ChemApp Applications in Multiphysics and Discrete Event Simulations

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GTT-User's Meeting 2018

COMSOL Certified Consultant

GTT-TECHNOLOGIES OFFICIAL AGENT

Overview

- Background
  - M4Dynamics
  - Multiphysics Simulation
  - Discrete Event Simulation
- M4Dynamics™ COMSOL® ChemApp© Interface
  - Multiphysics and thermochemistry

    M4D-CCI™
- M4Dynamics™ Arena® ChemApp© Interface
  - Discrete Event Simulation and thermochemistry

    M4D-ACI™

Background – M4Dynamics

- Based in Toronto, since 2015:
  - Consulting in Multiphysics and Thermodynamic based Process Simulation
  - Software development
  - Training
  - Custom physics models, COMSOL Application Development and Hosting

Discrete Event Simulation

- Used in Extractive Metallurgy to:
  - Scheduling simulation of metallurgical plants → several unit operation connected in a flowsheet, a series of events trigger actions between the unit operations
  - Identify operational bottlenecks and find opportunities to optimize resources
  - Evaluate impact, for example, of equipment capacity and utilization on overall plant performance
  - Often, these type of simulation consider time spans of several days or years to obtain statistically significant results

Discrete Event Simulation

- Motivation:
  - This type of simulation can be viewed as a very high level heat and mass balance flowsheet
  - However, it lacks of any thermochemistry component or tool
  - It relies on “recipes” of operation:
    - How many inches of metal level / hour are generated on a furnace before a tapping event is triggered
    - Duration of blow in a converter
  - This events might be set by constant values but they don’t depend on composition, temperature, heat balance, etc. → thermochemistry component

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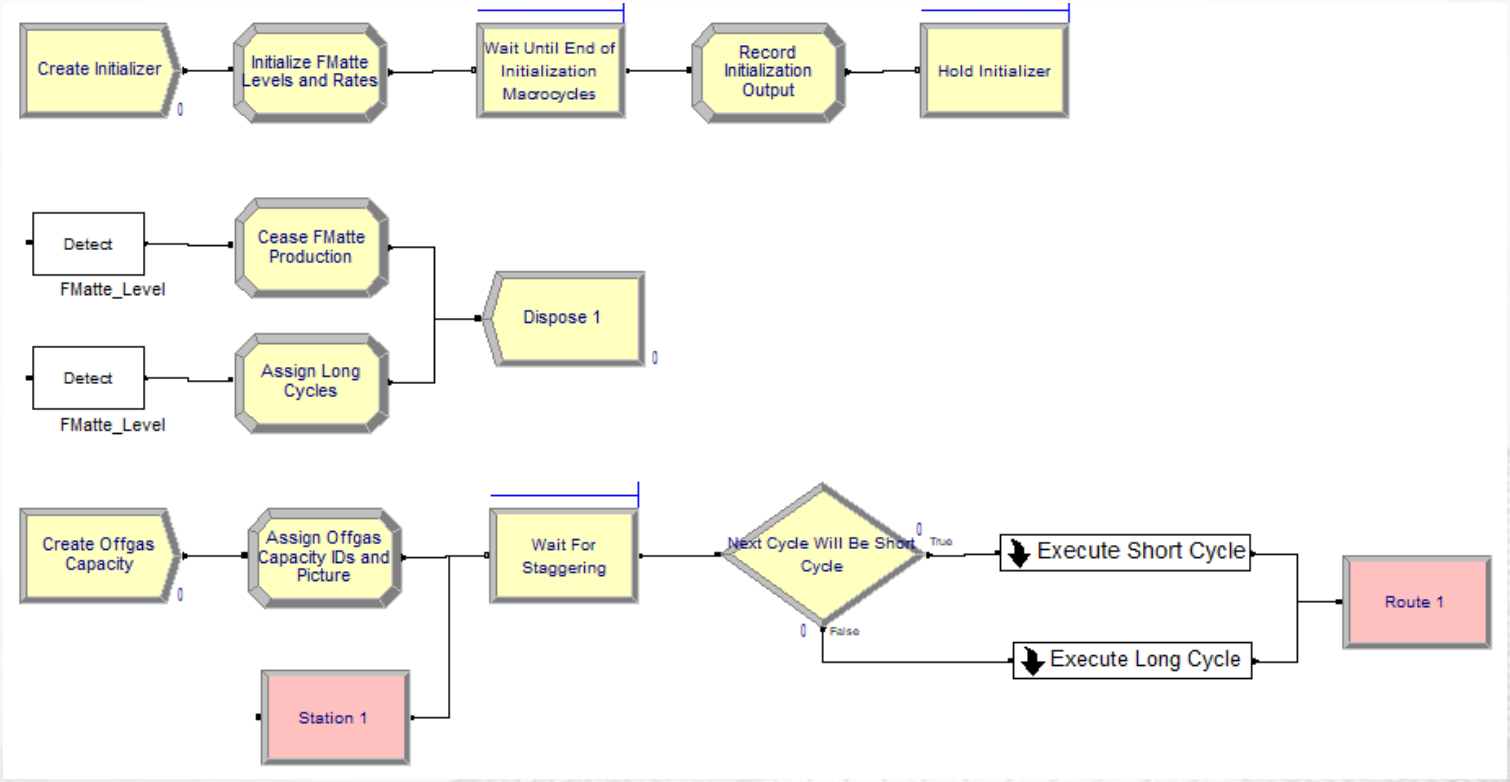
M4Dynamics™ Arena® ChemApp© Interface

