the Microfluidics Module

- Slip Flow (applicable for small Knudsen number (0.01 < Kn < 0.1)
  - Viscous flow in the bulk
  - Velocity slip at the boundaries
- Stokes flow (low Re (<< 1))
  - The contribution of advective inertial forces can be neglected
- Laminar flow (intermediate Re (~1-2000))
  - Steady or Unsteady flow

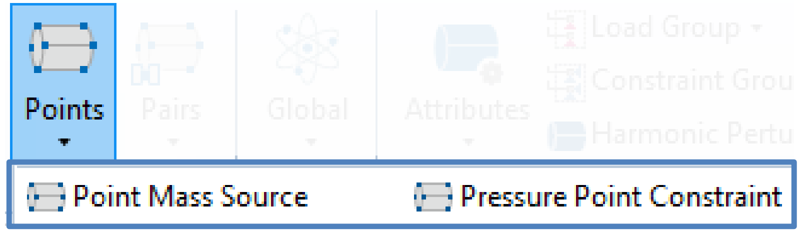
Physics Features for Laminar Flow

Domain conditions:

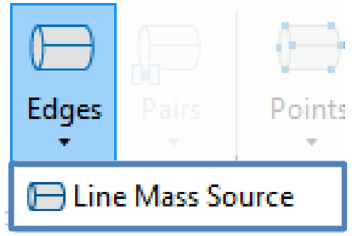
Boundary conditions:



Point conditions:

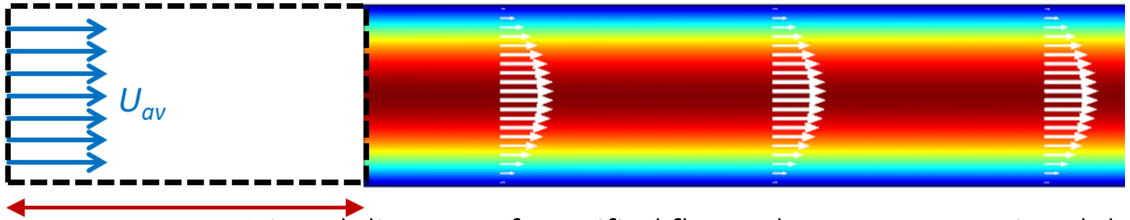


Edge conditions:



Laminar Inflow and Laminar Outflow

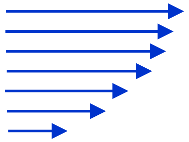
- Defines a laminar velocity profile for inlets/outlets with boundaries of any shape
  - Internally, a Navier-Stokes equation (D-1) is solved and projected on the boundary
  - Corresponds to a virtual domain that is attached upstream to the inlet



L_{entr} Virtual distance of specified flow value to computational domain

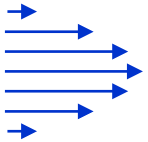
$$L_{entr} \gg 0.06\, Re * D$$

Constrain outer edges to zero

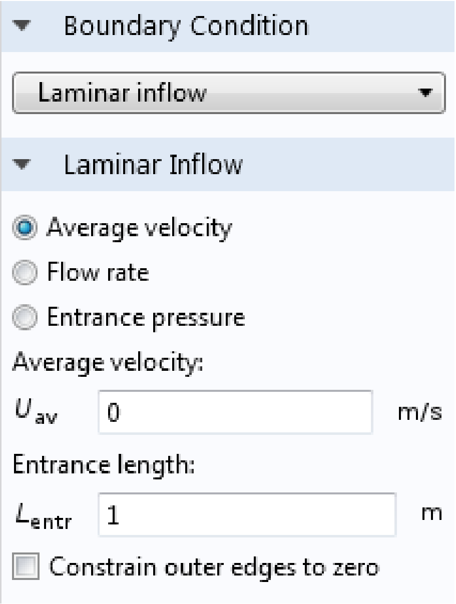


Velocity profile is defined by adjacent boundaries of real domain

Constrain outer edges to zero



Force laminar velocity profile to zero at adjacent boundaries of real domain



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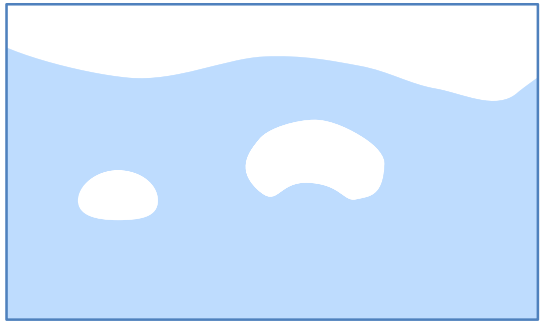
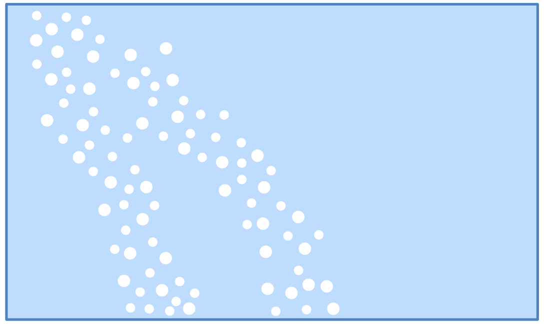
Multiphase Flow, Categorization

- Separated multiphase flow models:
  - For bubbles, droplets, phase boundaries, or particles that are relatively few and of the order of magnitude of the model domain
  - For multiphase flow in microfluidics
  - For free surfaces in otherwise single-phase fluids that are also in macroscopic systems



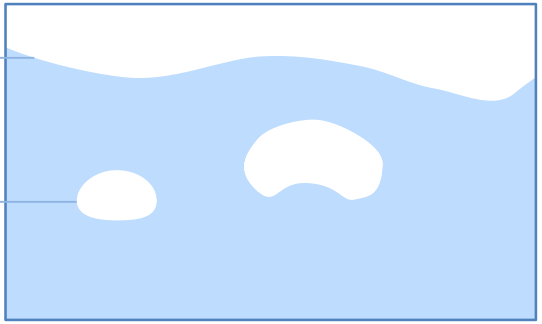
- Dispersed multiphase flow models (part of CFD Module only):
  - For bubbly flows with a large number of relatively small bubbles
  - For emulsions and aerosols
  - For large numbers of solid particles in fluids
  - For macroscopic multiphase flow (almost always required)



