An Introduction to COMSOL Multiphysics v4.3b & Subsurface Flow Simulation

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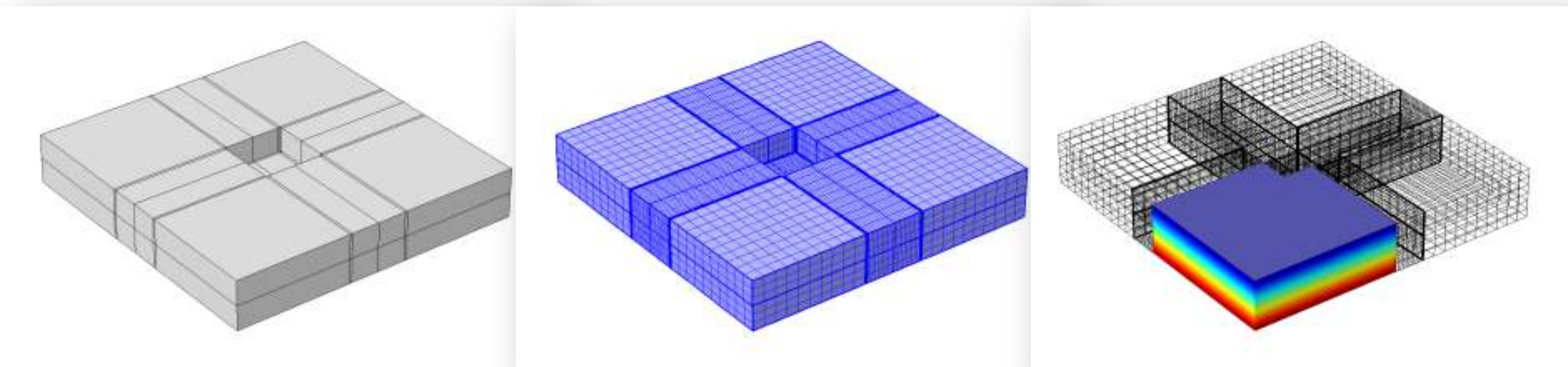
Agenda

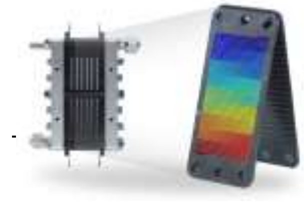
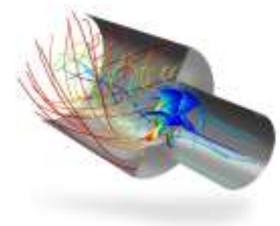
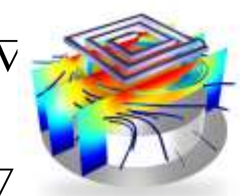
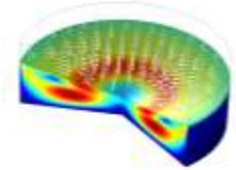
- Provide an overview of COMSOL 4.3b
- Our products, solutions and applications
- Subsurface Flow Module
- Demo: Vapor Intrusion Modeling



$$\nabla\times\left(\mu_r^{-1}\nabla\times\mathbf{E}\right)-k_0^2\left(\varepsilon_r-j\sigma/\omega\varepsilon_0\right)\mathbf{E}=\mathbf{0}$$

$$\nabla\cdot\left(-\left(1/\rho_0\right)\left(\nabla p-q\right)\right)-\left(\omega^2/\left(\rho_0 c_S^2\right)\right)=Q$$

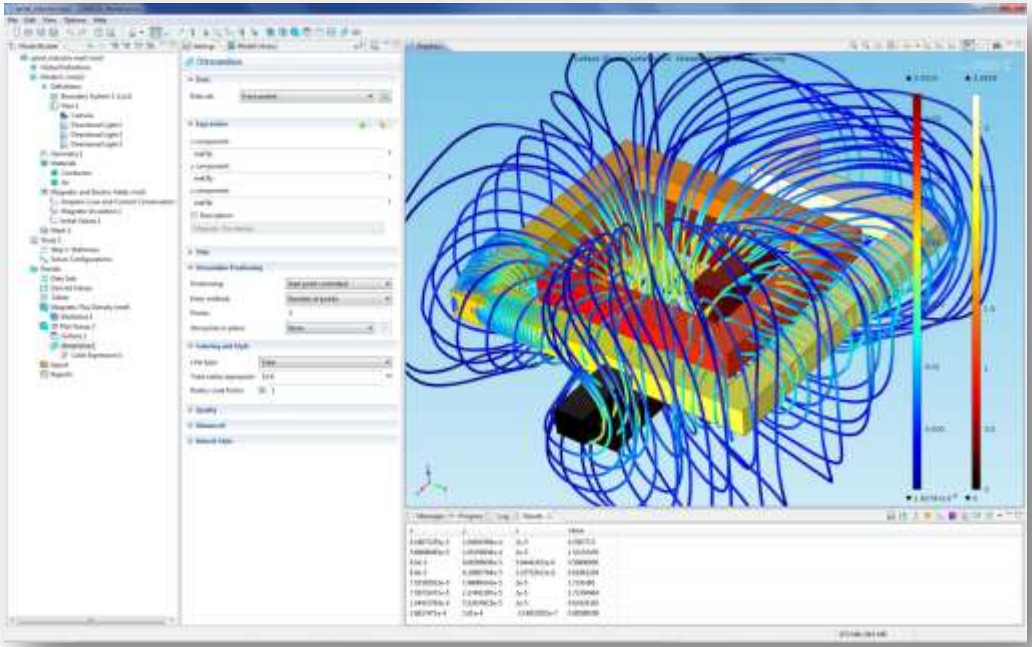
$$\nabla\cdot\left(\mathbf{C}:(\boldsymbol{\varepsilon}-\boldsymbol{\varepsilon}_{\dots}-\boldsymbol{\varepsilon}_{\dots})+\sigma_0\right)=\mathbf{F}$$

	PEM Fuel Cells
	Flow in Propeller
	Temperature Sensor
	Plasma Formation
	Miniature Liquid Lens

COMSOL is a Fully Integrated Software Suite

Based upon the finite element method, COMSOL is designed from the ground up to address arbitrary combinations of physical equations

- All modeling steps are available from one and the same environment:
  - CAD Import
  - Geometry Modeling
  - Meshing
  - Multiphysics problem setup
  - Solving
  - Visualization
  - Postprocessing
  - Export/Import of data