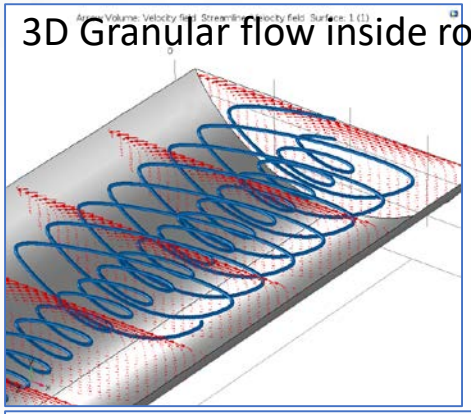
- Arena model for Smelter/Converter



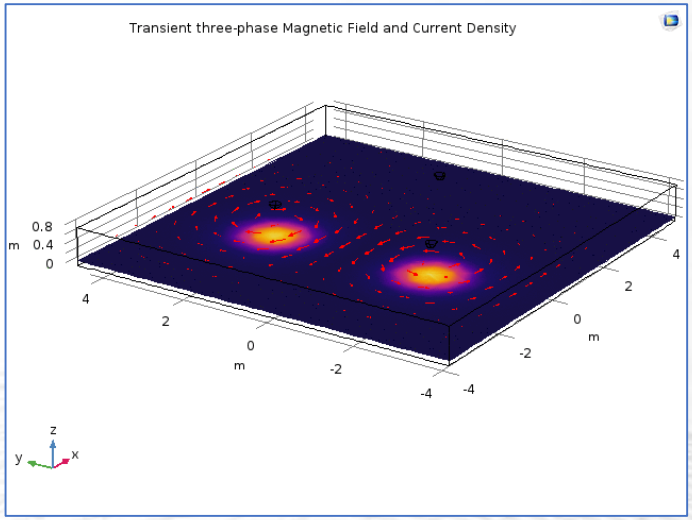
Cu Smelter model: Smelter + Converting simulation based on discrete event simulation
Courtesy of Prof. Alessandro Navarra

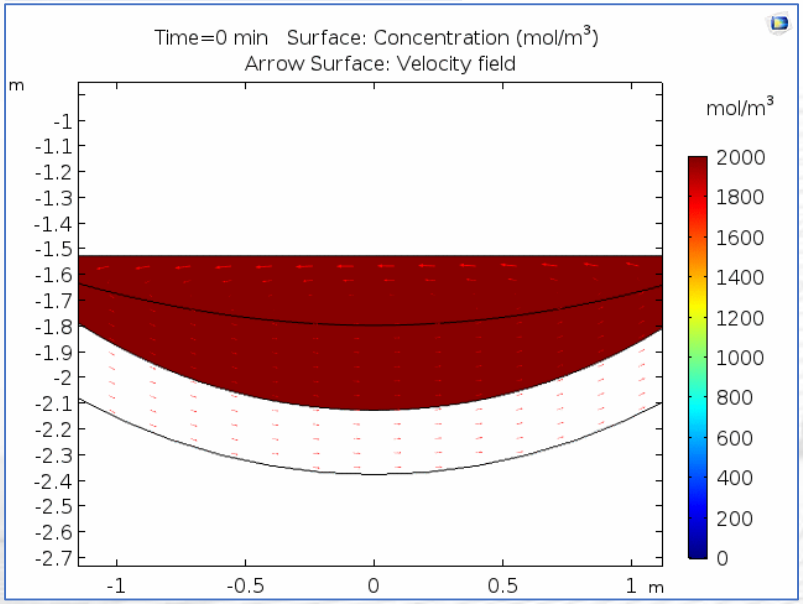
Multiphysics Simulation

3D Granular flow inside rotary kiln

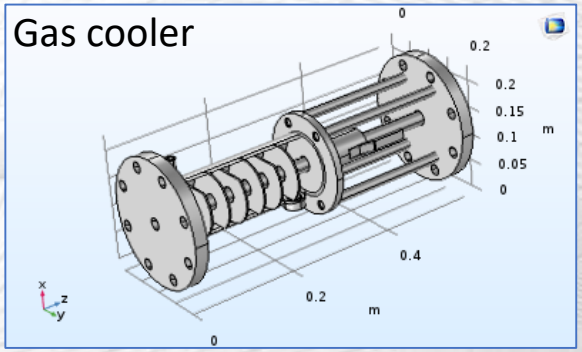


Magnetic field and current density on 3-electrode furnace





Concentration of reactants inside rotary kiln



M4D consulting

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M4Dynamics™ COMSOL® ChemApp© Interface

Motivation:

- We use COMSOL as Multiphysics simulation software. It is based on FEA:
  - Vast range of physics: Fluid flow, mechanical, thermal, structural, electrical,… All sharing common PDE formulation
  - Based on space discretization: 0D, 1D, 2D, 3D
  - Steady state, time-dependant, and other analysis
  - Allows detailed simulation of metallurgical reactors combining heat and mass transfer, fluid flow, etc
  - Does not have a thermochemistry component

