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

\[ \nabla \cdot \left( -\frac{1}{\rho_0} \left( \nabla p - q \right) \right) - \left( \frac{\omega^2}{\rho_0 c_s^2} \right) = \mathbf{Q} \]

\[ \nabla \cdot \left( C : \left( \mathbf{\varepsilon} - \mathbf{\varepsilon} - \mathbf{\varepsilon} \right) + \sigma_0 \right) = \mathbf{F} \]
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
Finite Element Modeling

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

1. Draw
2. Physics
3. Mesh
4. Solve
5. Postprocess
COMSOL Multiphysics® 4.3b Product Suite
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
Brinkman Equations

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

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

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

Convective term  
Forchheimer drag  
Non-linear effects
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

\[
S \left( \frac{\partial p}{\partial t} + \nabla \cdot \left[ \frac{k}{\eta} \nabla (p + \rho g D) \right] \right) = Q
\]
Fracture Flow

- Slow flow in thin shells and fractures (Darcy’s Law)
- Available only in Subsurface Flow Module

\[
d_f \frac{\partial}{\partial t}(\varepsilon_f \rho) + \nabla_T \cdot (\rho \mathbf{q}_f) = d_f Q_m
\]

\[
\mathbf{q}_f = -\frac{\kappa_f}{\mu} d_f (\nabla_T \rho + \rho g \nabla_T D)
\]

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)

\[
(C + S S) \frac{\partial H}{\partial t} + \nabla \cdot \left( k_s k \rho \nabla (H + D) \right) = Q
\]
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
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
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

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

Aldicarb and Aldicarb Sulfoxide after 10 days
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.
Chemical Reactor Design

• Flow and reactions in a porous reactor

• Plots indicate flow field and reaction $A + B \rightarrow C$

<table>
<thead>
<tr>
<th>Physics involved</th>
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<td>1. Flow (both free and porous)</td>
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<td>2. Chemical reactions</td>
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Pore Scale Flow

- Creeping Flow
- Image import for calculation of porosity and permeability
Natural Convection in Porous Media

- Conduction and convection
- Both include diffusion and mechanical spreading
Demo: Vapor Intrusion Modeling

Darcy’s law
\[ \nabla \cdot (\rho u) = Q_m \]

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

Mass Transfer
\[ \frac{\partial c_i}{\partial t} + \nabla \cdot (-D \nabla c_i + u c_i) = R_i \]

Mass Flux of Contaminant through Crack

\[ J_{ck} = \frac{Q_s c_{ck}}{A_{ck}} \exp\left( \frac{Q_s d_{ck}}{D_{ck} A_{ck}} \right) \]

\[ \exp\left( \frac{Q_s d_{ck}}{D_{ck} A_{ck}} \right) - 1 \]

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

1. This Meeting
2. Work through the quick-start booklet
4. Browse the Model Library Examples & Documentation
   These are continuously being updated
   Over 2000 papers & presentations
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