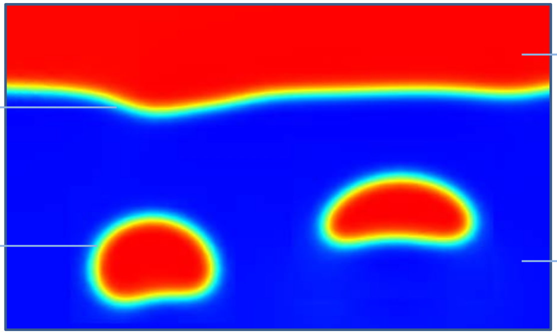
Multiphase Flow, Categorization

- Separated multiphase flow models

Interface described in detail



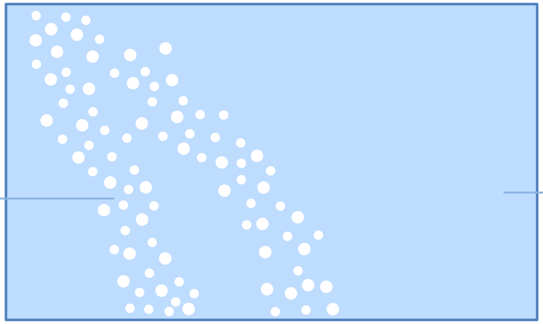
Isosurfaces



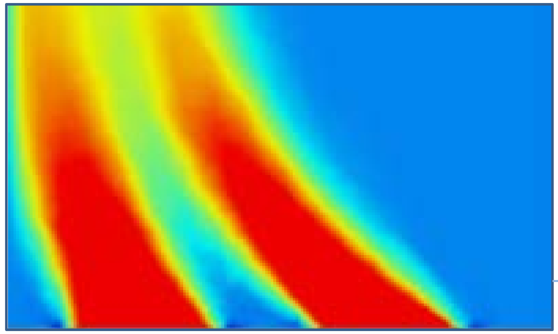
Phase field, ϕ
$\phi = 1$ (red)
$\phi = -1$ (blue)

- Dispersed multiphase flow models

Dispersed phase



Continuous phase

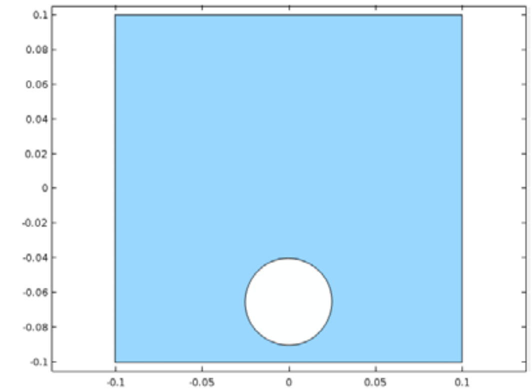


Volume fraction field, ϕ
$0 < \phi < 1$

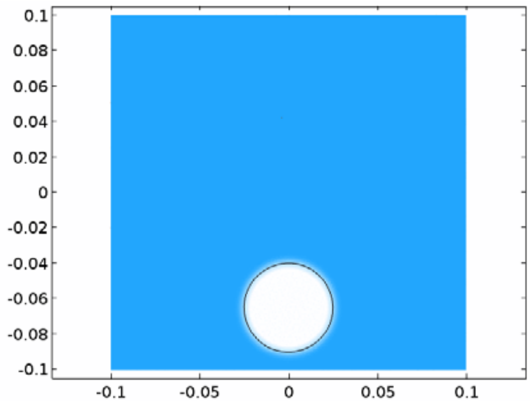
Multiphase Flow, Separated Flows

- Tracks the exact surface location using the level set or phase field models, or by using moving mesh
- Accurate modeling of surface-tension effects
- Includes a surface-tension coefficient library
- Level set and phase field can handle topology changes while moving mesh cannot
- Moving mesh can be very accurate and it is also simple to add forces and other boundary conditions at the phase boundary

Moving mesh



Phase field



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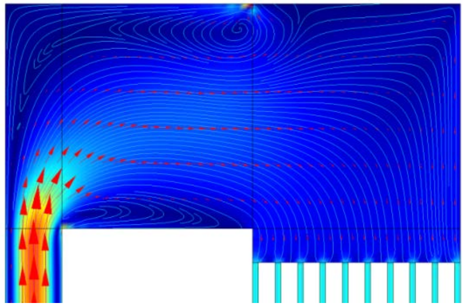
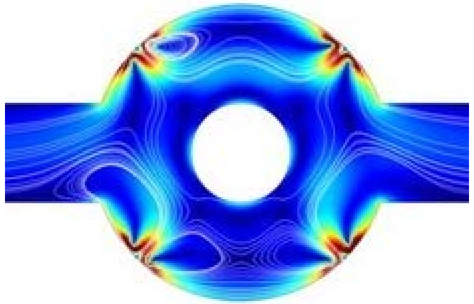
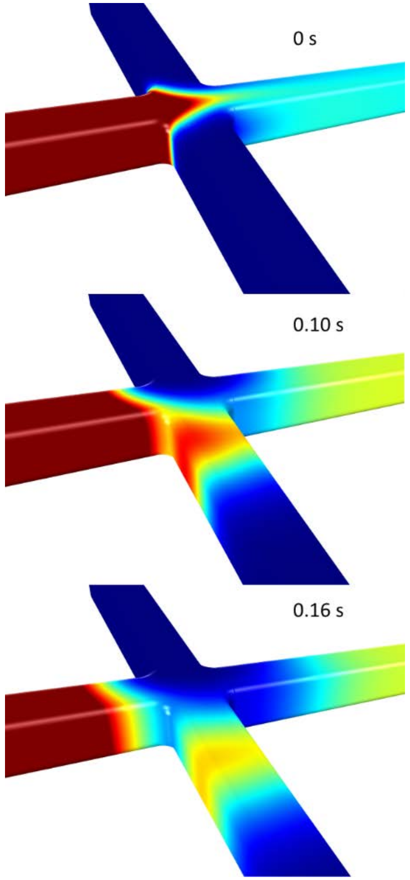
Electrokinetic Flow

- Utilizes electric fields to move fluids
- Primarily used to pump or mix fluids
- Based on two main phenomena
  - Electroosmosis
    - Explicit modeling of electric double layers on small length scales
    - On larger scales, the electroosmotic mobility can be specified as part of a slip boundary condition
  - Electrophoresis and dielectrophoresis







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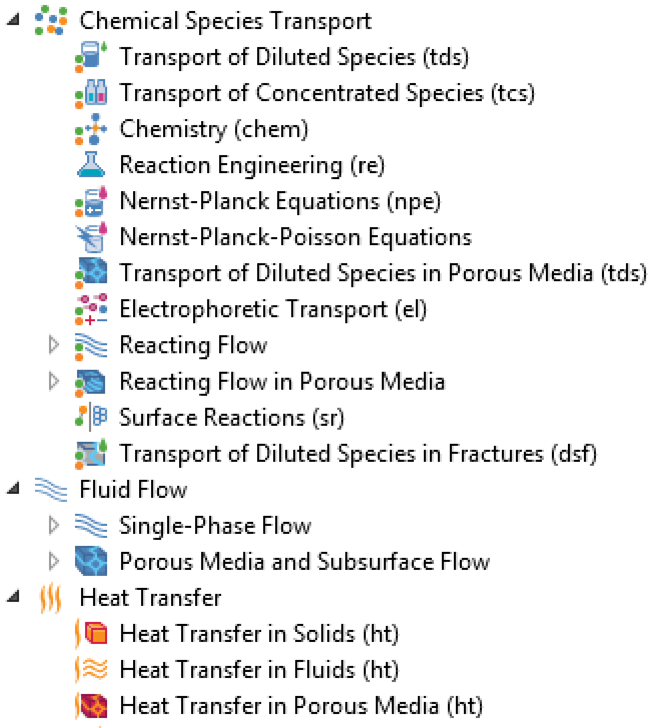
Chemical Reaction Engineering Module