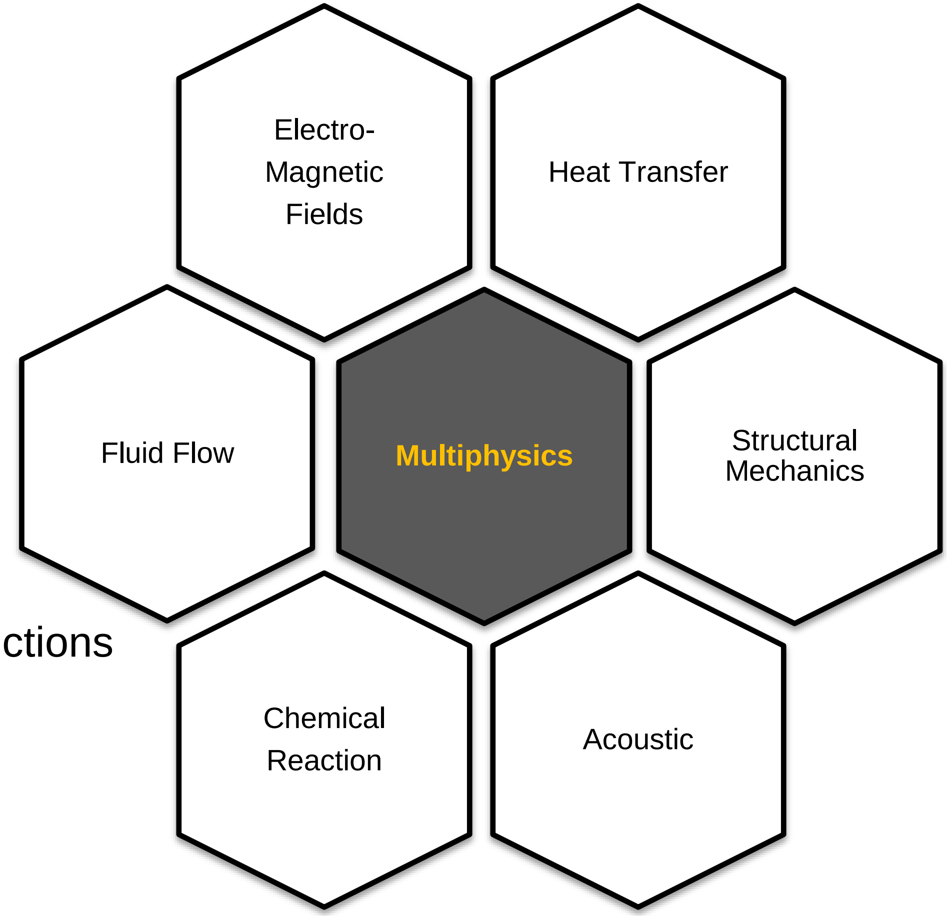
Why COMSOL Multiphysics?

- Inherently Multiphysics
  – Solve single physics
  – Couple as many physics as you want

- Easy to use
  – *COMSOL Desktop*
  – Same user-interface for all physics

- Adaptable
  – Custom materials and interpolation functions
  – Parameterize anything
  – Option to add equations

- High-Performance Computing (HPC)
  – Multicore & Multiprocessor: for all license types
  – Clusters: for floating network licenses



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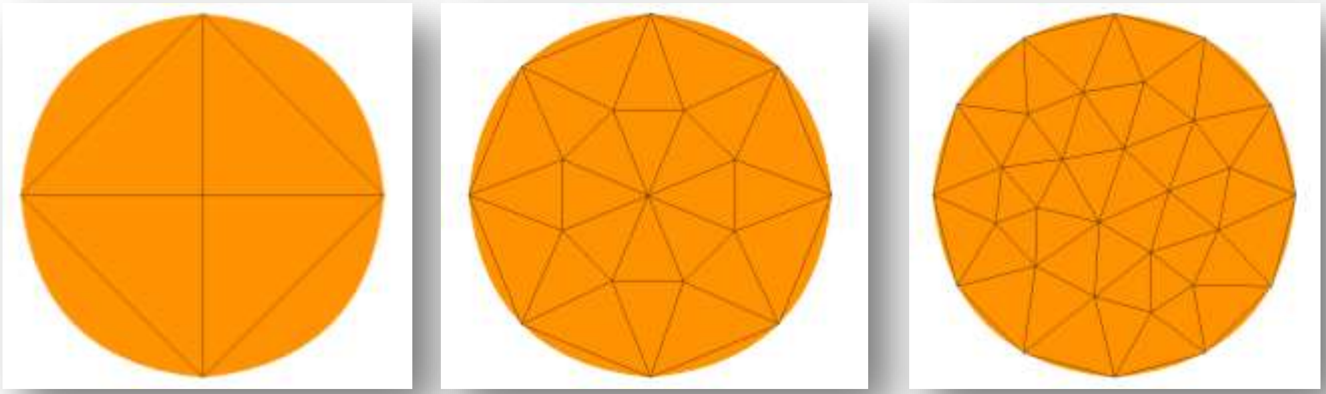
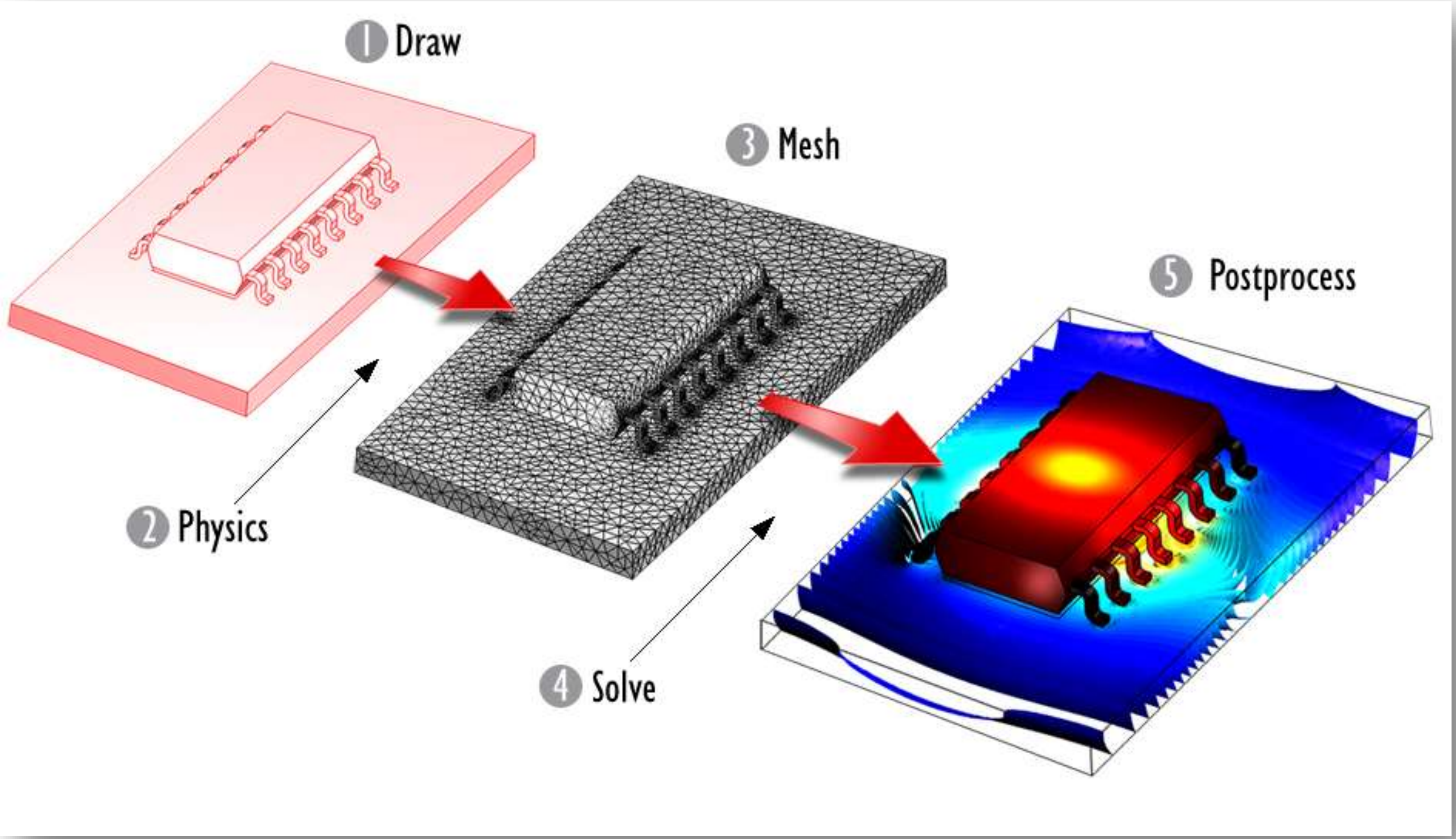
Finite Element Modeling



