Slag Modeling based on Coal-Ash Compositions

GTT Workshop

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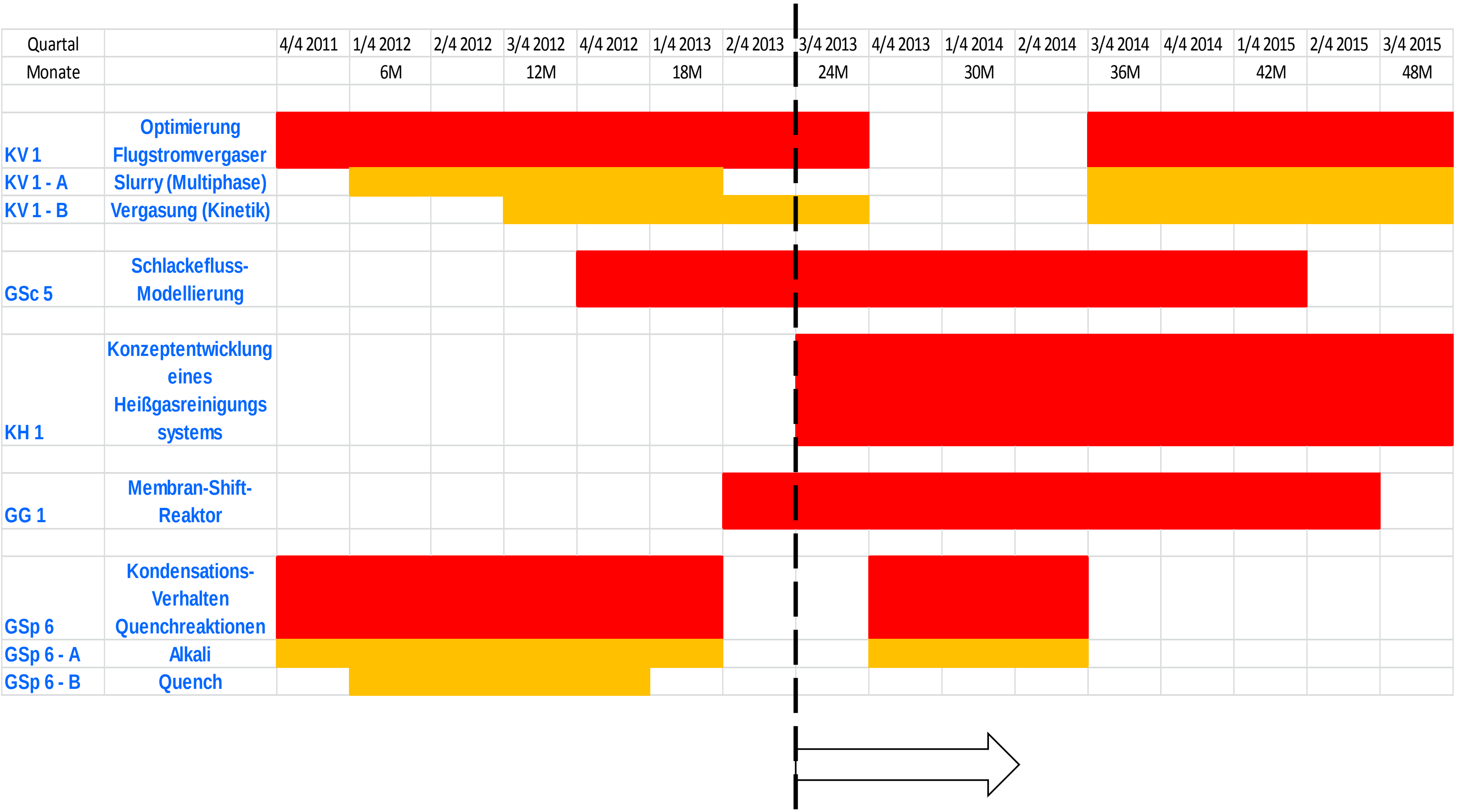
Inhalt