The Chemical Reaction Engineering Module

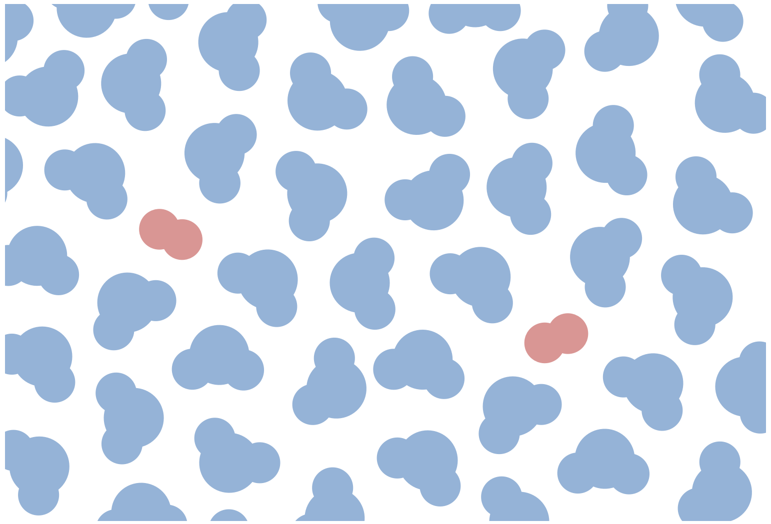
- Chemical species transport and reactions
  - Concentrated solutions (Maxwell-Stefan), dusty gas, dilute solutions
  - Free and porous media
- Reaction kinetics
  - Mass action law
  - Type in analytical expressions of concentrations
  - Homogeneous and heterogeneous reactions
- Fluid flow
  - Laminar flow and porous media flow
- Heat transfer and heat of reactions
  - Conduction, convection and radiation (surface to ambient)



The transport and reaction interfaces in the Chemical Reaction Engineering Module

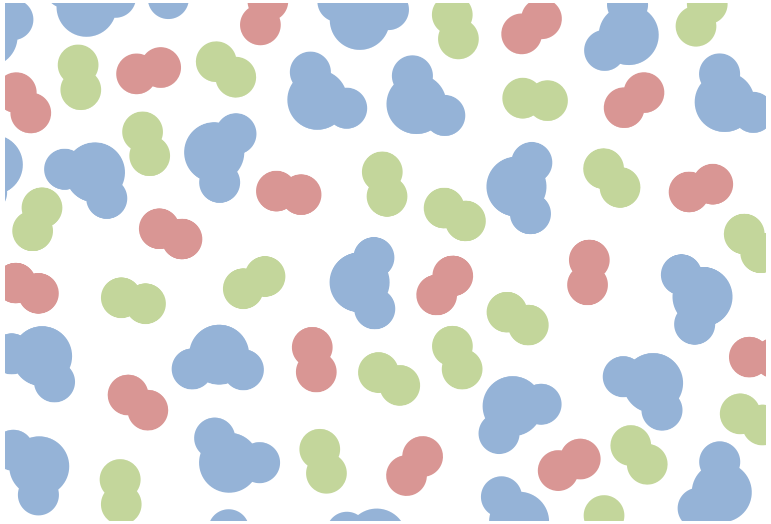
Transport in Diluted Solutions

- Solute interacts only with solvent
- Solution density equals solvent density
- Chem. Reaction Engineering Module:
  - Fick's law
  - Knudsen and dusty gas



Transport in Multicomponent Solutions

- All species interact with each other
- Solution density is the sum of all species density
- Chem. Reaction Engineering Module:
  - Maxwell-Stefan
  - Mixture averaged
  - Knudsen and dusty gas



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Reaction Model

- Steam reforming:

$$CH_4 + H_2O \rightleftharpoons 3H_2 + CO$$
$$CO + H_2O \rightleftharpoons H_2 + CO_2$$

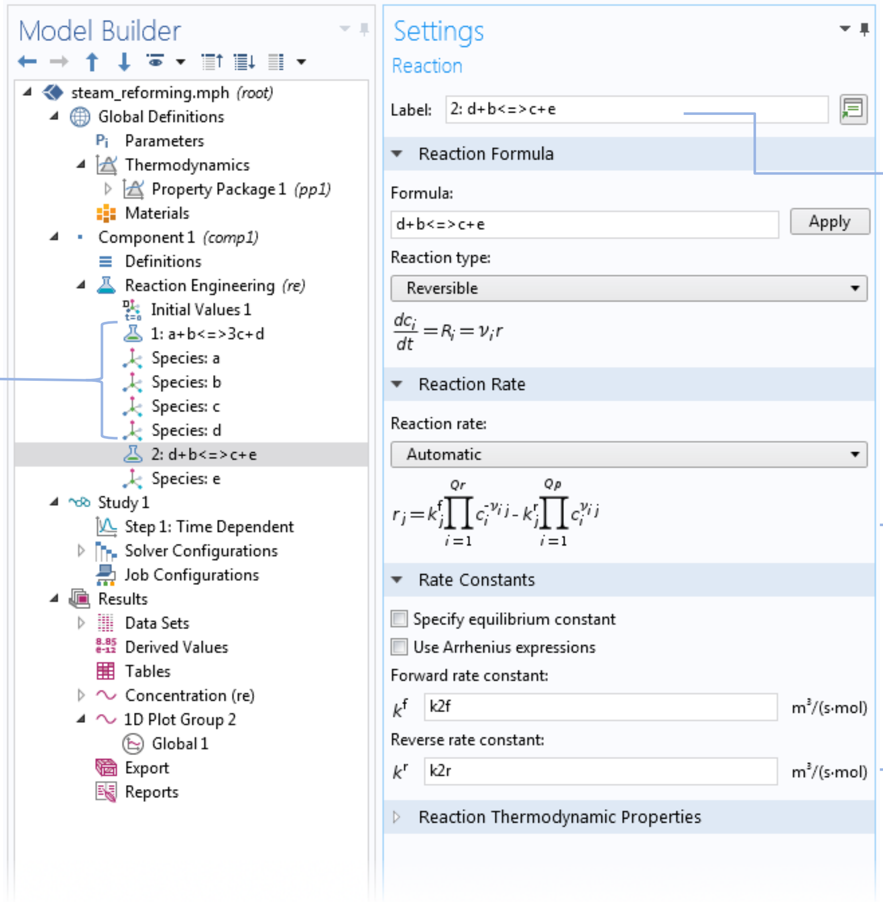
  - Kinetics through mass action law or user defined

- Simplified input:

$$a + b \rightleftharpoons 3c + d$$
$$d + b \rightleftharpoons c + e$$

- Last step: thermodynamic properties

Perfectly Mixed System



1. Just type in the chemical reactions.

2. The material balances for the species are automatically generated as you type in the chemical equations.

3. The kinetics are automatically formulated according to the mass-action law. If needed, you can replace the rate law with your own expressions.

4. Automatic units of rate constants, depending on kinetics expressions.

Models for batch, semibatch, continuous stirred tank reactors, and plug-flow reactors are predefined.