4 Elements | 24 Elements | 48 Elements

I. Decompose or Discretize the Problem
II. Approximate the Solution for each elements/Nodes
III. Assemble the Element Equations & Solve

COMSOL Modeling Process



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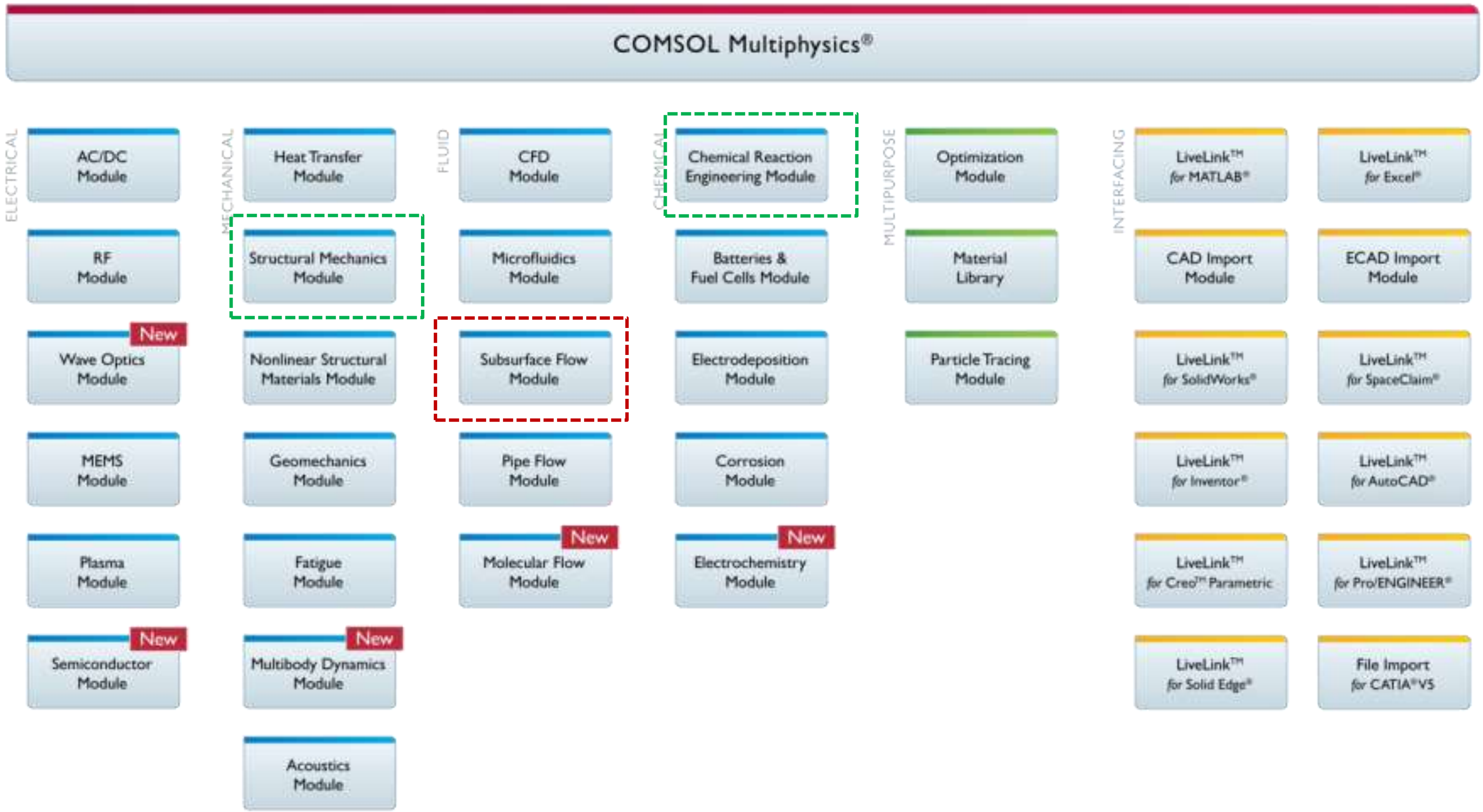
COMSOL Multiphysics® 4.3b Product Suite



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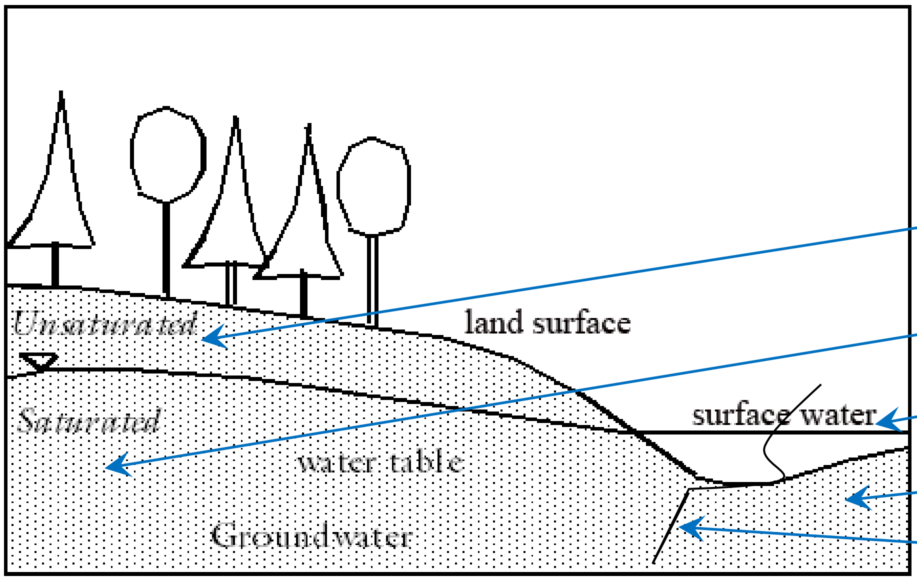
Physics Interfaces for Porous Media Flow

- Richard’s equation: Variably saturated porous media
- Darcy’s law: Slow flow in porous media
- Brinkman equation: Fast flow in porous media
- Navier-Stokes equation: Free flow