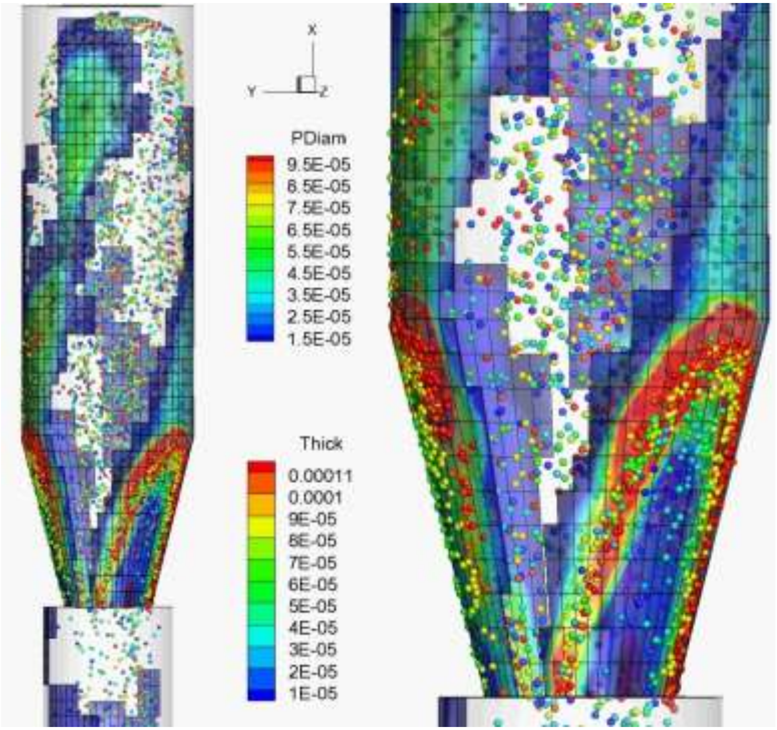
- HotVeGas Project
- P³ - Particle Post Processor
- Slag Modeling
  - Overview
  - Models
  - Performance

HotVeGas Project (Computational Fluid Dynamics)



P³ - Particle Post Processor

- In-House-Code at the Institute
- Developed by M. Losurdo
- Parameters for Slag not included



Particle Deposition and Slag Flow in a generic Gasifier

P³ - Particle Post Processor

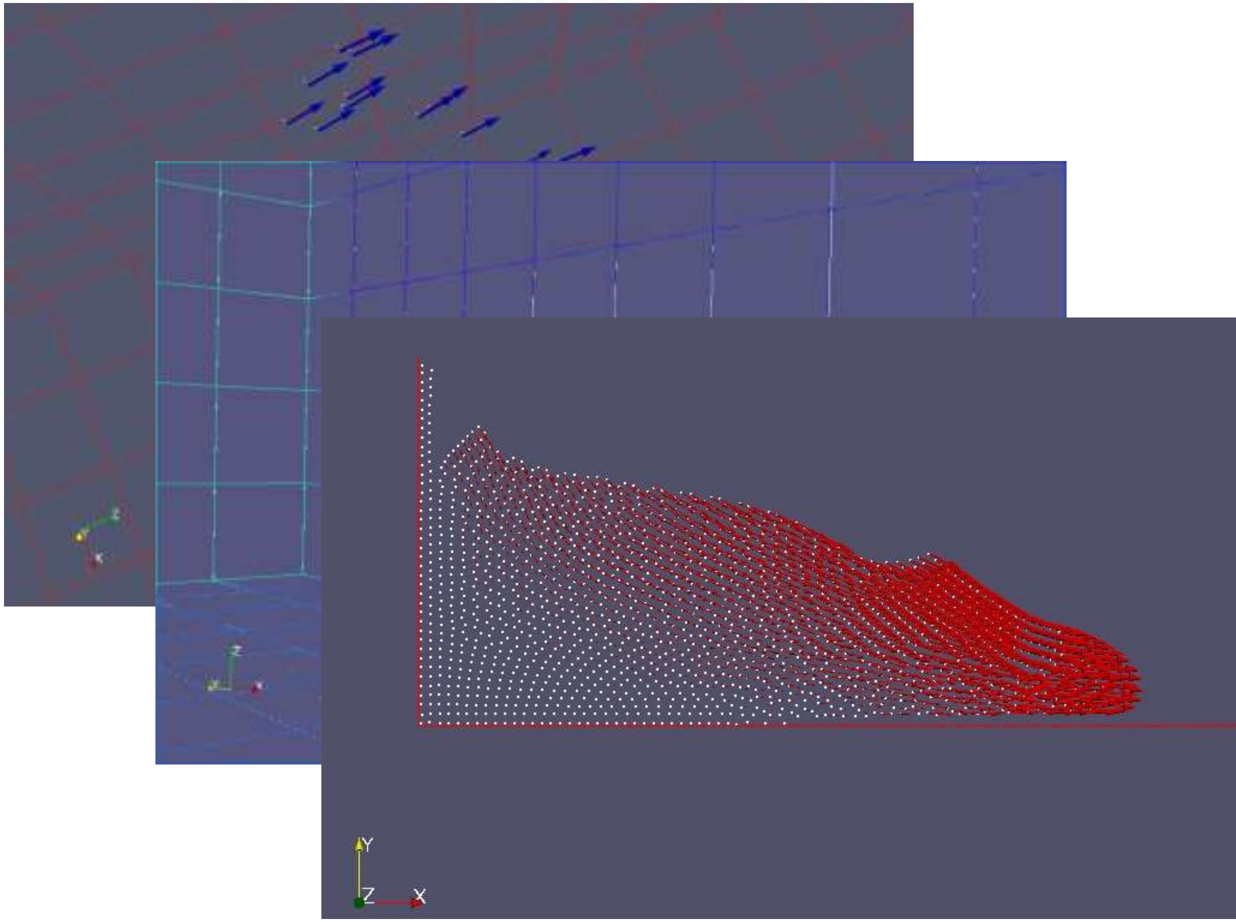
CFD Post-Processing:

Based on Flow Field Simulation:

1) Particle Tracking

2) Deposition

3) Slag Flow



P^3 - Particle Post Processor

Open Source SPH Code based on:

Liu and Liu, Smoothed Particle Hydrodynamics – A Meshfree Particle Method, 2003

Code for hydrodynamics

- Heat Conduction and Radiation missing ⟶ no melting process
- Constant Viscosity ⟶ no dependency on temperature
- Newtonian flow ⟶ no non-Newtonian flow for lower temperatures
- Equation of State ⟶ valid for hydrodynamics

P³ - Particle Post Processor

Grid-based methods

- Eulerian
- Lagrangian
- Hybrid

↓

- Finite Difference
- Finite Element
- Finite Volume

Meshfree methods

- Lagrangian

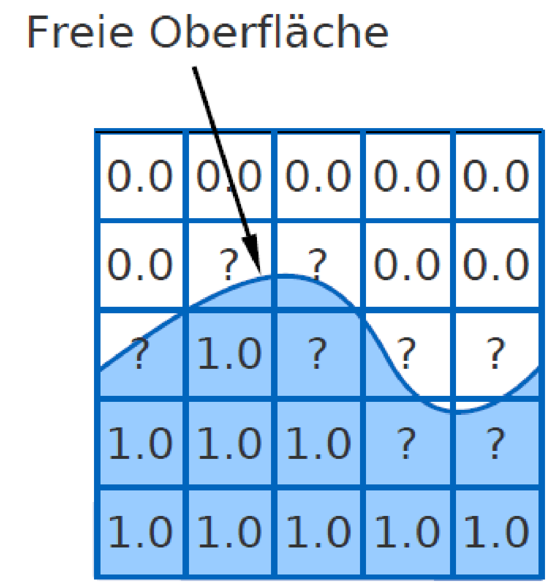
↓

- Molecular Dynamics
- Discrete Element Method
- Smoothed Particle Hydrodynamics

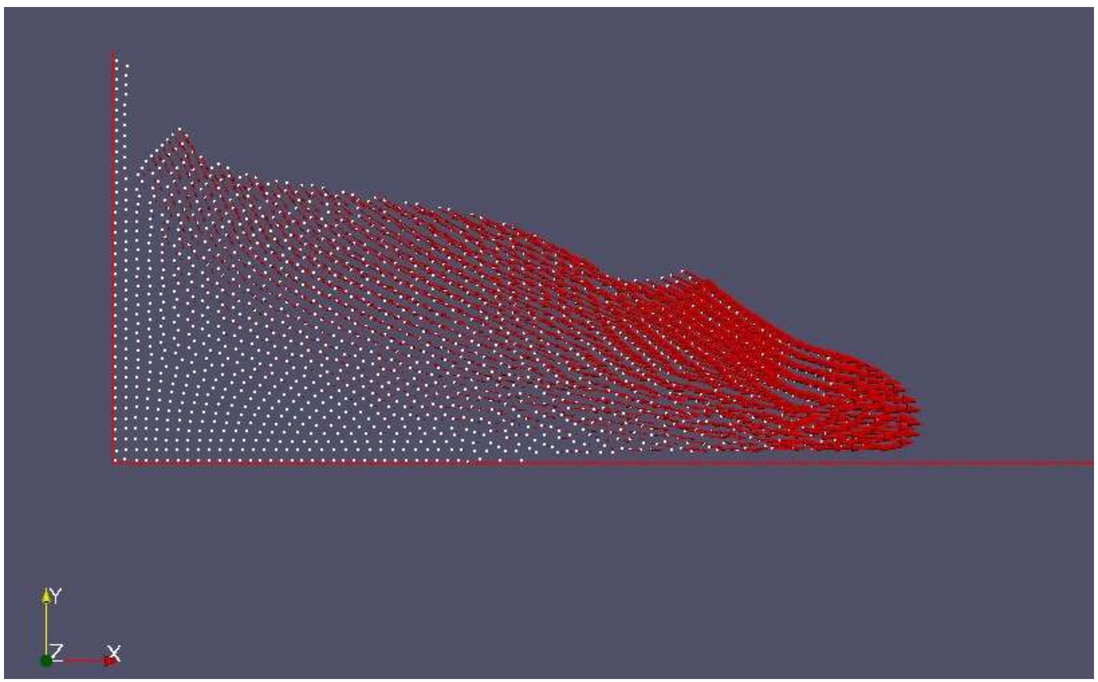
Smoothed Particle Slagdynamics

Why SPH?