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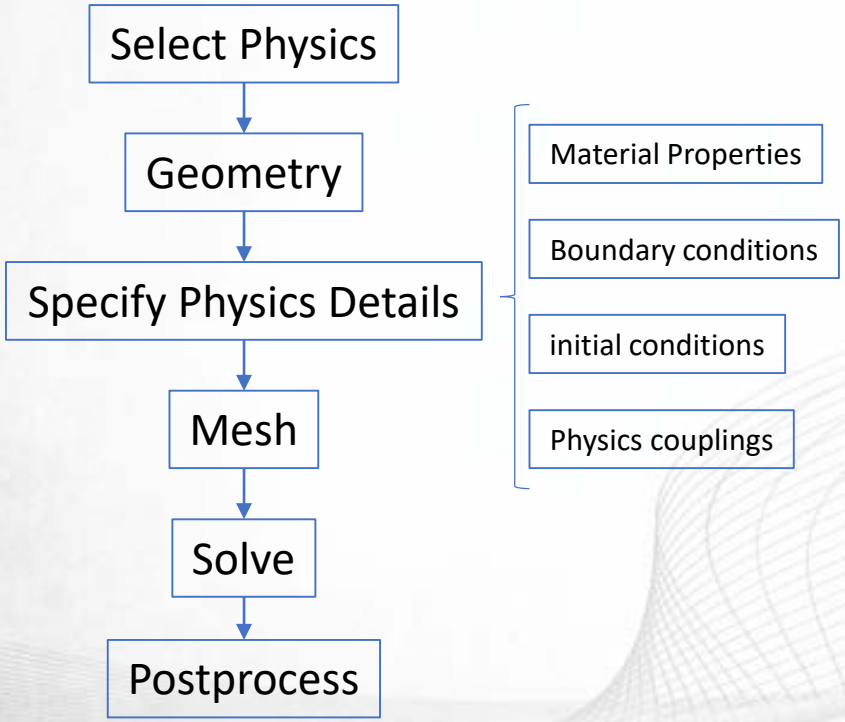
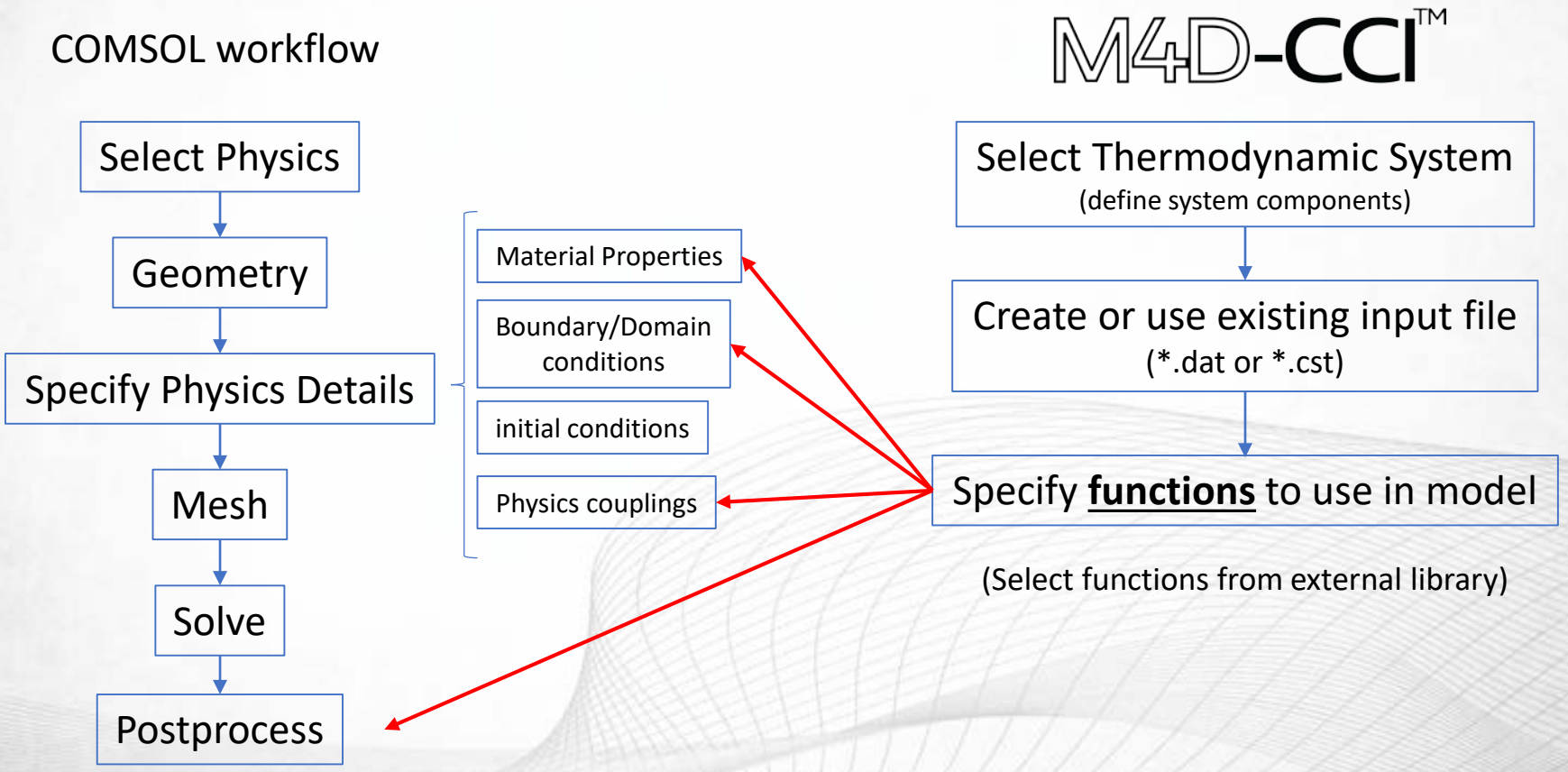
Typical COMSOL Workflow

COMSOL workflow



Adding thermochemistry library to the workflow



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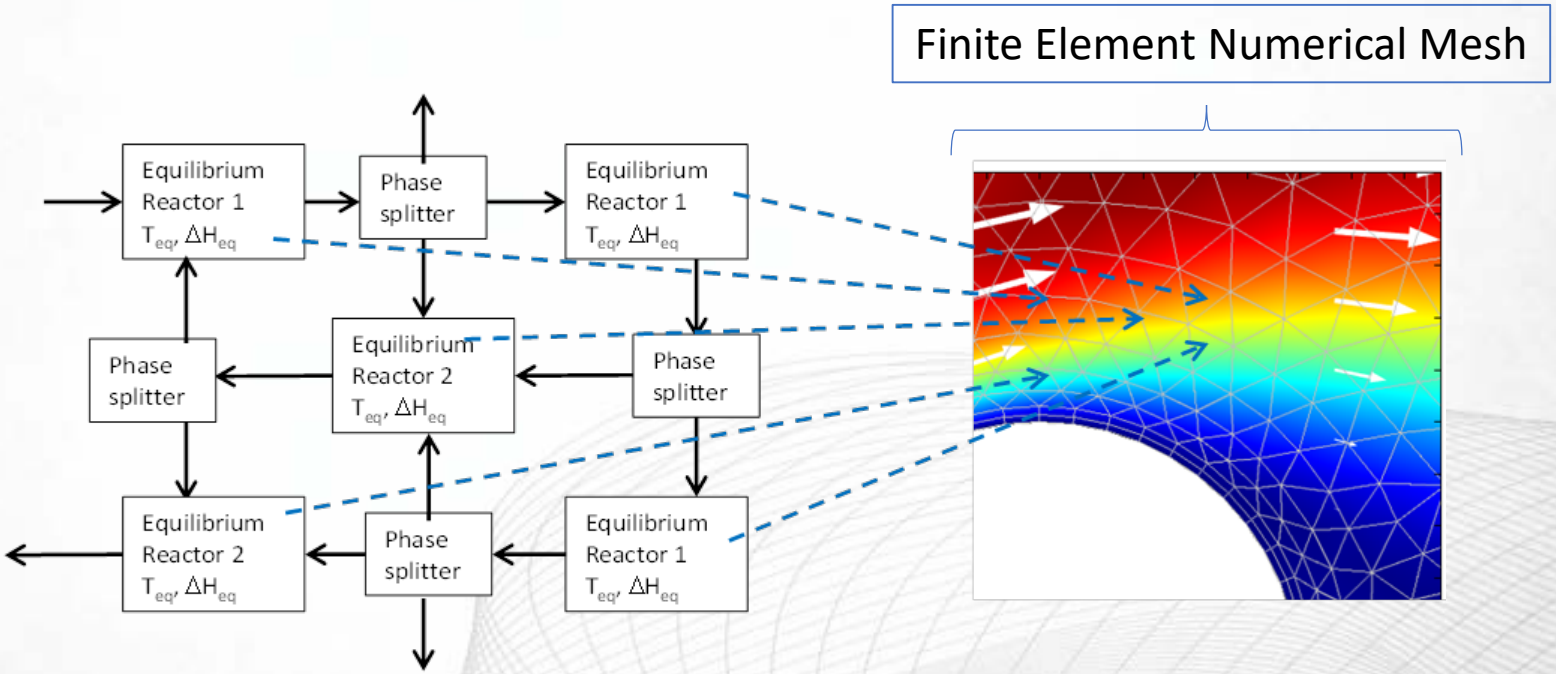
Concept