Fracture Flow: Flow along surfaces



Richard’s equation

Darcy’s law

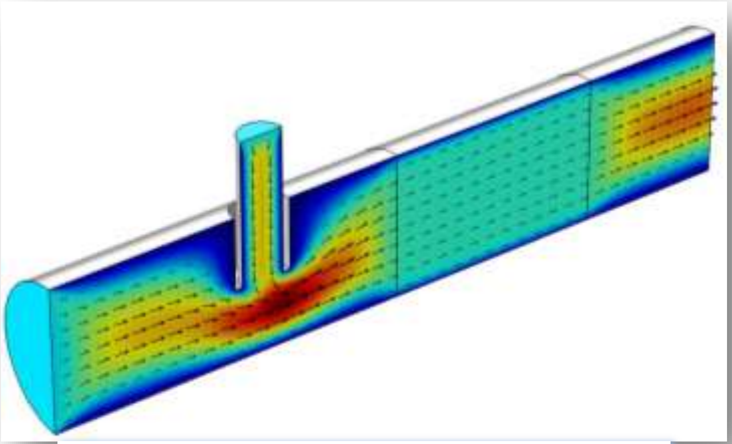
Navier Stokes

Brinkman equations

Fracture Flow

Brinkman Equations

- Fast flow in saturated porous media
- Convective term
- Forchheimer drag
- Compressible or incompressible fluid



Porous reactor with coupled Navier-Stokes, Brinkman Equation and multiple species transport

$$\frac{\partial}{\partial t}(\varepsilon_p \rho) + \nabla \cdot (\rho \mathbf{u}) = Q$$

$$\frac{\rho}{\varepsilon_p}\left(\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla)\frac{\mathbf{u}}{\varepsilon_p}\right) = -\nabla p + \nabla \cdot \left[\frac{1}{\varepsilon_p}\left\{\mu(\nabla \mathbf{u} + (\nabla \mathbf{u})^T) - \frac{2}{3}\mu(\nabla \cdot \mathbf{u})\mathbf{I}\right\}\right] - \left(\frac{\mu}{\kappa} + Q\right)\mathbf{u} - \beta_F |\mathbf{u}| \mathbf{u}$$

Convective term

Forchheimer drag

Non-linear effects

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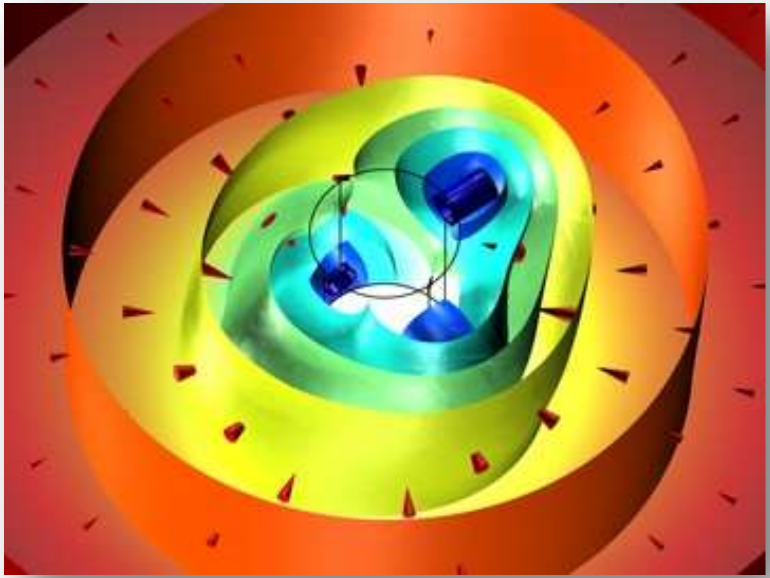
Darcy's Law

- Slow flow in saturated porous media
- Subsurface Flow Module includes Pressure Head and Hydraulic Head formulations, intended for hydrology problems
- Compressible or incompressible flow, variable density and viscosity, anisotropic permeability

$$S\frac{\partial p}{\partial t}+\nabla\cdot\left[\frac{k}{\eta}\nabla(p+\rho gD)\right]=Q$$



3D simulation of a Perforated Well with Darcy's law

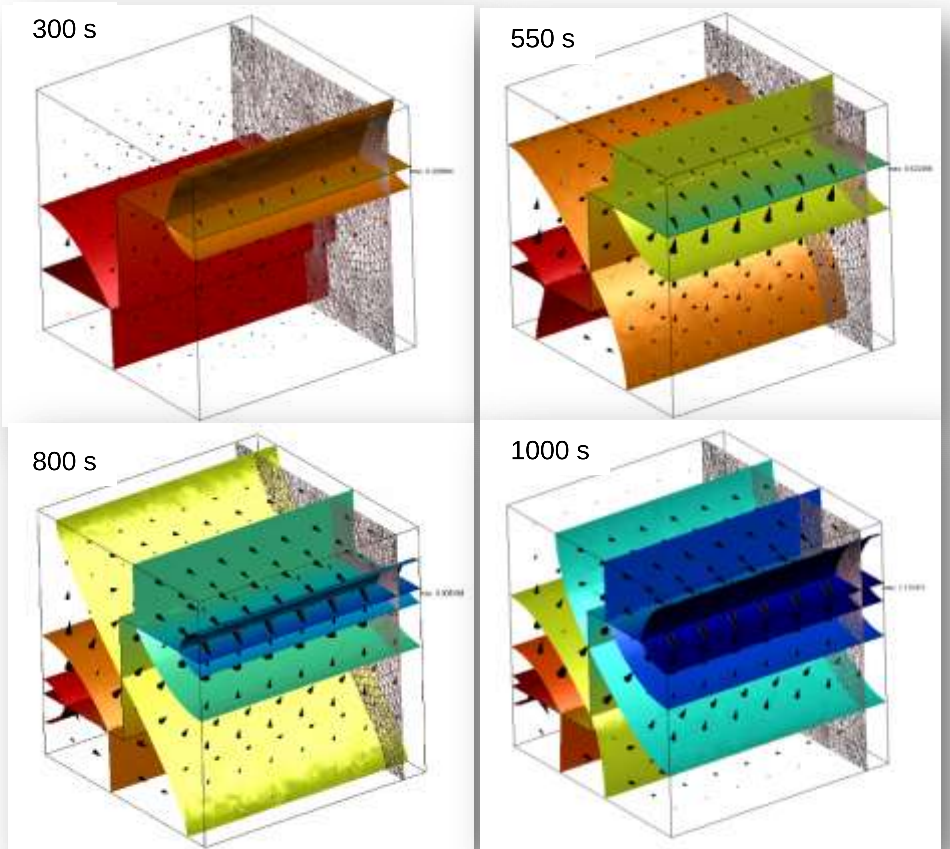
Fracture Flow

- Slow flow in thin shells and fractures (Darcy's Law)

- Available only in Subsurface Flow Module

$$d_{\mathrm{f}}\frac{\partial}{\partial t}(\varepsilon_{\mathrm{f}}\rho) + \nabla_T \cdot (\rho \mathbf{q}_{\mathrm{f}}) = d_{\mathrm{f}} Q_{\mathrm{m}}$$