- Free Surfaces
- Large Deformation and Separation
- No Meshing



Pugachev – Numerische Berechnung Energetischer Systeme

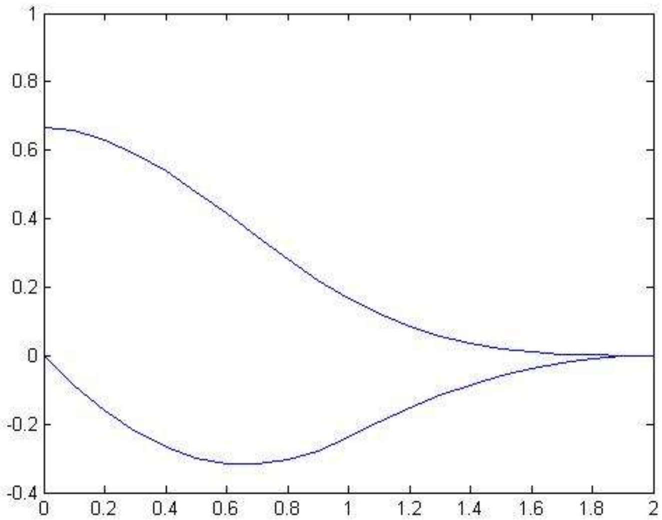


Dam break scenario
with a viscous fluid in SPH

Smoothed Particle Slagdynamics

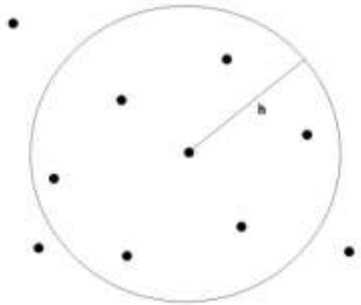
SPH Basics

- Domain represented by Interpolation points (Particles)
- Each Particle contributes to neighbouring Particle
- Contribution dependent on Smoothing Function



Cubic Smoothing-Kernel (top) with Gradient (bottom)

$$A(r) = \sum_j m_j \frac{A_j}{\rho_j} W(|r - r_j|, h)$$



Smoothed Particle Slagdynamics

Navier-Stokes Equation (Lagrangian form)

Continuity

$$\frac{D\rho}{Dt} = -\rho \frac{\partial v^\beta}{\partial x^\beta} \quad \Rightarrow \quad \frac{D\rho_i}{Dt} = \sum_{j=1}^{N} m_j v_{ij}^\beta \frac{\partial W_{ij}}{\partial x_i^\beta}$$

Momentum

$$\frac{Dv^\alpha}{Dt} = \frac{1}{\rho} \frac{\partial \sigma^{\alpha\beta}}{\partial x^\beta} \quad \Rightarrow \quad \frac{Dv_i^\alpha}{Dt} = \sum_{j=1}^{N} m_j \frac{\sigma_i^{\alpha\beta} + \sigma_j^{\alpha\beta}}{\rho_i \rho_j} \frac{\partial W_{ij}}{\partial x_i^\beta}$$

Energy

$$\frac{De^\alpha}{Dt} = \frac{\sigma^{\alpha\beta}}{\rho} \frac{\partial v^\alpha}{\partial x^\beta}$$

$$\Rightarrow \quad \frac{De_i}{Dt} = \frac{1}{2} \sum_{j=1}^{N} m_j \frac{p_i + p_j}{\rho_i \rho_j} v_{ij}^\beta \frac{\partial W_{ij}}{\partial x_i^\beta} + \frac{\mu_i}{2\rho_i} \epsilon_i^{\alpha\beta} \epsilon_i^{\alpha\beta}$$

Smoothed Particle Slagdynamics

Problems

- Heat Conduction and Radiation missing
- non-Newtonian flow for lower temperatures
- Equation of State for free surface flows

Slag mainly described by

- Viscosity
- Thermal Conductivity

To Do

- coupling temperature and viscosity
- modelling solid or liquid behavior of slag