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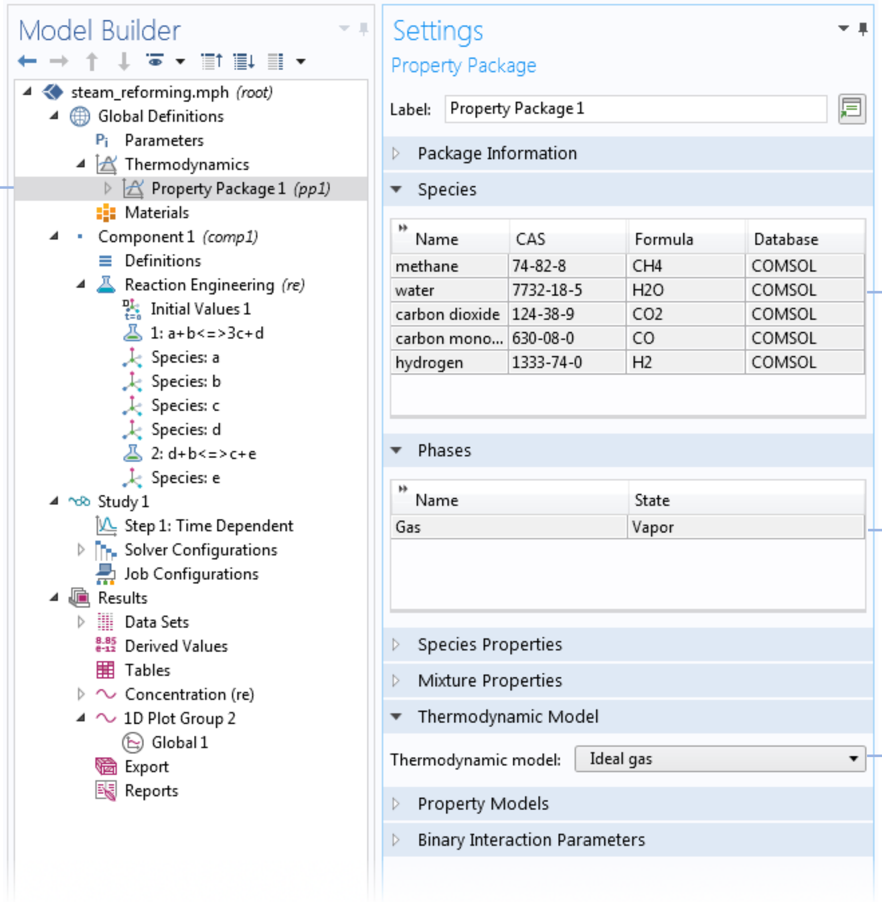
Thermodynamic Properties

1. Add a *Property Package* node.



2. Add compounds from the database.

3. Select phase.

4. Select thermodynamic model.

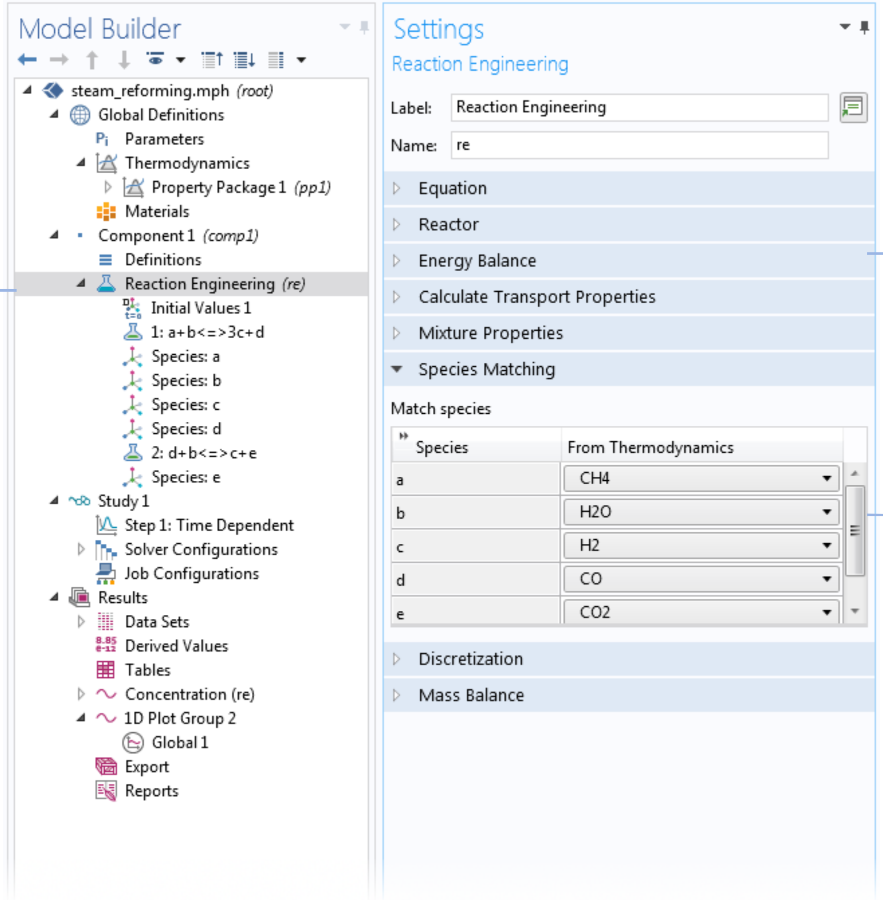
At this stage, the thermodynamic property package is decoupled from the species list in the *Reaction Engineering* node.

Thermodynamic Properties, Species Matching

1. Select the *Reaction Engineering* node.

2. Activate energy balance.

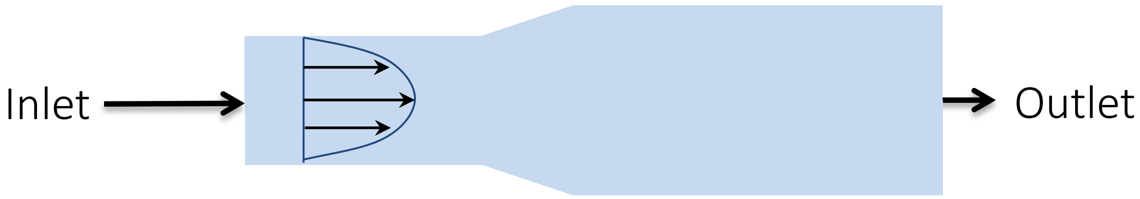
3. Match species.



The thermodynamic property package is now coupled to the species list in the *Reaction Engineering* node.