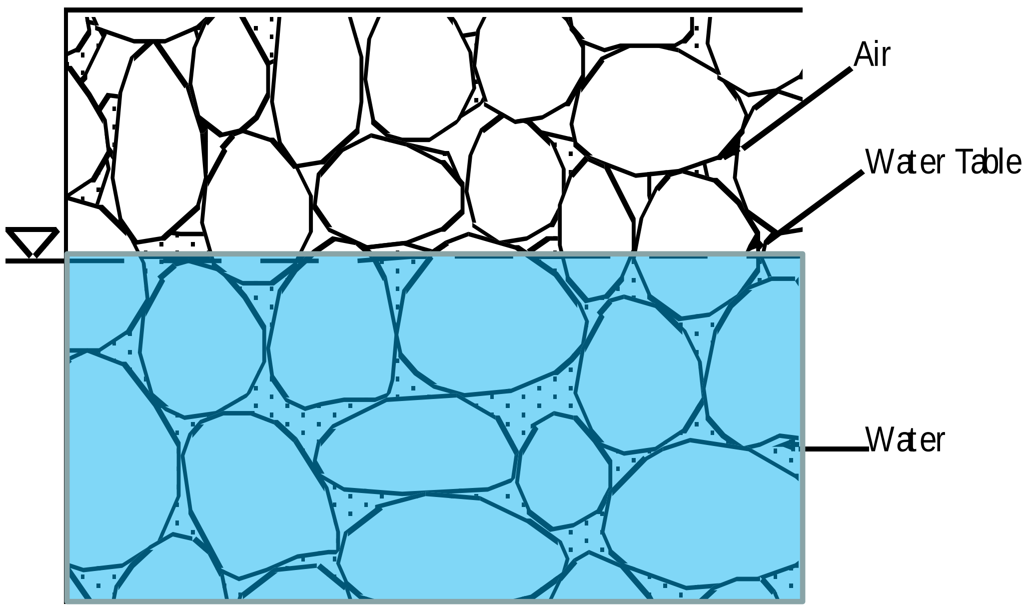
$$\mathbf{q}_{\mathrm{f}} = -\frac{\kappa_{\mathrm{f}}}{\mu} d_{\mathrm{f}}(\nabla_{\mathrm{T}} p + \rho g \nabla_{\mathrm{T}} D)$$



Darcy's law with Fracture flow

Richard’s Equation – Variably Saturated Flow

- Slow flow for variably saturated porous media
- Available only in Subsurface Flow Module
- Van Genuchten and Brooks & Corey retention models
- Normally coupled to Solute Transport



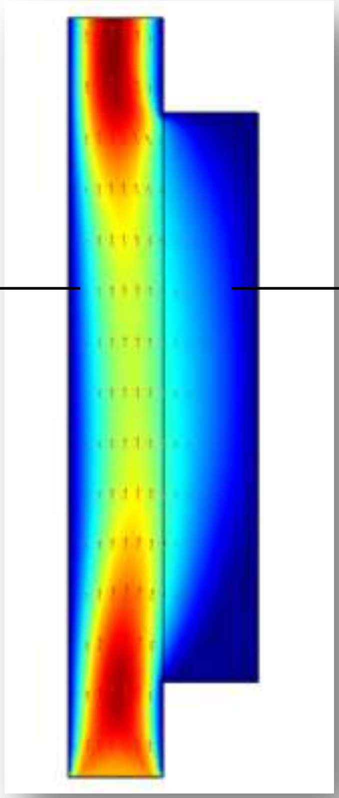
- C = Specific moisture capacity
- S = Storage effects (compressibility)

$$(C + S\varepsilon S)\frac{\partial H_p}{\partial t} + \nabla \cdot \left[\frac{k_s}{h} k_\rho \nabla (H_p + D) \right] = Q$$

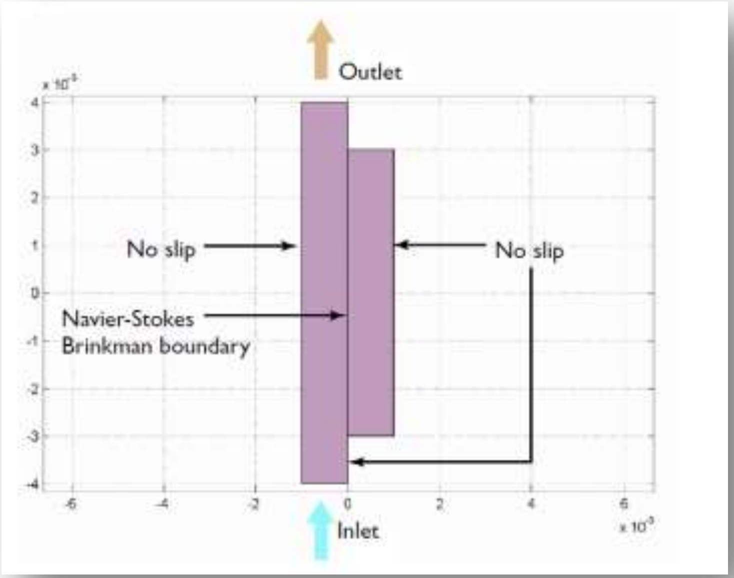
Free and Porous Media Flow

- Laminar flow coupled to flow in porous media
  - Navier-Stokes and Brinkmann Equation
- Joint stabilization scheme
- Convective term in Porous Media Flow
- Forchheimer drag in Porous Media Flow

Free Flow

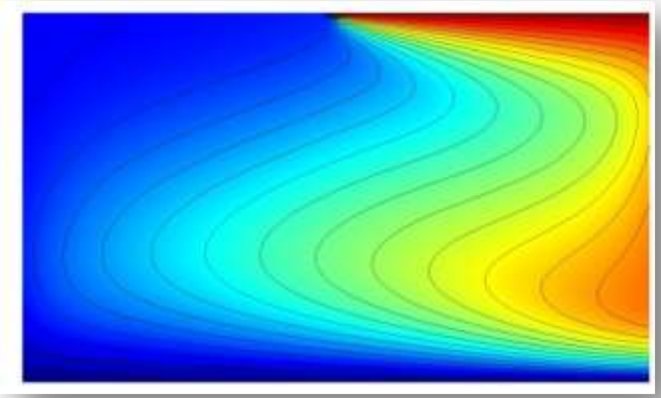


Porous Media

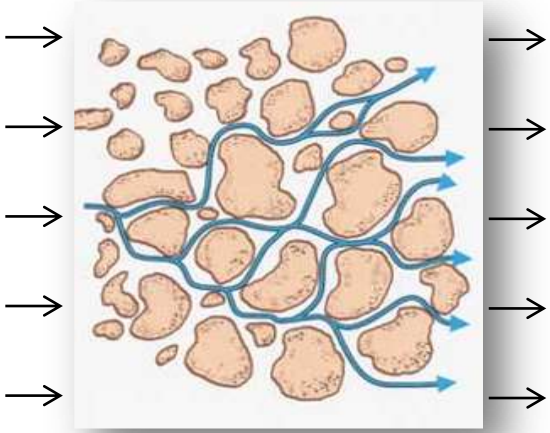


Solute Transport

- Transport of mass, but in Porous media for Subsurface Flow applications
- Multiphysics
  - Darcy's Law, Richards' or Brinkman Equations
- Interface features
  - Sorption, Dispersion, Diffusion, and Volatilization in porous media