Smoothed Particle Slagdynamics

Modify Energy Equation

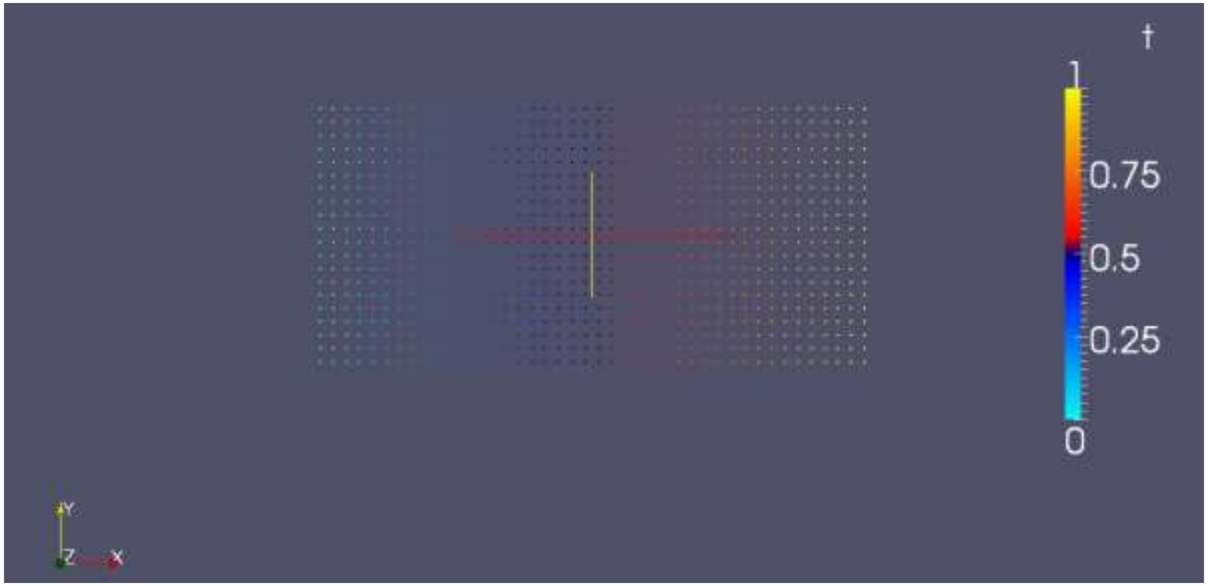
$$\frac{De_i}{Dt} = \frac{1}{2}\sum_{j=1}^{N} m_j \frac{p_i + p_j}{\rho_i \rho_j} v_{ij}^{\beta} \frac{\partial W_{ij}}{\partial x_i^{\beta}} + \frac{\mu_i}{2\rho_i} \epsilon_i^{\alpha\beta} \epsilon_i^{\alpha\beta}$$

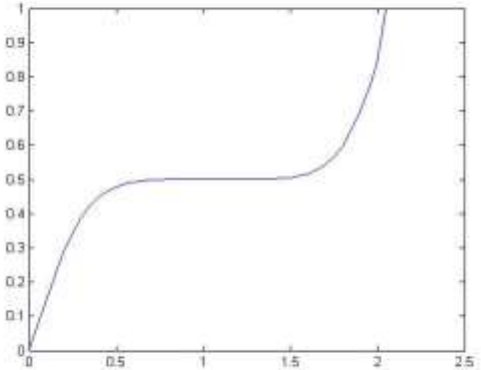
$$\frac{De_i}{Dt} = \frac{1}{2}\sum_{j=1}^{N} m_j \frac{p_i + p_j}{\rho_i \rho_j} v_{ij}^{\beta} \frac{\partial W_{ij}}{\partial x_i^{\beta}} + \frac{\mu_i}{2\rho_i} \epsilon_i^{\alpha\beta} \epsilon_i^{\alpha\beta} + \sum_{j=1}^{N} m_j \frac{\kappa_{ij}}{\rho_i \rho_j} T_{ij} x_{ij}^{\beta} \partial \frac{W_{ij}}{\partial x_i^{\beta}}$$

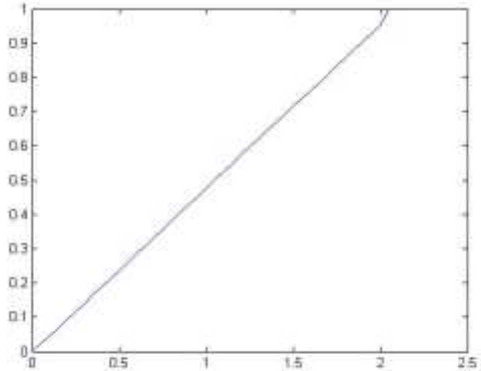
Heat Conduction

Smoothed Particle Slagdynamics

Example: Heat Conduction







Temperatur over length
Top: after 4K Iterations
Bottom: after 400K Iterations

Smoothed Particle Slagdynamics

Modelling of non-Newtonian Flow

- For lower temperatures
- Cross Model implemented
- Parameters needed

$$\rho\upsilon(\dot{\gamma})=\upsilon_{\infty}+\frac{\upsilon_{0}-\upsilon_{\infty}}{(1+(K\dot{\gamma})^{m})}$$