Analogy to Local Equilibrium Concept



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How to use

- M4D-CCI is built as an “external function” in COMSOL → like an add-in
- It allows to:
  - Evaluate thermodynamic properties → it can help define complex material properties.
  - Perform equilibrium calculations based on COMSOL variables → one-way coupling
  - Affect COMSOL variables based on equilibrium results → two-way coupling

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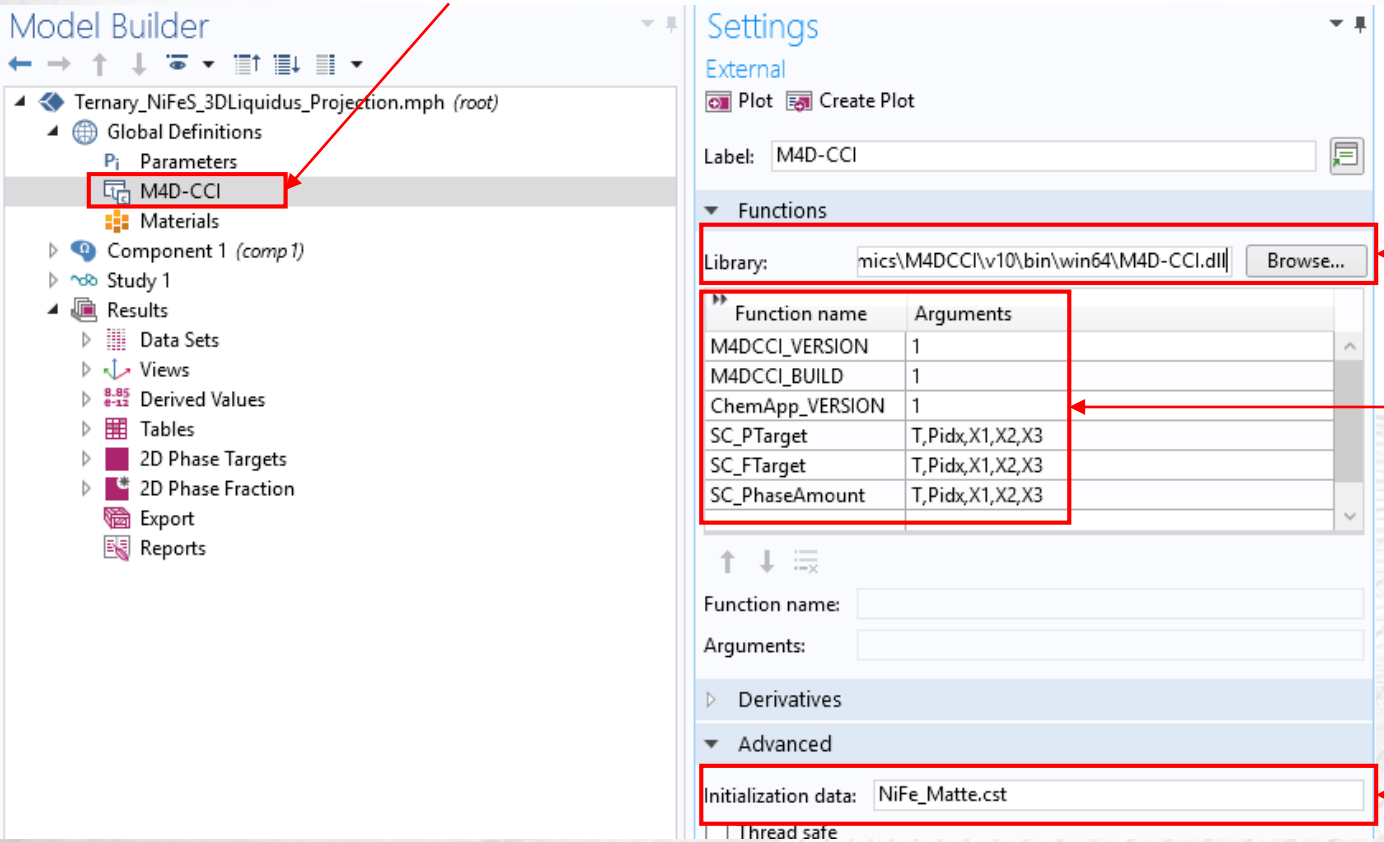
How to use – Defining external function in COMSOL

External function decl.



