Modeling high viscosity slag flows in entrained flow gasifiers using a Volume of Fluid (VOF) approach

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interSlagFoam

Agenda

- Motivation
- Fundamentals
- ChemApp® in OpenFOAM
- Modeling viscosity
- First Results
- Summary
- Outlook
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Motivation

- Gasification = thermo-chemical conversion ($\lambda < 1$)
- Technology – entrained flow gasifier (high temperatures)
- Feedstock – coal
  - Contains carbon and ash (Si, Fe, Ca, Na, K)
- Products:
  - Synthesis gas (mainly $H_2$, CO)
  - Slag (residue, but necessary for process)
importance of slag modeling:
- wall protection in gasifier, closed slag film necessary
- Radiant cooler (exhaust heat steam generating system)
→ Fouling, plugging and corrosion

cooled wall  slag film  gas phase

ten wall region

radiant cooler

slag
particles
cooling fin

Therefore simulation of slag flow behavior important
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Fundamentals - general

- Solver for wall near region only:
  - Source terms come from prescribed external field or
  - basic lagrangian-solver (OpenFOAM, FLUENT, CFX)
- Two-way coupling between solvers with dynamic mesh

- Features of interSlagFoam (iSF) in comparison to interFoam:
  - Temperature equation
  - Added source terms (mass, momentum, energy)
  - Wall heat treatment
  - Coupling with ChemApp©

- Neglected physics:
  - No gas phase reactions in iSF
  - No velocity and turbulence backcoupling
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Fundamentals - principle

interSlagFoam  
Solver interface  
Lagrangian solver (e.g. coalFoam)

slag  
Coal/ash particles
- Continuity equation:

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

- Momentum equation:

\[
\frac{\partial (\rho \mathbf{u})}{\partial t} + \nabla \cdot (\rho \mathbf{u} \mathbf{u}) = \nabla \cdot (\mu \nabla \mathbf{u}) + \rho \mathbf{g} - \nabla p + \mathbf{F}_{\text{mom}}
\]

- Volume Of Fluid (VOF) equation:

\[
\frac{\partial \alpha}{\partial t} + \nabla \cdot (\alpha \mathbf{u}) = \frac{S_\alpha}{\rho_{\text{slag}}}
\]

- Temperature equation:

\[
\frac{\partial \rho c_p T}{\partial t} + \nabla \cdot (\rho c_p T \mathbf{u}) = \nabla \cdot (\lambda \nabla T) + S_T
\]
- library for calculation of complex multicomponent and multiphase chemical equilibrium
- Sketch of integrating ChemApp© into simulations:

![Diagram showing integration of CFD and ChemApp© with additional models for density, viscosity, and slag phases]
Phase diagram for ternary system:

ASlag-Liq + Al₆Si₂O₃(s) [liquidus + solidus]

Mullite + Al₂O₃(s) + CaAl₂Si₂O₈(s) [solidus]

very complex system, real slag has much more than 3 species → ChemApp© is needed
Slagmodeling
Solidus and Liquidus lines

800 K
1800 K
cooled wall slag film gas phase

SiO₂ - CaO - Al₂O₃
1400 K

SiO₂ - CaO - Al₂O₃
1600 K

SiO₂ - CaO - Al₂O₃
1800 K

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Modeling viscosity

- Modeling of viscosity essential for slag flow simulation
- Different models already implemented
- Urbain, Kalmanovitch-Frank, Random Model for testing
- Model coefficients depending on slag composition (phases)

\[ \mu = a(x_i) \cdot T \cdot \exp \left( \frac{b(x_i) \cdot 10^3}{T} \right) \]

Urbain Model

![Graph showing viscosity vs temperature for Urbain Model](image)

amount solid - liquid

![Graph showing amount solid and liquid vs temperature](image)
Device for slag flow measurement in laboratory scale

Operating conditions:
- $p = 1$ bar
- $T_{\text{gas}} = 1800$ K
- $T_{\text{wall}} = 800$ K

Slag data:
- $\eta_{\text{max}} = 100$ Pas
- $\rho = 2550$ kg/m$^3$
- $\lambda = 1.5$ W/m$^2$K

Mesh information:
- 8500 hexahedral cells
- Cell resolution: 0.1 mm
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First results – slag flow device

- Slag layer thickness between 21 and 30 mm
- $\text{Re}_{\text{slag}} \in [10^{-6}, 10^{-2}]$
- $\text{Pr}_{\text{slag}} \in [3.2 \times 10^3, 5 \times 10^4]$
First results – quarter cylinder

- Fully 3D test case for slag flow and source term behavior

Operating conditions:
- $p = 1$ bar
- $T \in [1250, 2000]$ K

Slag data:
- Urbain model ($\eta_{\text{max}} = 200$ Pas)
- $\sigma = 0.5$ N/m
- Real slag composition
  (8 elements, > 100 phases)

Mesh information:
- 40,000 hexahedral cells
- Size: $\Theta$ 25 cm, length 100 cm
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First results – quarter cylinder

- Case description
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First results – quarter cylinder

- Animations of slag layer formation and downstream flow

slag flow and velocity magnitude/ profile

viscosity behavior under different temperatures
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First results – mesh deformation

- Mesh deformation due to fouling done with dynamicMesh

- Example: simpleFoam calculation on quarter cylinder case
  - based on „static“ condition of slag flow
  - backcoupling via deformed mesh
Summary

- Development of a near wall region slag flow solver
- Added temperature equation and source terms for slag
- Different viscosity models implemented
- ChemApp© library successful coupled
- First results for slag layer formation and slag flow
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Outlook

- Completion of programming interSlagFoam
  - Adding of missing models

- Validation with experiments
  - Literature
  - Slag flow device (design phase, construction end of this year)

- Performance speed up of ChemApp© using Look-up tables

- Future goal:
  - Simulation of slag flow behavior of complete entrained flow gasifiers with radiant cooler
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