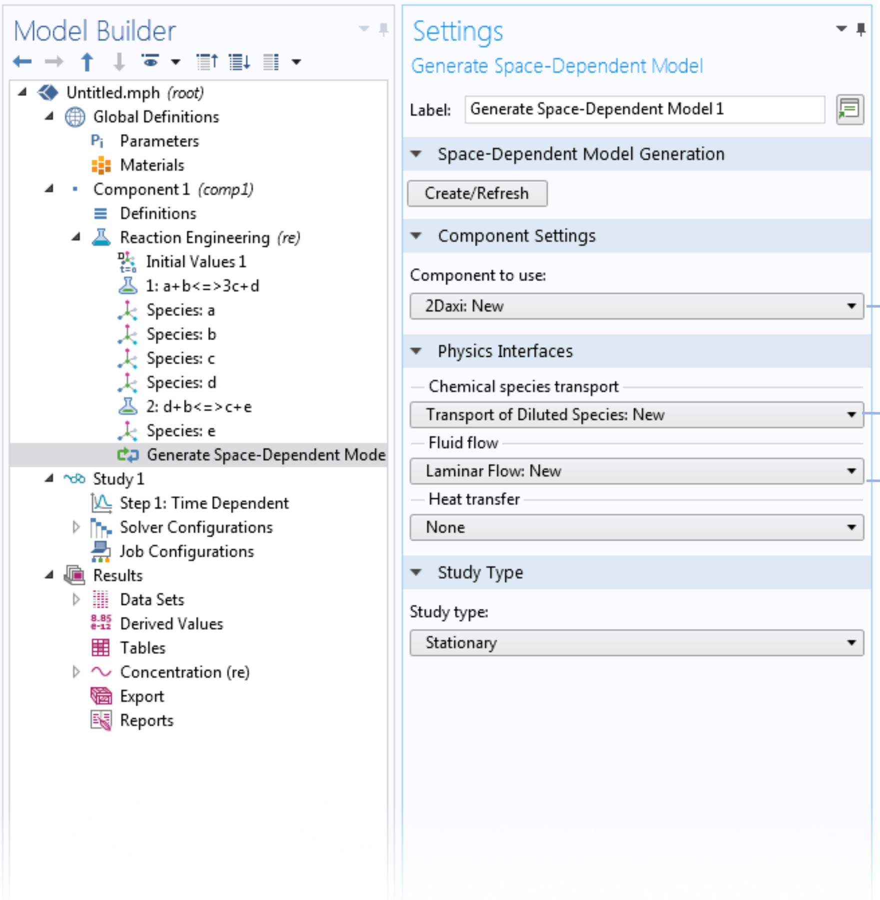
Space-Dependent Model

- Reactor model:
  - Tubular reactor with laminar flow



Generate Space-Dependent Model

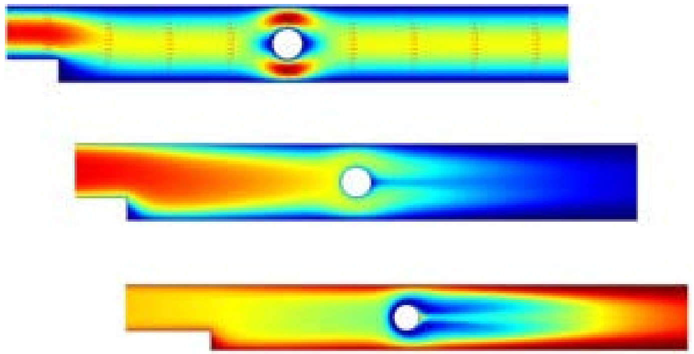
1. Add the *Generate Space-Dependent Model* node.



2. Select space dimension.

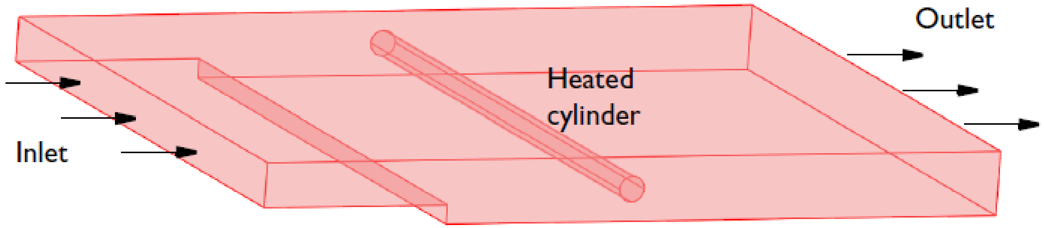
3. Select type of transport.

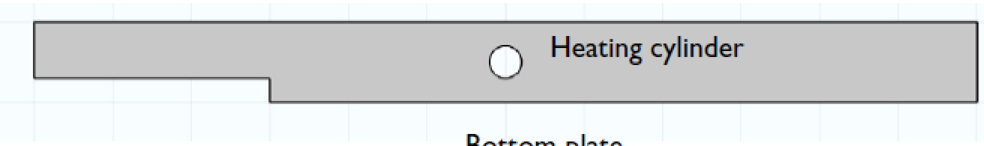
Demo: Thermal Decomposition



Geometry

- 3D geometry can be approximated with 2D cross section





Thermal Decomposition

- Thermal Decomposition:

$$A \xrightarrow{k} F$$

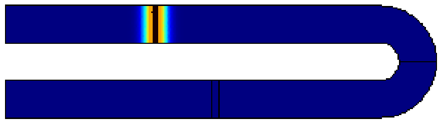
(Fragments (F) concentration is assumed constant)

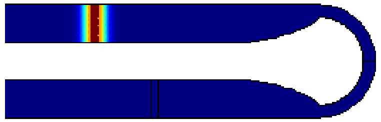
- Reaction Rate: $\text{rate} = kc_A$

- Rate constant: $k = A\exp\left(-\frac{E}{R_g T}\right)$

- Heat of reaction: $Q = -\text{rate} \cdot H$

Demo: Modeling Band Dispersion in a Curved Microchannel





Background

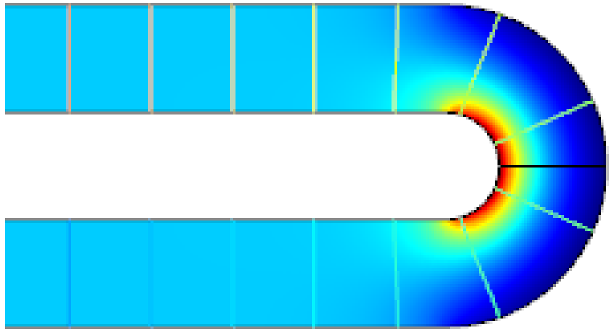
- The curved microchannel geometry induces dispersion in the analyte band as the later traverses through the geometric turn.

- The turn-induced dispersion could affect the detection downstream. One of the proposed solutions is geometric optimization. By altering the microchannel geometry, the turn-induced dispersion could be minimized.

- This model studies the band dispersion (of neutral species) in an Electroosmotic flow (EOF) – different geometry set-ups can be studied and the design can also be optimized (would require Optimization Module)

Understanding the Turn-Induced Dispersion

- One of the most obvious reasons for the dispersion is difference in the inner and outer path lengths, also known as Racetrack effect.
- The other important reason is the difference in solute velocity in the curved section, which arises due to difference in potential gradient.