M4D-CCI.dll

These functions are defined in M4D-CCI

Thermodynamic input file

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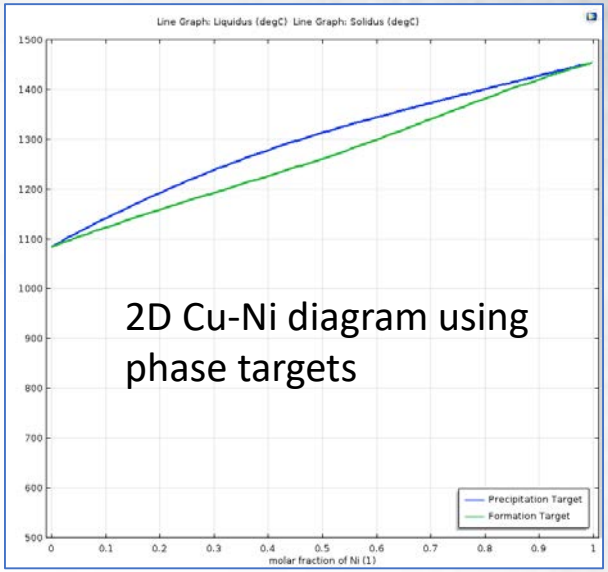
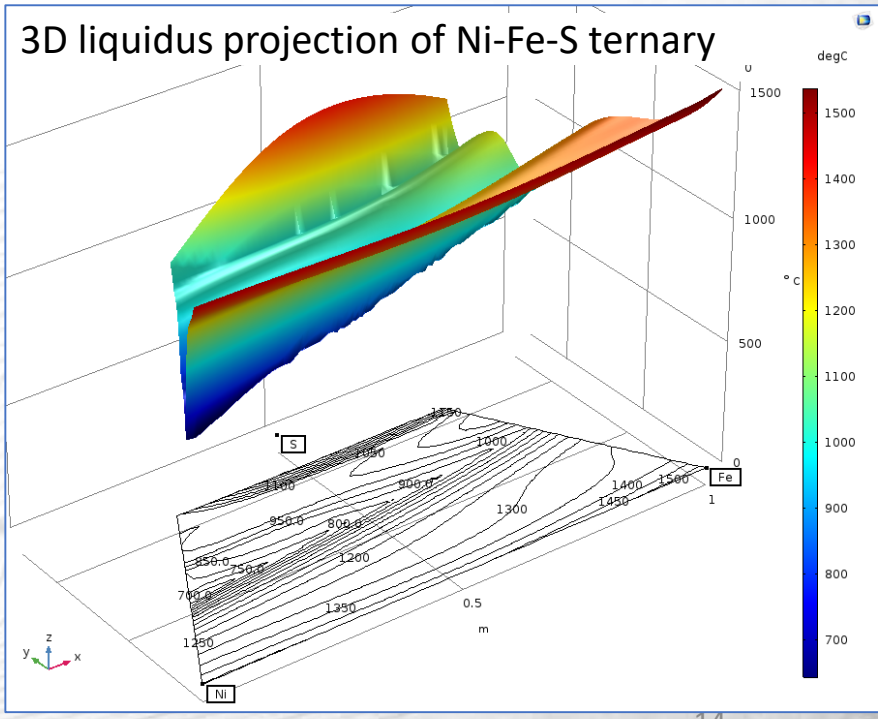
Examples of use

- Equilibrium Calculations - General
  - Thermodynamic functions: G, H, S, Cp
  - Amount, fractions, activities, etc. of phases, system components, phase constituents,
  - fraction,
  - Phase Target: precipitation and formation targets
  - Fixed chemical potential calculation of amount and fraction of phases, phase constituent and system components



2D Cu-Ni diagram using phase targets



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Examples of use

- Equilibrium Calculations – Chemical Reaction Kinetics

$$\frac{dc_i}{dt} = R_i$$

$$R_i = \sum_j R_j = \sum_j v_{ij} r_j$$

$$r_j = k_j^f \prod_{i=1}^{Q_r} c_i^{v_{ij}} - k_j^r \prod_{i=1}^{Q_p} c_i^{v_{ij}}$$

$$k_j^f = A_j^f e^{\left(\frac{-Ea_j^f}{R_g T}\right)}$$

$$k_j^r = \frac{k_j^f}{K_{e,j}}$$

$$K_{e,j} = e^{\left(\frac{-\Delta G_j^o}{R \cdot T}\right)}$$

For a set of ODE's with c_i as the variable to solve for

The source term depends on the rate of reactions

Which depends on the rate constants for each reaction

At equilibrium, reverse and forward rate constants are related by the equilibrium constant

Equilib constant is calculated by M4D-CCI for each reaction

i: species index, j: reaction index, f: forward, r: reverse; e: equilibrium

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Examples of use

- Equilibrium Calculations – Reaction Kinetics + Energy Balance

All of the previous +:

$$V \sum_i c_i \cdot C_{p,i} \cdot \frac{dT}{dt} = Q$$

$$Q = -V \sum_j H_j \cdot r_j$$

The system's temperature depends on the heat source from chemical reactions

The volumetric heat source, depends on Enthalpy of reactions and rate of reactions

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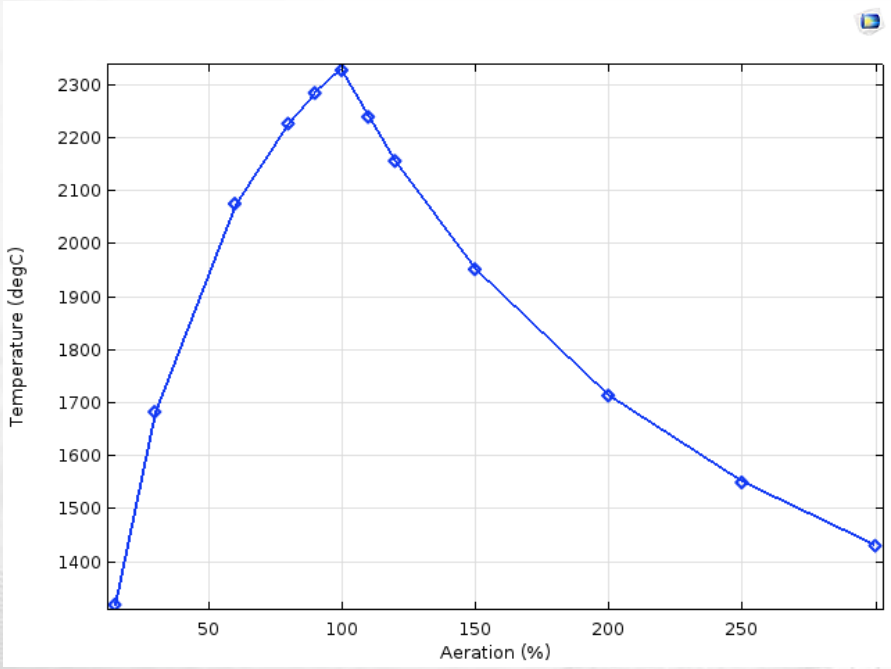
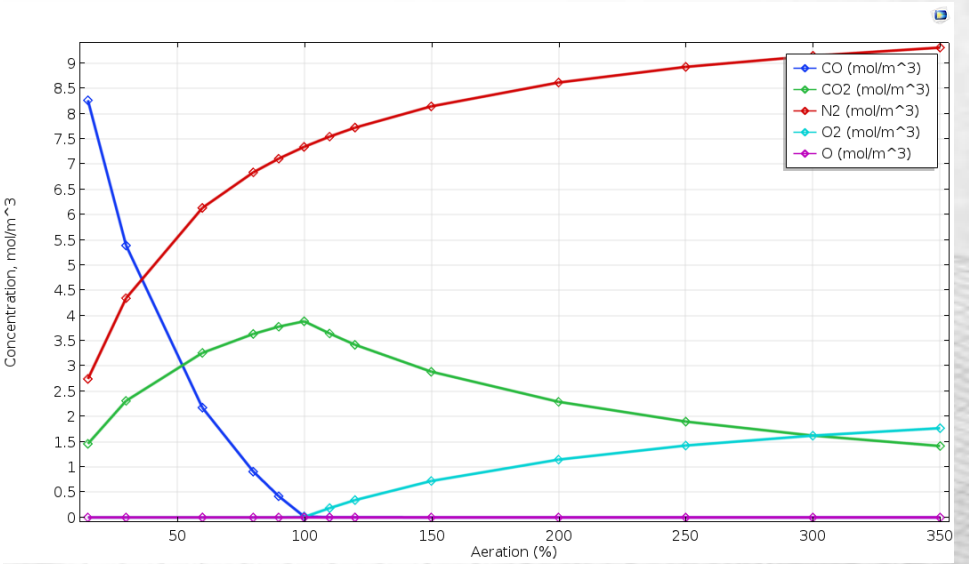
Examples of use