Concentration (rainbow) and velocity (streamlines) plot



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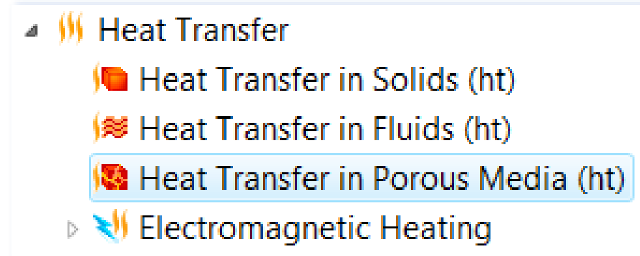
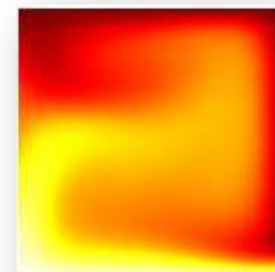
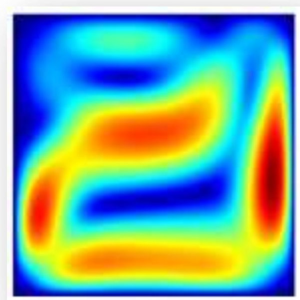
Heat Transfer

- Heat transfer in Solids and Fluids
- Heat Transfer in Porous Media
- Extended version in Subsurface Flow Module
  - Add up to 5 different Immobile Fluids
  - Geothermal Heating
  - Thermal Dispersion
- Multiphysics
  - Darcy's Law, Richards' or Brinkman Equations



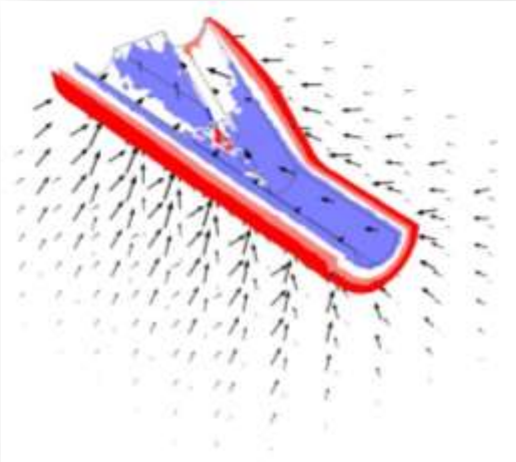




Temperature (Thermal) and velocity (rainbow) plot

Poroelasticity Interface

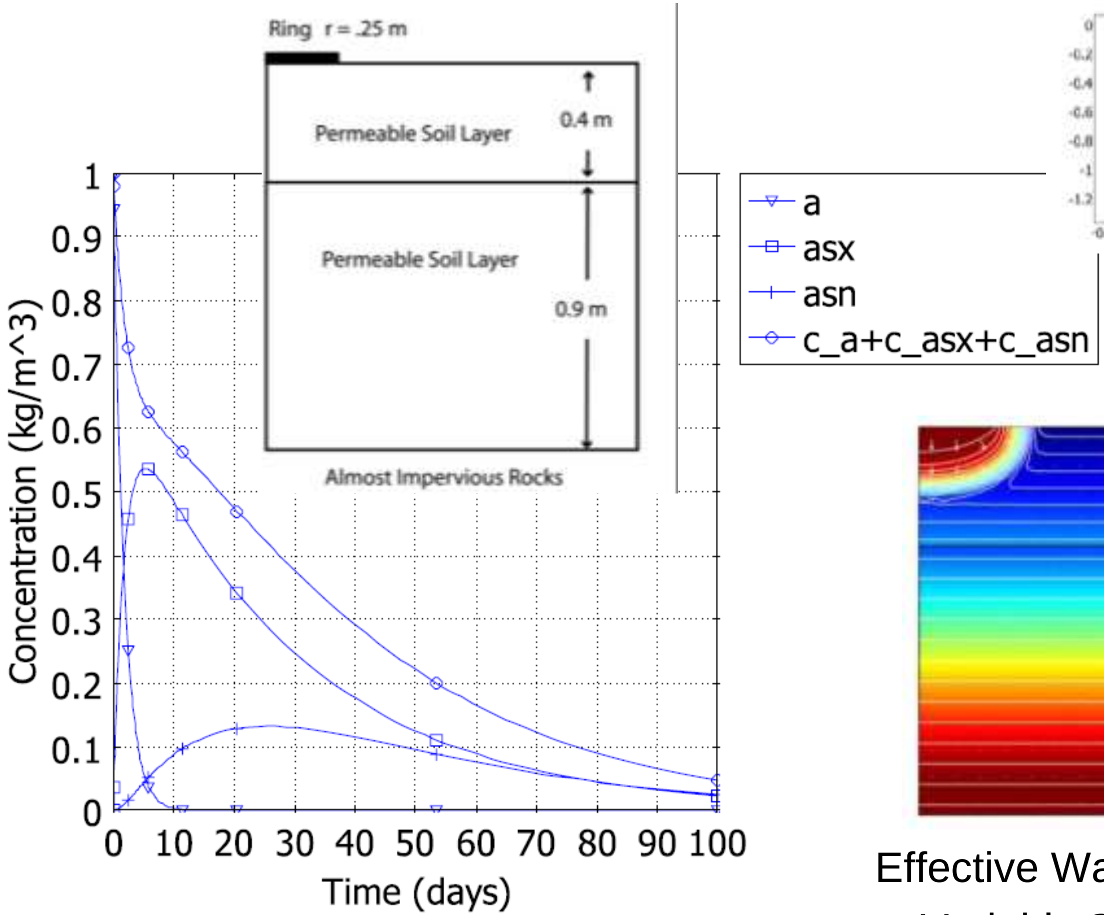
- Biot's theory for poroelasticity
- Deformation in porous matrix due to changes in pore pressure
- Poroelasticity uses Solid Mechanics and Darcy's Law
- It can model anisotropic porous media if used together to Solid Mechanics Module
- Application in hydrology, Oil&Gas, food, pulp&paper, pharmaceutical industries, biomechanics

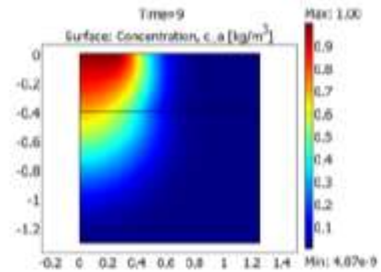


Failure analysis of a multilateral well

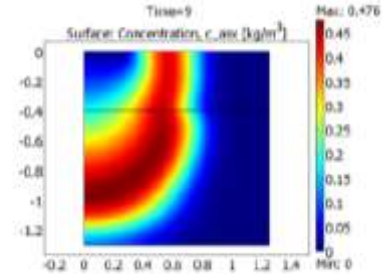
Multiphysics Applications

Pesticide DeToxification in Groundwater

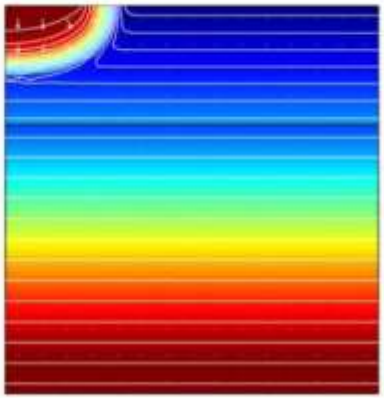


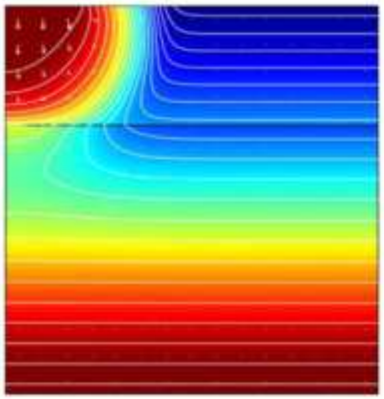


aldicarb
after 10 days



aldicarb sulfoxide
after 10 days





Effective Water Saturation + Pressure Contours of Variably Saturated Soil after 0.3 days + 1 day