Smoothed Particle Slagdynamics

Critical Viscosity Temperature T_{cv}

- Separates non-newtonian from newtonian fluid behavior
- Determined by composition of deposition

Non-Newtonian Behavior

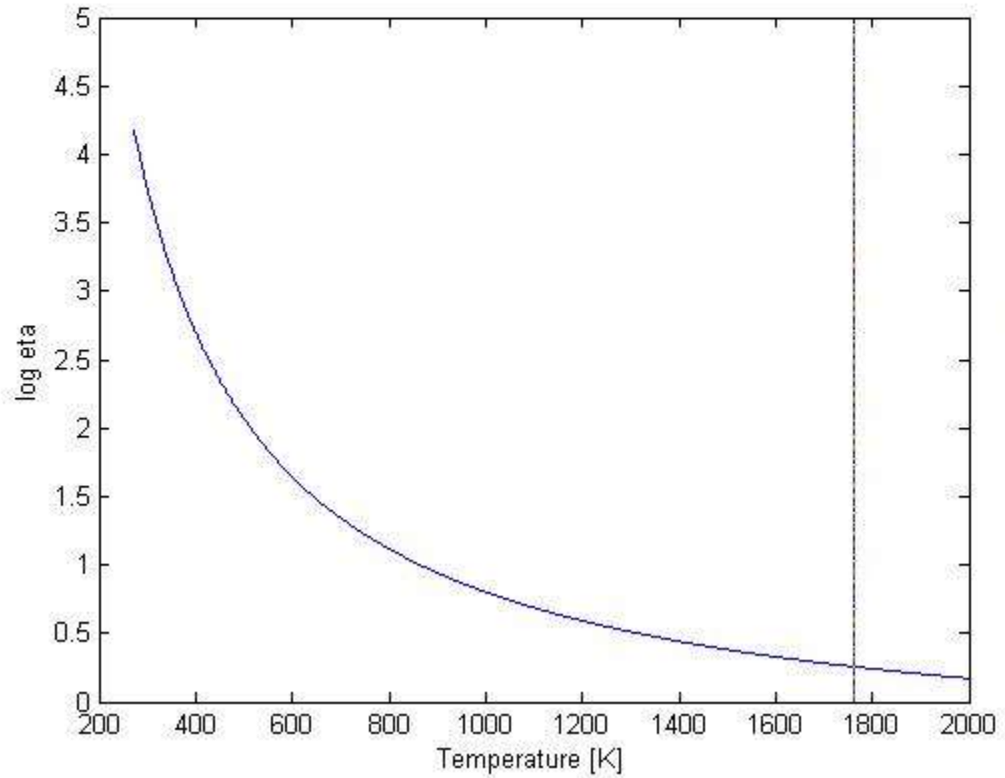
1)
- Modelled with newtonian model
- Determined by volume fraction of solids ⇒ FactSage

2)
- Solid behavior below T_{cv}

Smoothed Particle Slagdynamics

SiO_2	53.37 wt%
Al_2O_3	27.88 wt%
TiO_2	0.65 wt%
Fe_2O_3	5.36 wt%
CaO	6.94 wt%
MgO	1.30 wt%
Na_2O	0.33 wt%
K_2O	2.18 wt%

Critical Viscosity Temperature T_{cv}



- T_{cv} from acid/base-ratio (Seggiani)
- Viscosity from Arrhenius-type equation with silica-ratio (S):