- Equilibrium Calculations – Reaction Kinetics + Energy Balance

Example: 0D combustion of preheated CO + Air mixture



Effect of aeration on adiabatic flame T
Initial gas T = 650°C



Equilibrium concentration vs aeration

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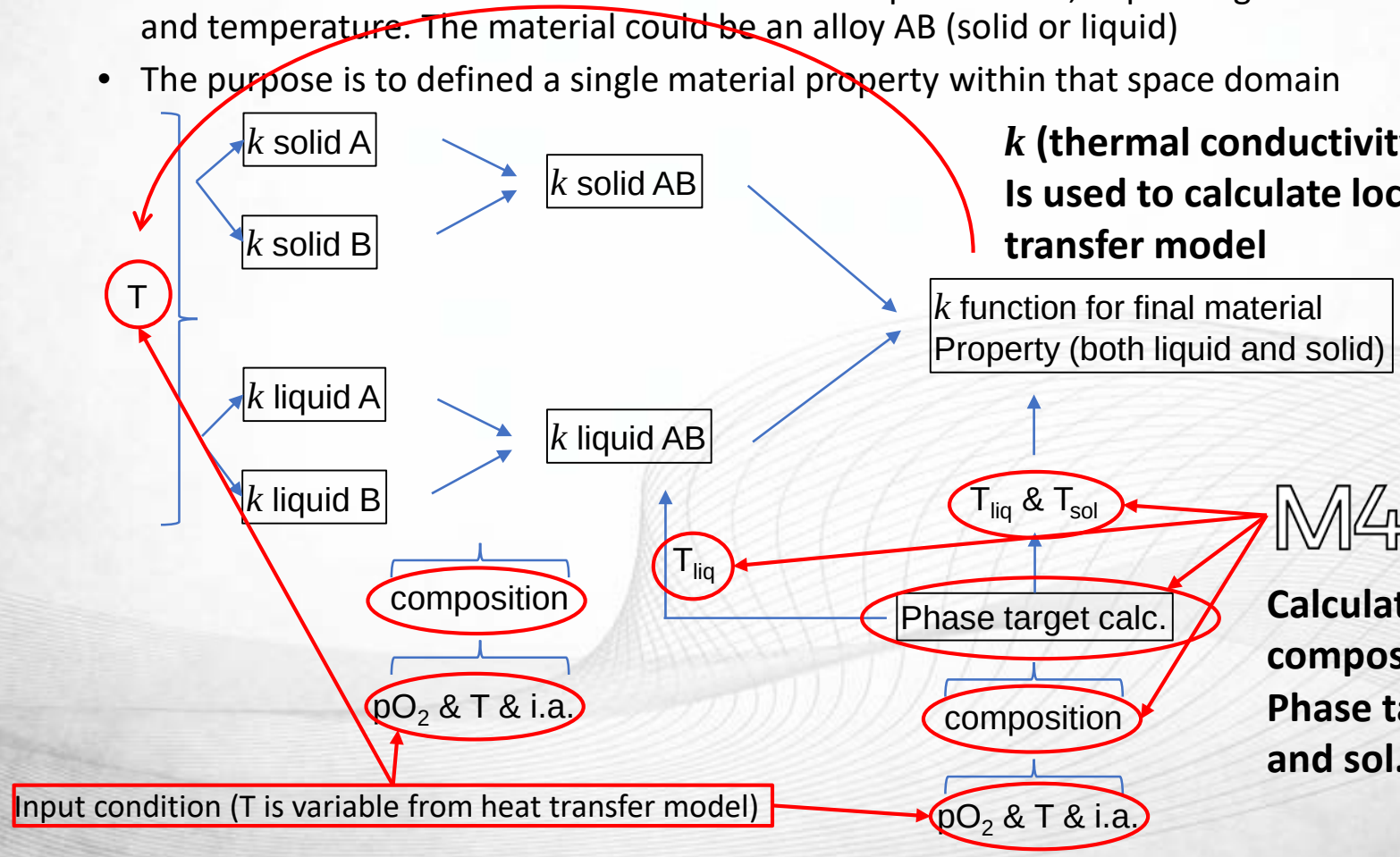
Examples of use

- Complex material properties:
  - Consider a material domain that can be either liquid or solid, depending on the local concentration and temperature. The material could be an alloy AB (solid or liquid)
  - The purpose is to defined a single material property within that space domain



k (thermal conductivity)
Is used to calculate local T on the heat transfer model

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Calculate local eq. compositions,
Phase targets → T liq and sol.