Equipotential Lines and Velocity Surface plot

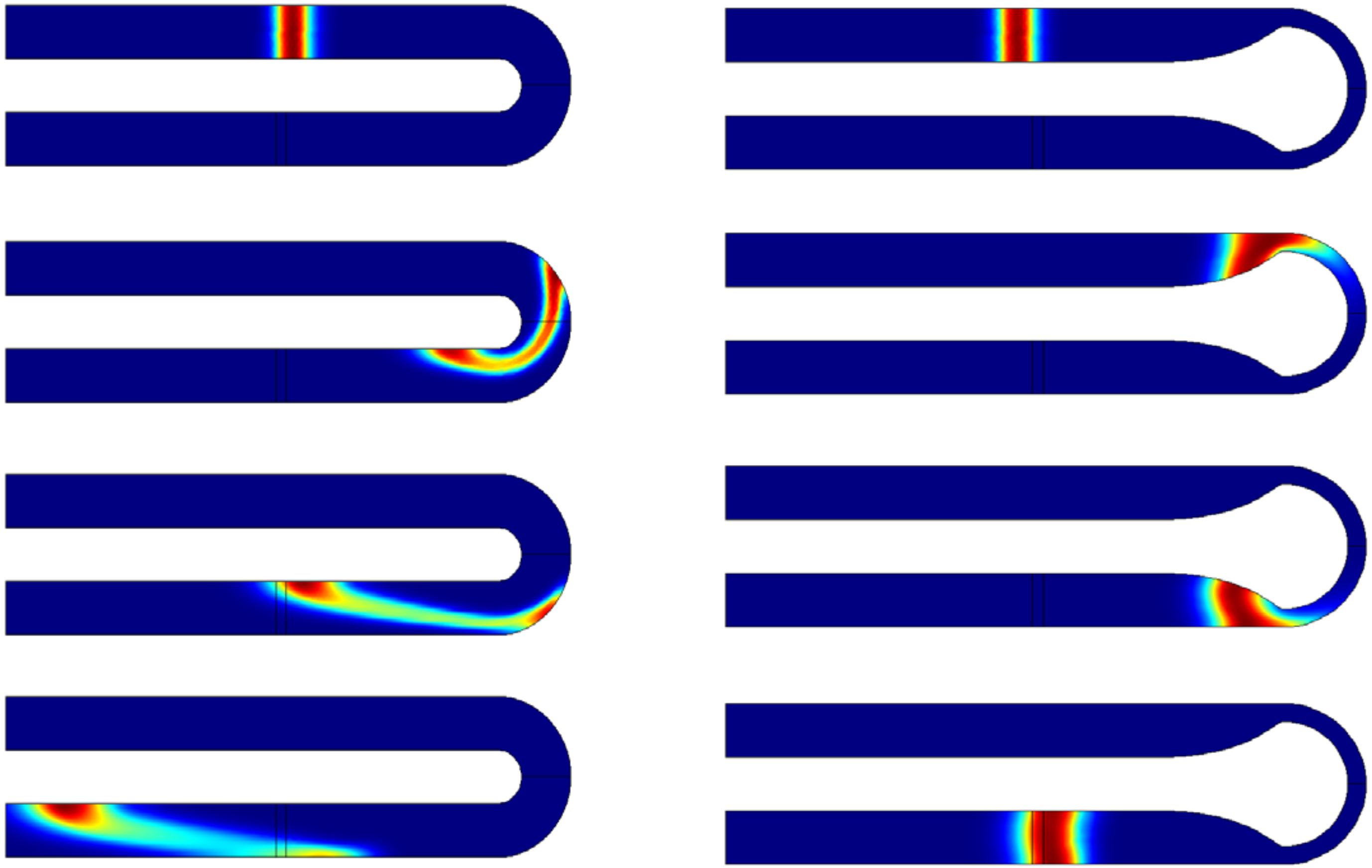
Solute traverses faster along the inner edge due to higher electric field (proportional to velocity)

Modeling

- The Electric Currents interface is used to model the electric field in the microchannel. The Creeping Flow interface is used to model the fluid flow using the simplified Electroosmotic velocity boundary condition. The Transport of Diluted Species interface is used to model the mass transport.

- The present model is developed for neutral species transport in EOF however the same idea is applicable for electrophoresis problems as well. This is because both fluxes, convective and migrational, vary linearly with concentration and electric field.

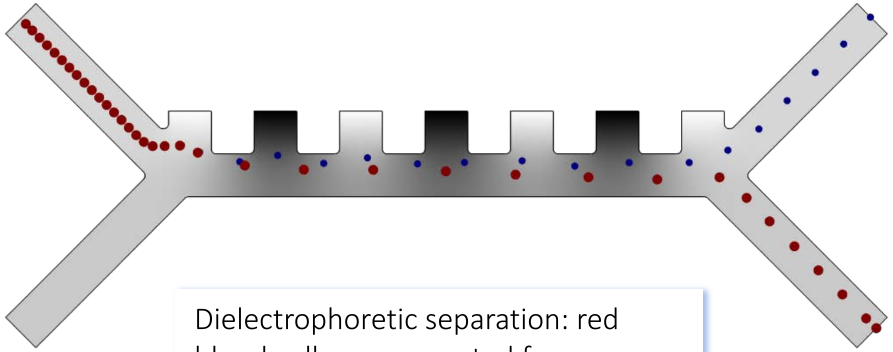
Results



Concentration surface plot for original and optimized geometry at different times

Demo

Dielectrophoretic Separation of Platelets from Red Blood Cells



Dielectrophoretic separation: red blood cells are separated from platelets using dielectrophoresis.

Dielectrophoresis

- Dielectrophoresis is the movement of particles in non-uniform electric fields due to the interactions of the particles' induced dipoles with the field gradients
- Dielectrophoretic force:

$$\mathbf{F}_{\text{ext}} = 2\pi r_p^3 \varepsilon_0 \,\text{real}(\varepsilon_f^*)\,\text{real}\left(\frac{\varepsilon_p^* - \varepsilon_f^*}{\varepsilon_p^* + 2\varepsilon_f^*}\right) \nabla |\mathbf{E}_{\text{rms}}|^2$$

- Shell feature can be added for particles with thin dielectric shells:

$$\varepsilon_{\text{eq}}^* = \varepsilon_s^* \frac{\left(\frac{r_0}{r_i}\right)^3 + 2\left(\frac{\varepsilon_p^* - \varepsilon_s^*}{\varepsilon_p^* + 2\varepsilon_s^*}\right)}{\left(\frac{r_0}{r_i}\right)^3 - \left(\frac{\varepsilon_p^* - \varepsilon_s^*}{\varepsilon_p^* + 2\varepsilon_s^*}\right)}$$