$$\log(\eta) = 4.468\, S^2 + 1.265\left(\frac{10^4}{T}\right) - 7.44$$

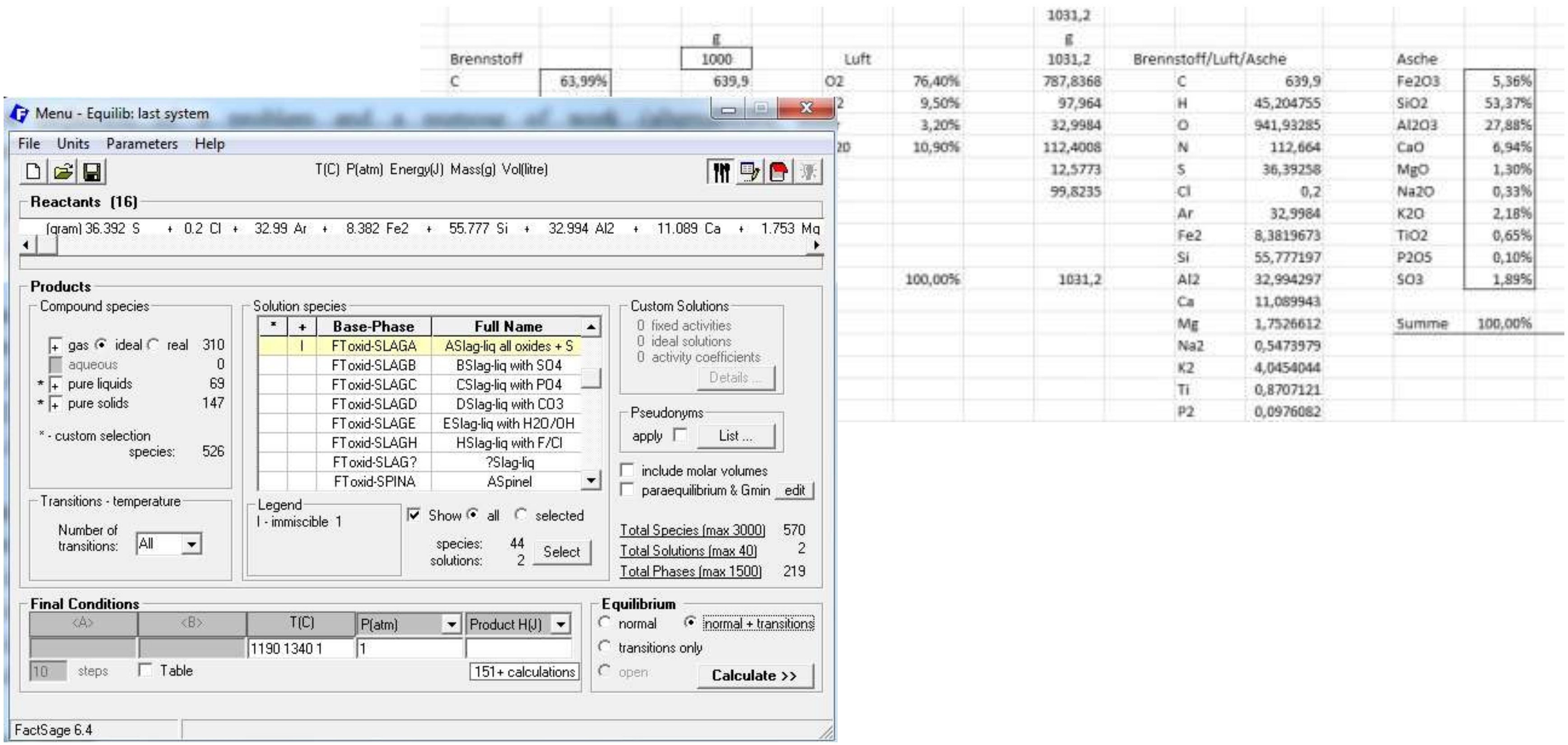
- Colloidal liquids with solids (Kondratiev):

$$\eta_S = eta_L (1 - V_S)^{-2.5}$$

Vs : Volume Fraction of Solids

Smoothed Particle Slagdynamics

Solid Fraction of Slag with FactSage



Smoothed Particle Slagdynamics

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CaO	6.94 wt%
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Na_2O	0.33 wt%
K_2O	2.18 wt%

Density

- With Partial Molar Volumes approach (Mills, Rhine)

$$V=(M_1x_1+M_2x_2+M_3x_3...)/\rho$$

$$V=x_1\bar{V}_1+x_2\bar{V}_2+x_3\bar{V}_3+...$$

$$\rho=\sum_i x_iM_i/x_i\bar{V}_i$$

M:	molecular weight
X:	mole fraction
$\bar{V}$:	partial molar volume

Smoothed Particle Slagdynamics

Heat Capacity and Thermal Conductivity

SiO_2	53.37 wt%
Al_2O_3	27.88 wt%
TiO_2	0.65 wt%
Fe_2O_3	5.36 wt%
CaO	6.94 wt%
MgO	1.30 wt%
Na_2O	0.33 wt%
K_2O	2.18 wt%

- With Partial Molar Heat Capacity approach (Kopp-Neumann)

$$C_p = x_1 \bar{C}_{p1} + x_2 \bar{C}_{p2} + x_3 \bar{C}_{p3} \ldots$$

- Thermal diffusivity $\alpha = 4.5 * 10^{-7} (m^2/s)$ (Mills, Rhine)