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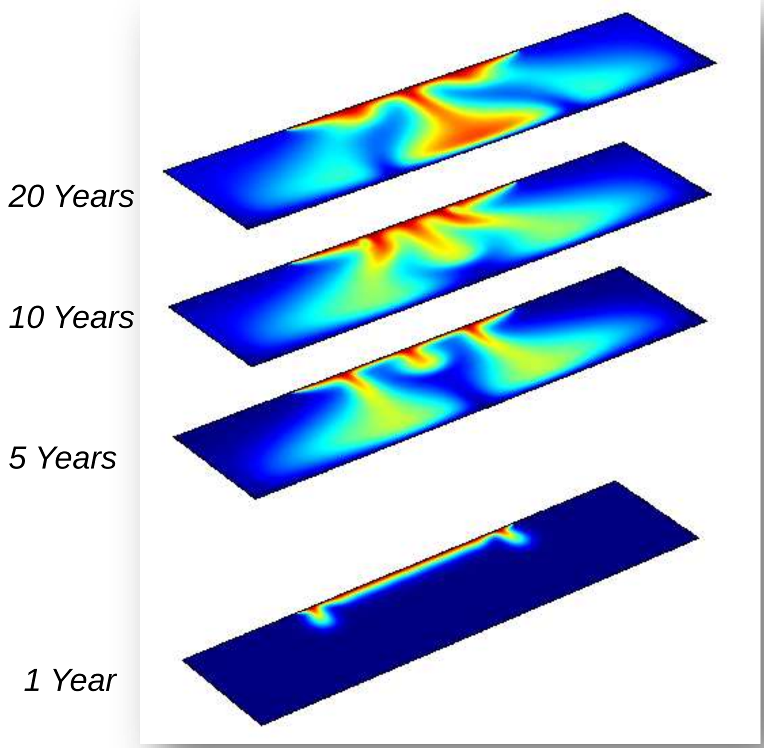
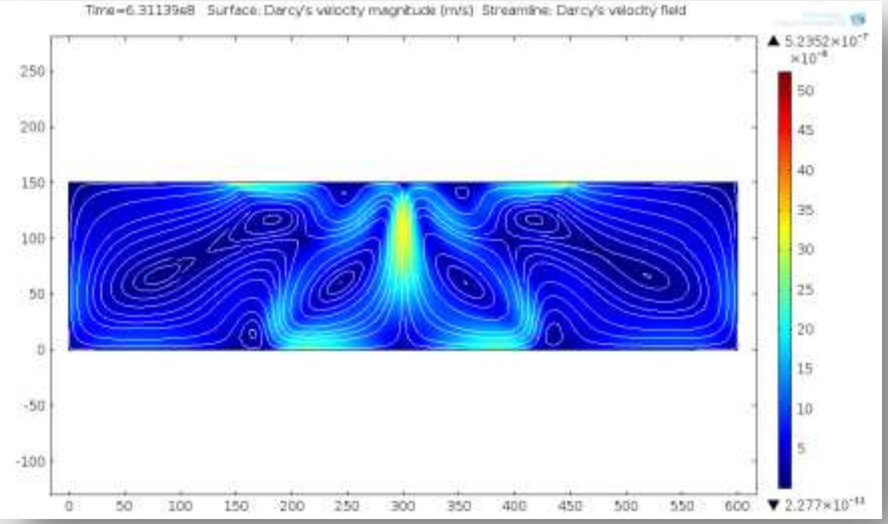
Density Driven flow in Porous Media

- Elder Problem: Density variations can initiate flow even in a still fluid.
- Fluid movement in salt-lake systems, saline-disposal basins, dense contaminant and leachate plumes, and geothermal reservoirs.
- 2-way coupling of two physics interfaces: Darcy's Law and Solute Transport.





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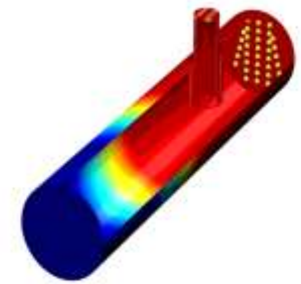
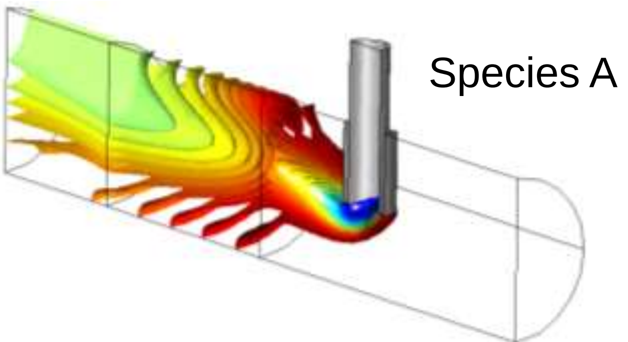
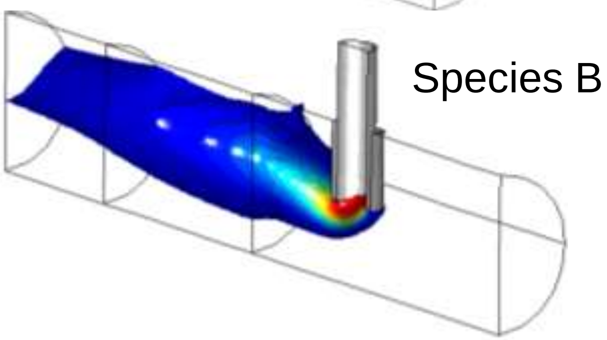
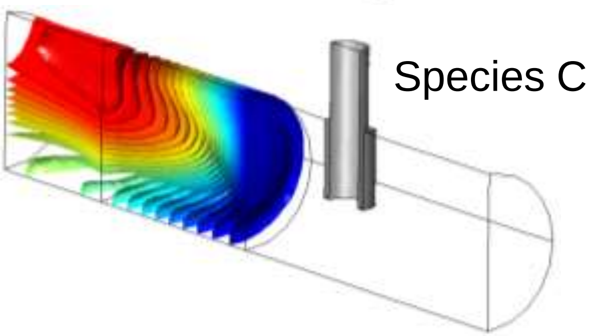
Chemical Reactor Design