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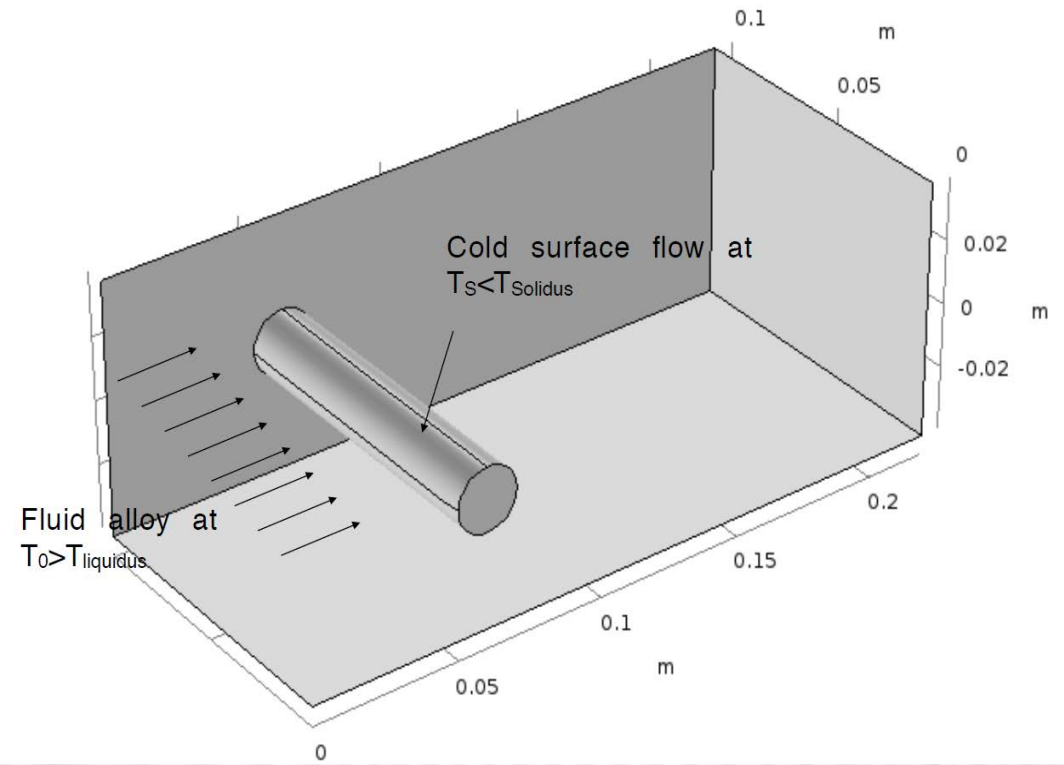
Examples of use

- Phase Change - Solidification of non-ideal liquid as function of space and time and composition



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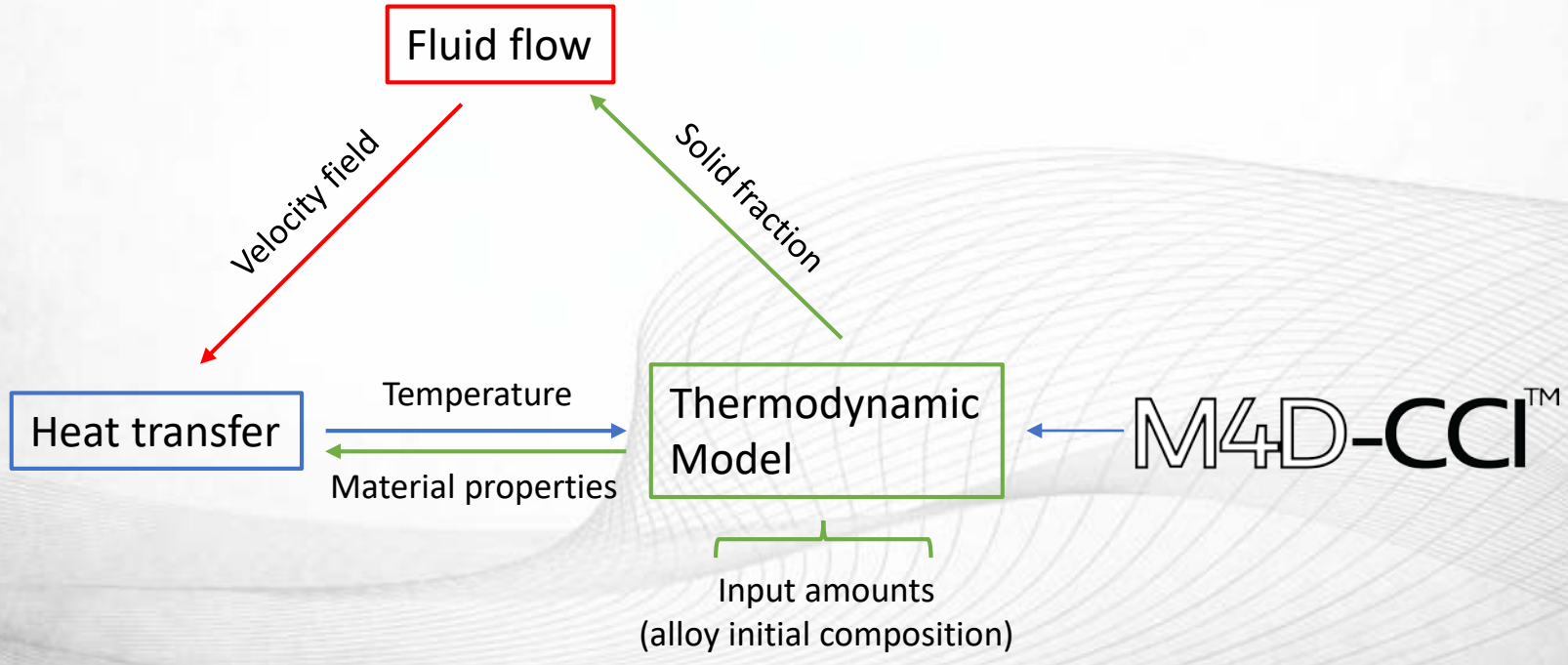
Examples of use

- Solidification model uses a fixed numerical grid to track liquid/solid interface
- Model approach:



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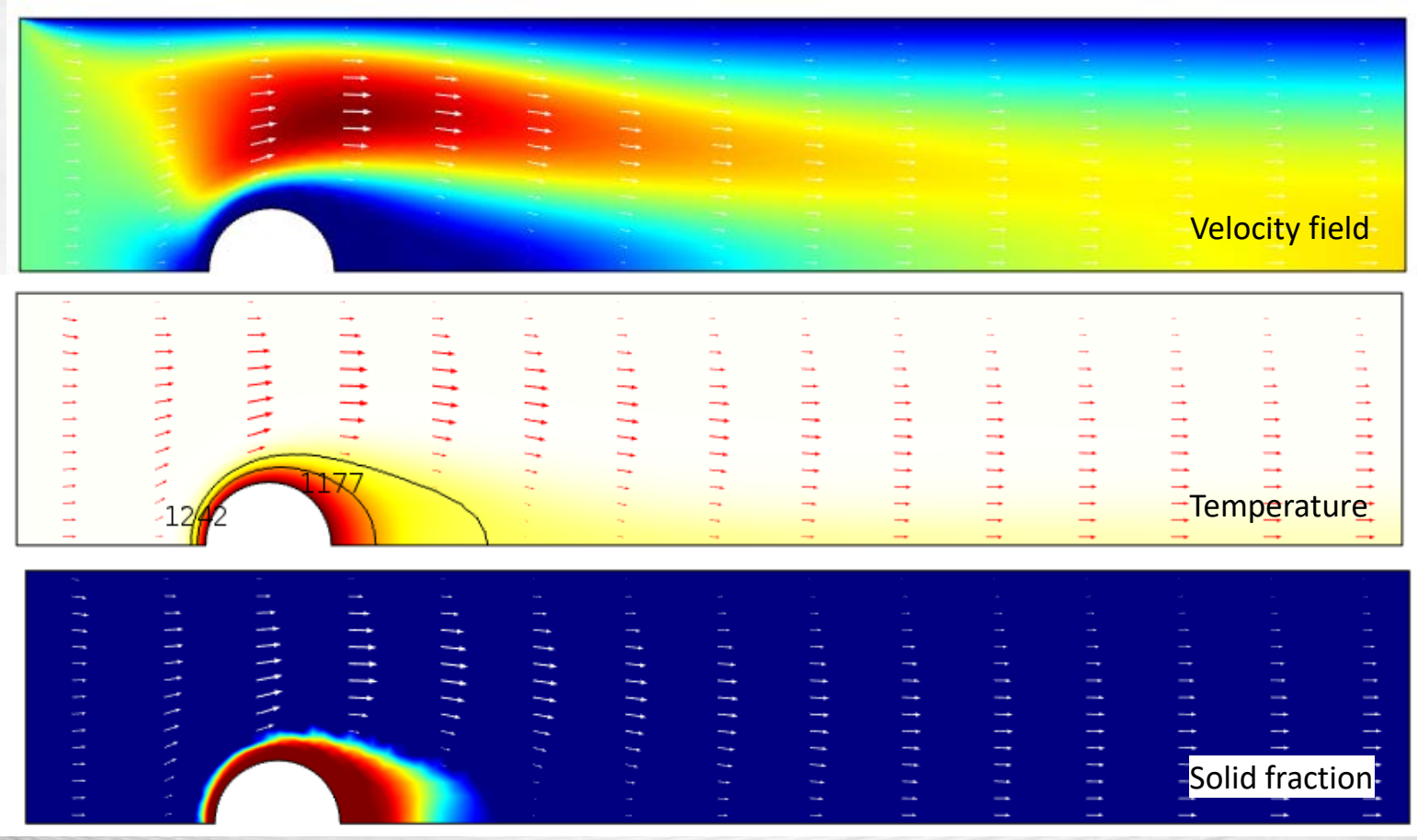
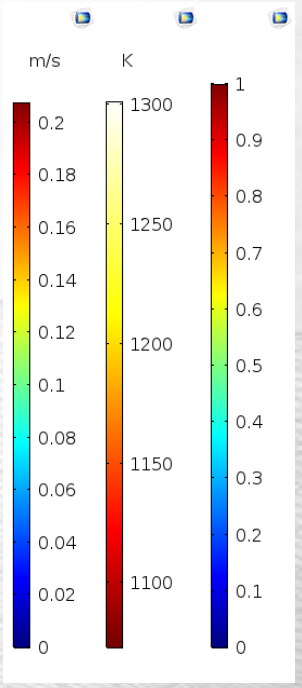
Examples of use

- Phase Change - Results





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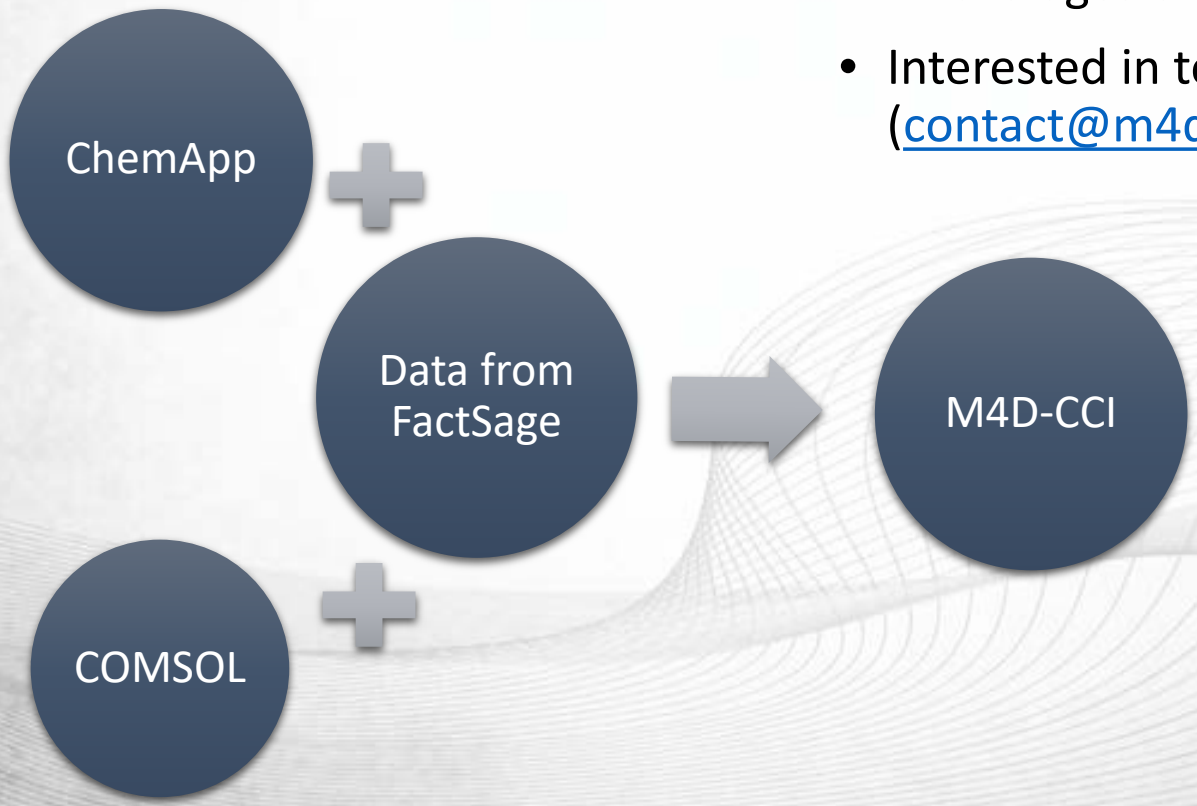
Current State of Development

- Compatible with COMSOL versions 5.1 up to 5.3a
- 64-bit ChemApp version
- Final stages of documentation
- Interested in testing it? (contact@m4dynamics.com)



Thanks!