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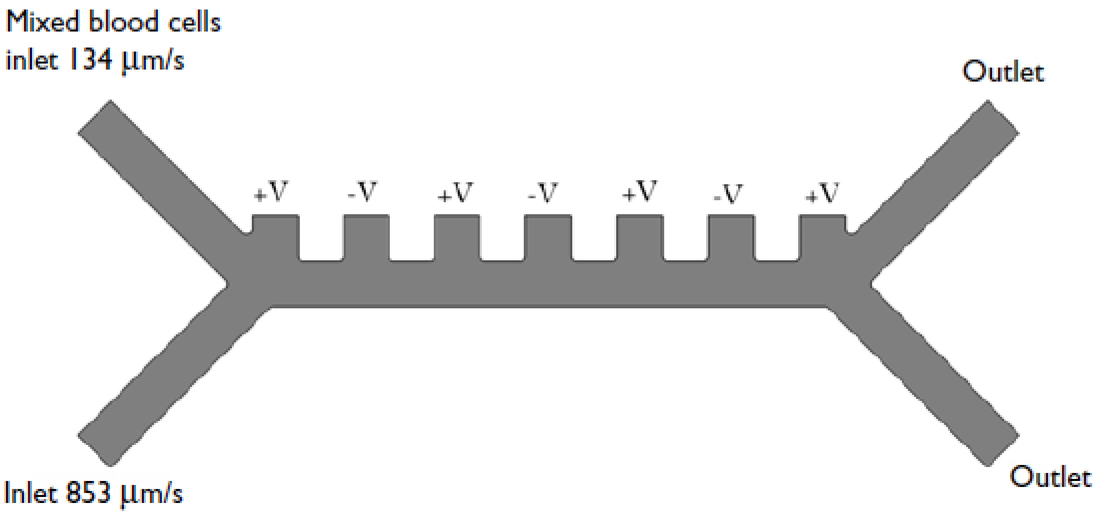
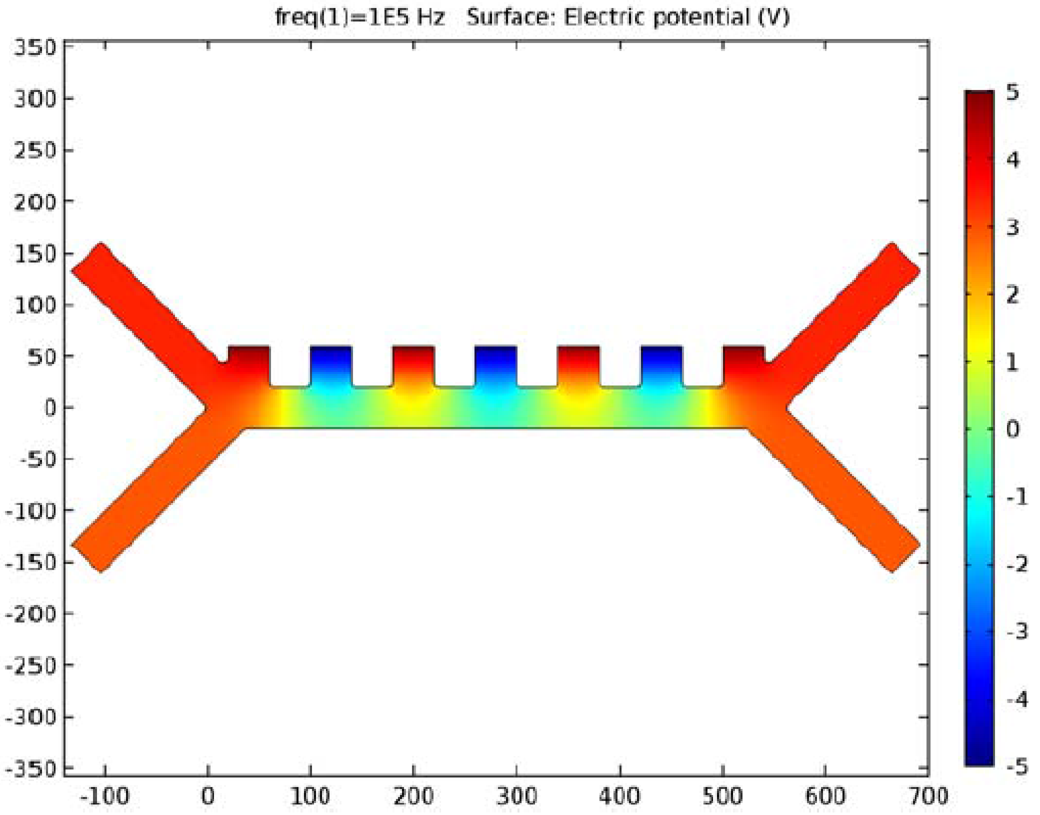
Dielectrophoretic separation