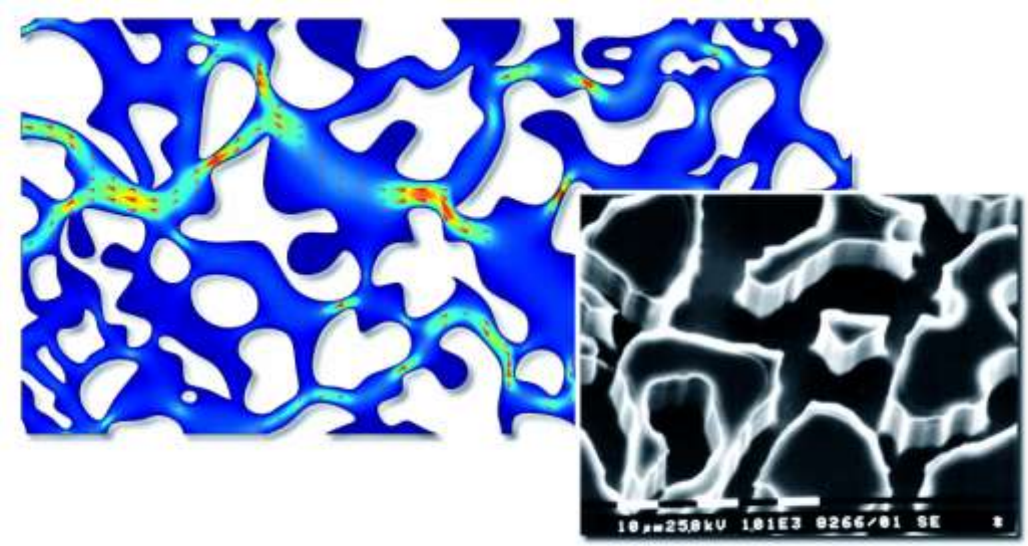


- Flow and reactions in a porous reactor
- Plots indicate flow field and reaction A+B$\longrightarrow$C

Physics involved
1. Flow (both free and porous) 2. Chemical reactions

Pore Scale Flow

- Creeping Flow
- Image import for calculation of porosity and permeability



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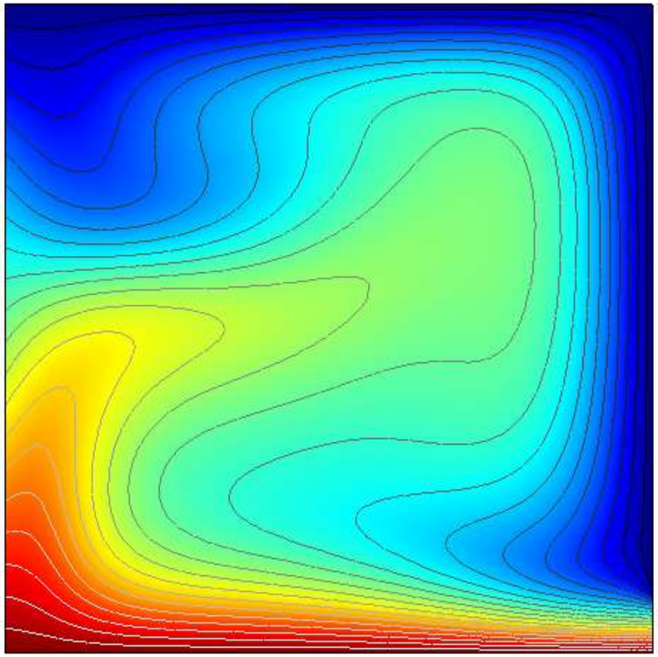
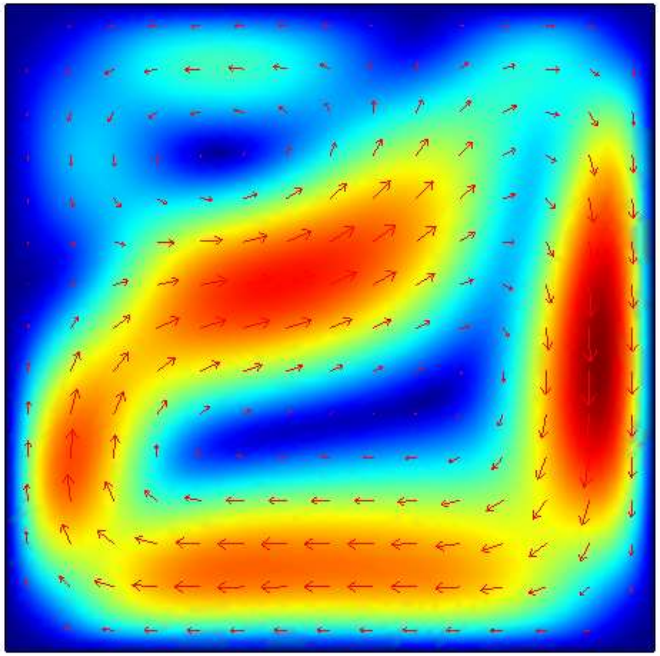
Natural Convection in Porous Media

- Conduction and convection
- Both include diffusion and mechanical spreading

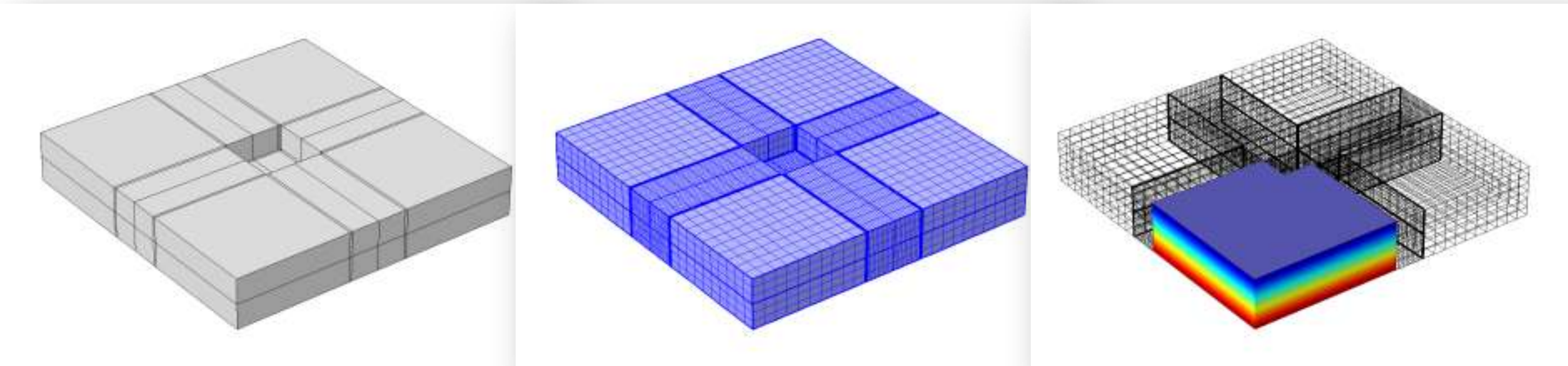


Temperature



Velocity

Demo: Vapor Intrusion Modeling



Darcy's law

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

$$\mathbf{u} = -\frac{k}{\mu}(\nabla p + \rho g \nabla D)$$

Mass Transfer

$$\frac{\partial c_i}{\partial t} + \nabla \cdot (-D\nabla c_i + \mathbf{u} c_i) = R_i$$

Mass Flux of Contaminant through Crack

Y. Yao et al. / Building and Environment 59 (2013)

$$J_{ck} = \frac{\frac{Q_s c_{ck}}{A_{ck}} \exp\left(\frac{Q_s d_{ck}}{D^{ck} A_{ck}}\right)}{\exp\left(\frac{Q_s d_{ck}}{D^{ck} A_{ck}}\right) - 1}$$

Getting started…

1. This Meeting
2. Work through the quick-start booklet
3. Webinars & tutorials: http://www.comsol.com/events/webinars/
4. Browse the Model Library Examples & Documentation
5. Browse Models: http://www.comsol.com/showroom/product/
   These are continuously being updated
6. Browse User Papers: http://www.comsol.com/papers/
   Over 2000 papers & presentations

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