- Geometry and boundary conditions

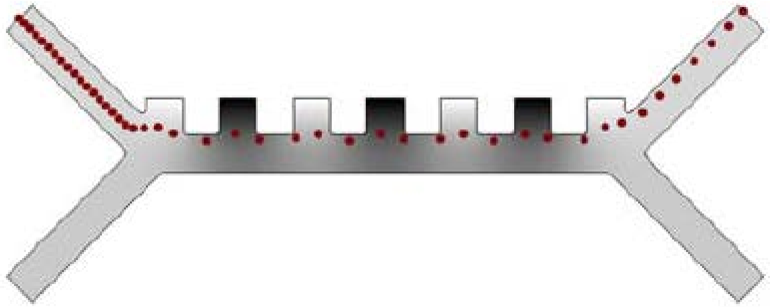


Results

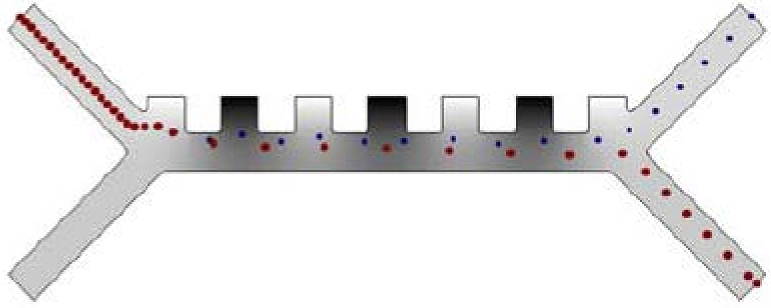
Electric potential distribution



Particle trajectories without dielectrophoresis

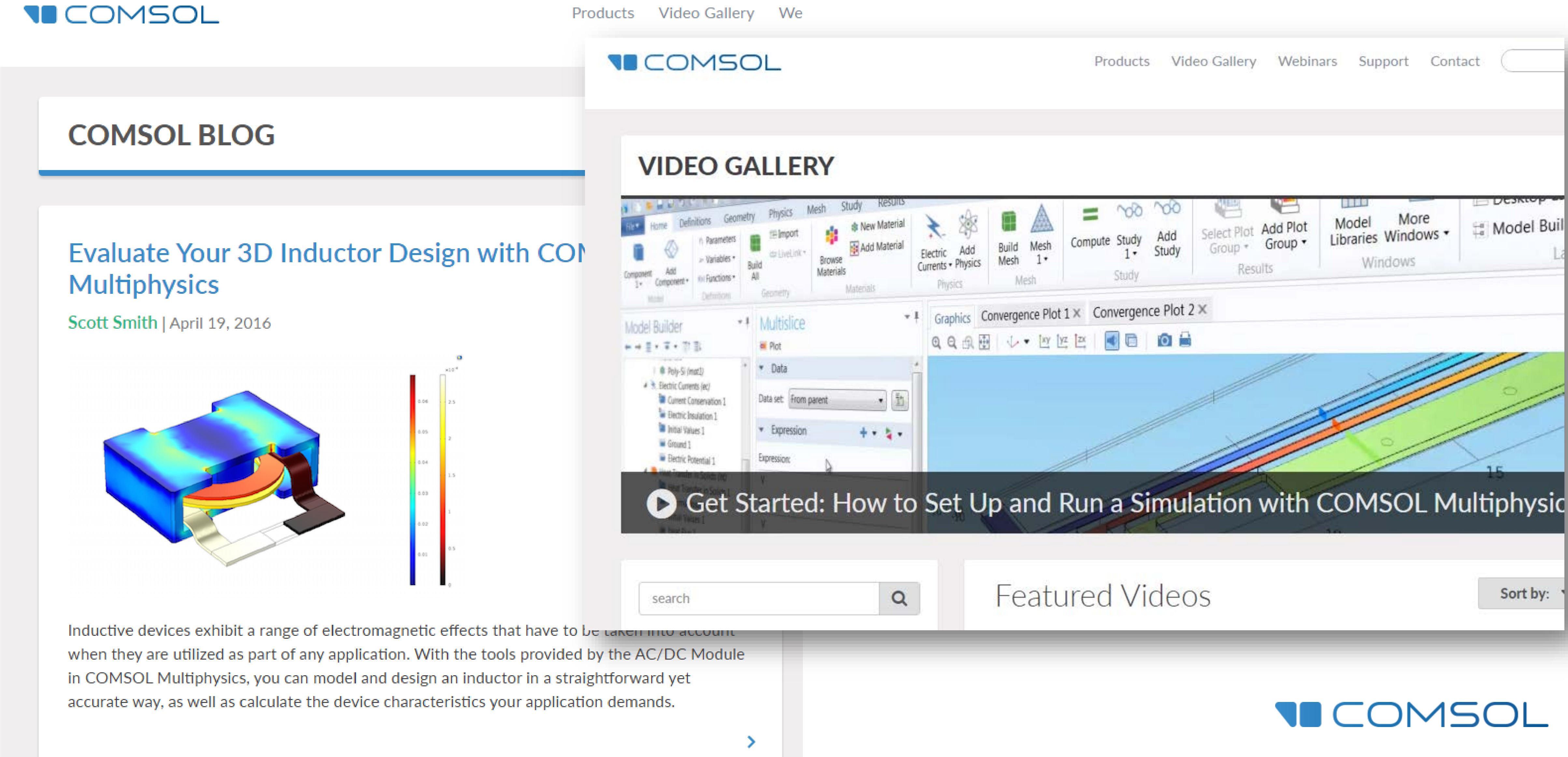


Particle trajectories with dielectrophoresis
(Red: Red Blood Cells, Blue: Platelets)



Q & A

COMSOL Resources on the Web



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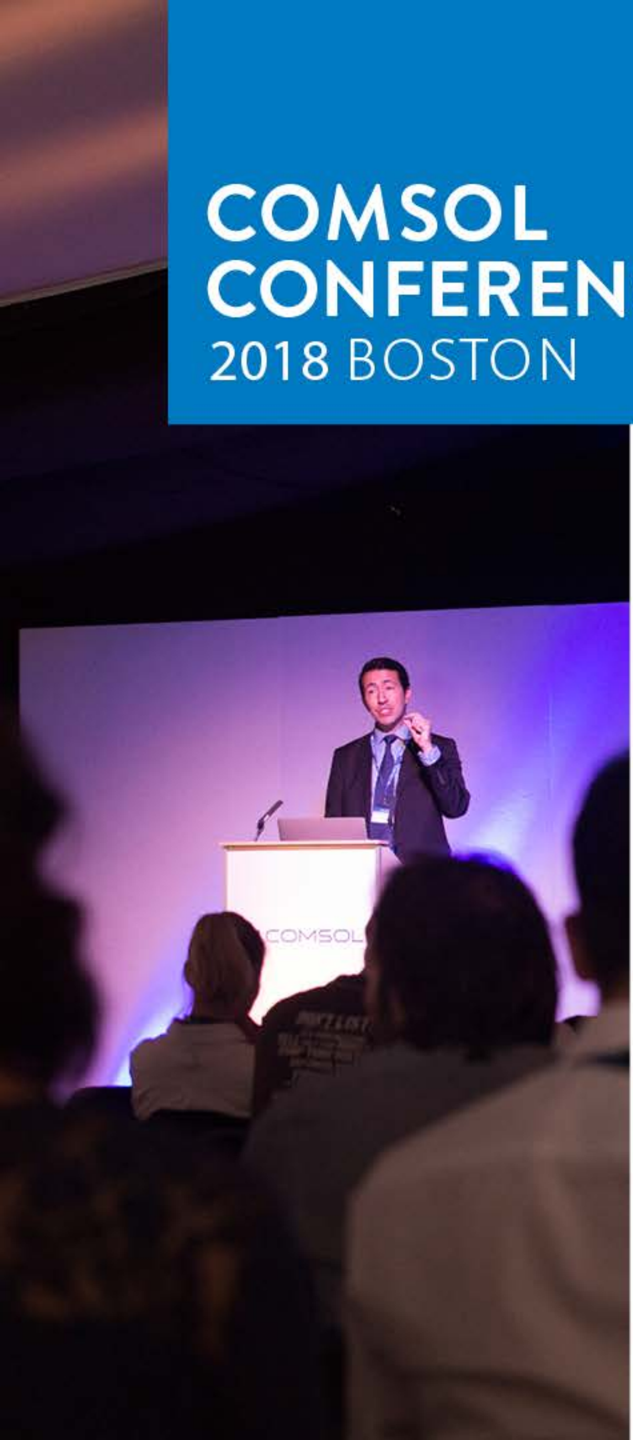

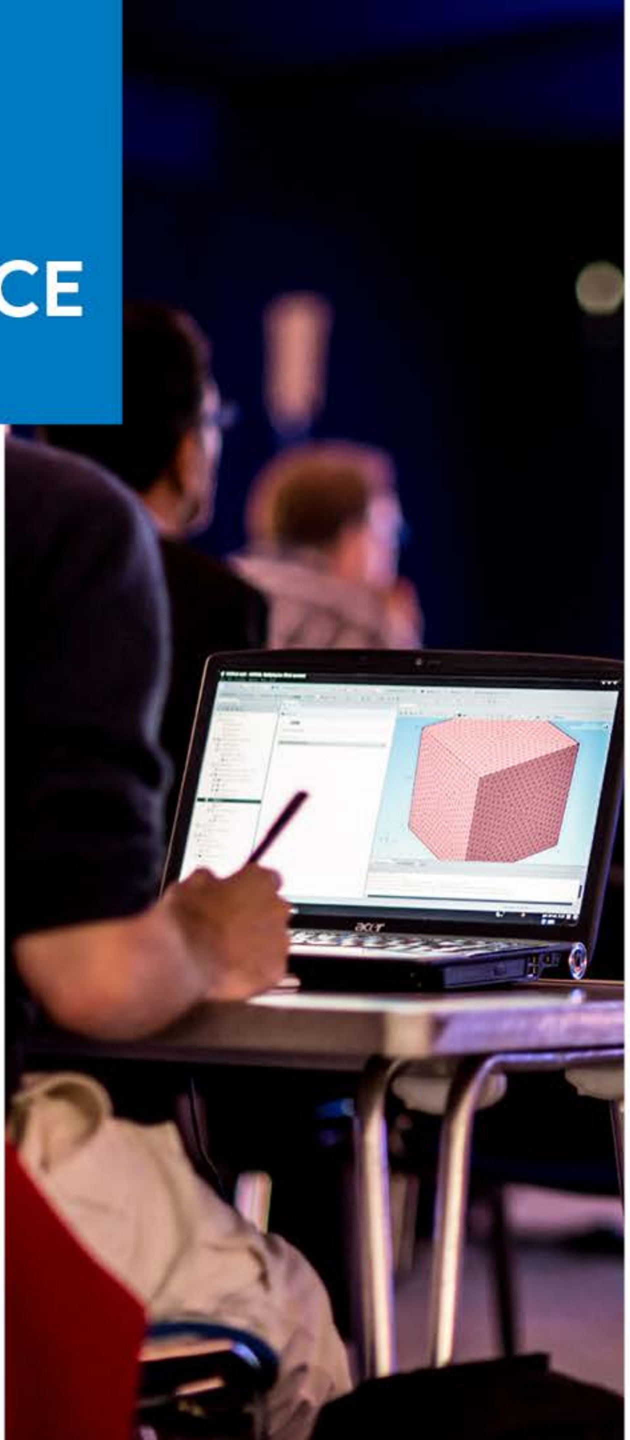

SAVE THE DATE

October 3–5

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