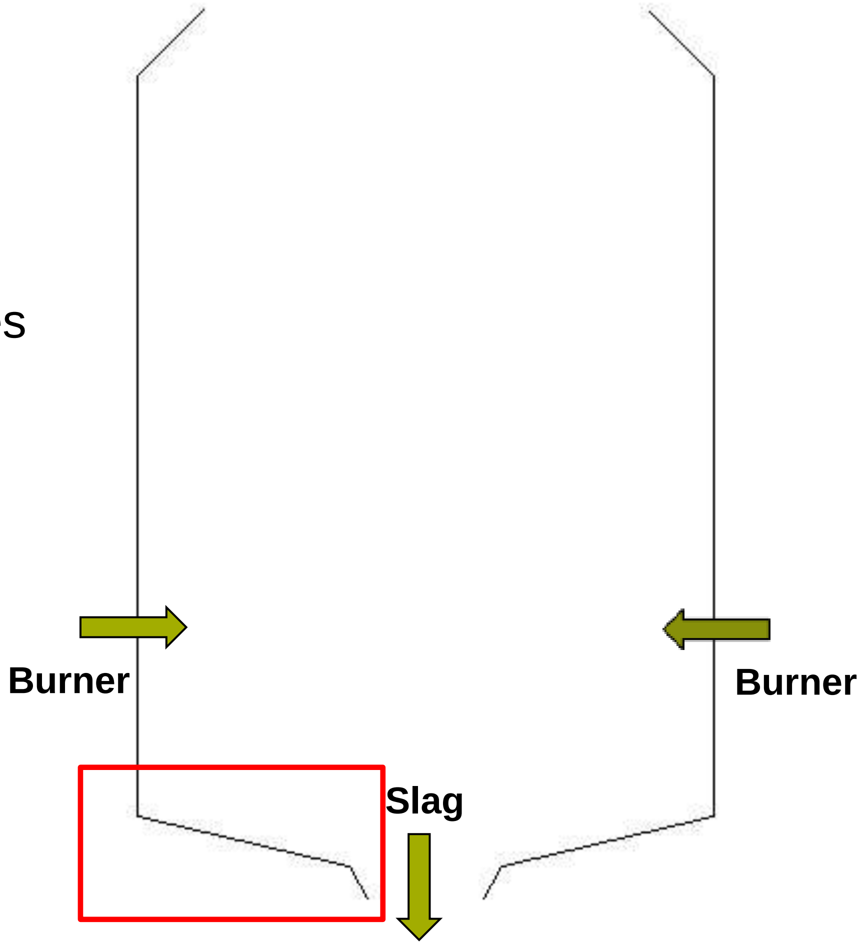
$$\lambda = \alpha C_p \rho$$

C_p: partial molar heat capacity
X: mole fraction

Smoothed Particle Slagdynamics

Performance

- 10 seconds slag simulation = 6.5 d
- # slag particles << # boundary particles
- Search for interacting particles:
  - All-pair search $O(N^2)$
  - Linked-list algorithm $O(N)$
  - Tree search algorithm $O(N \log N)$



Walls of Prenflo coal gasifier

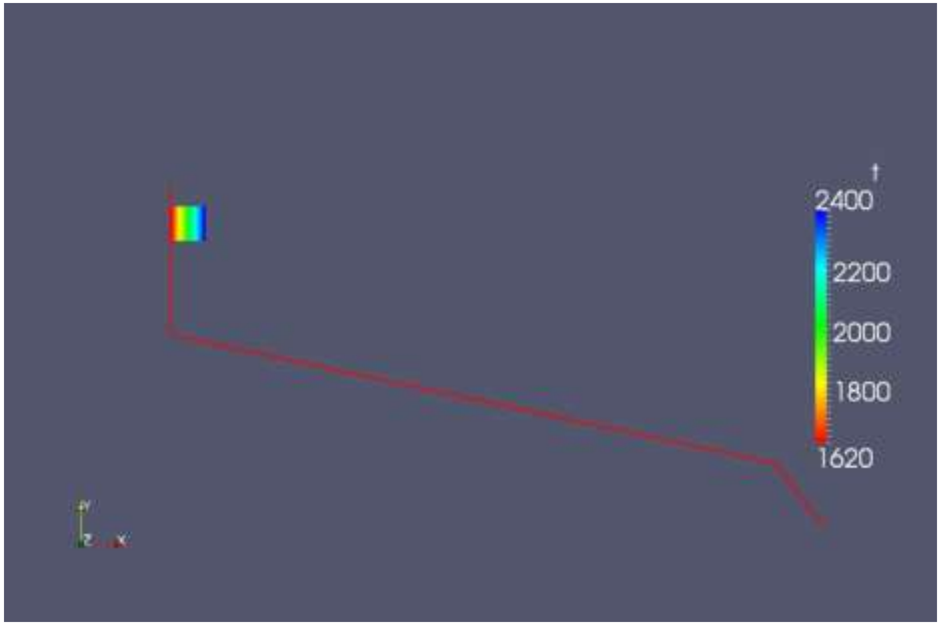
Smoothed Particle Slagdynamics

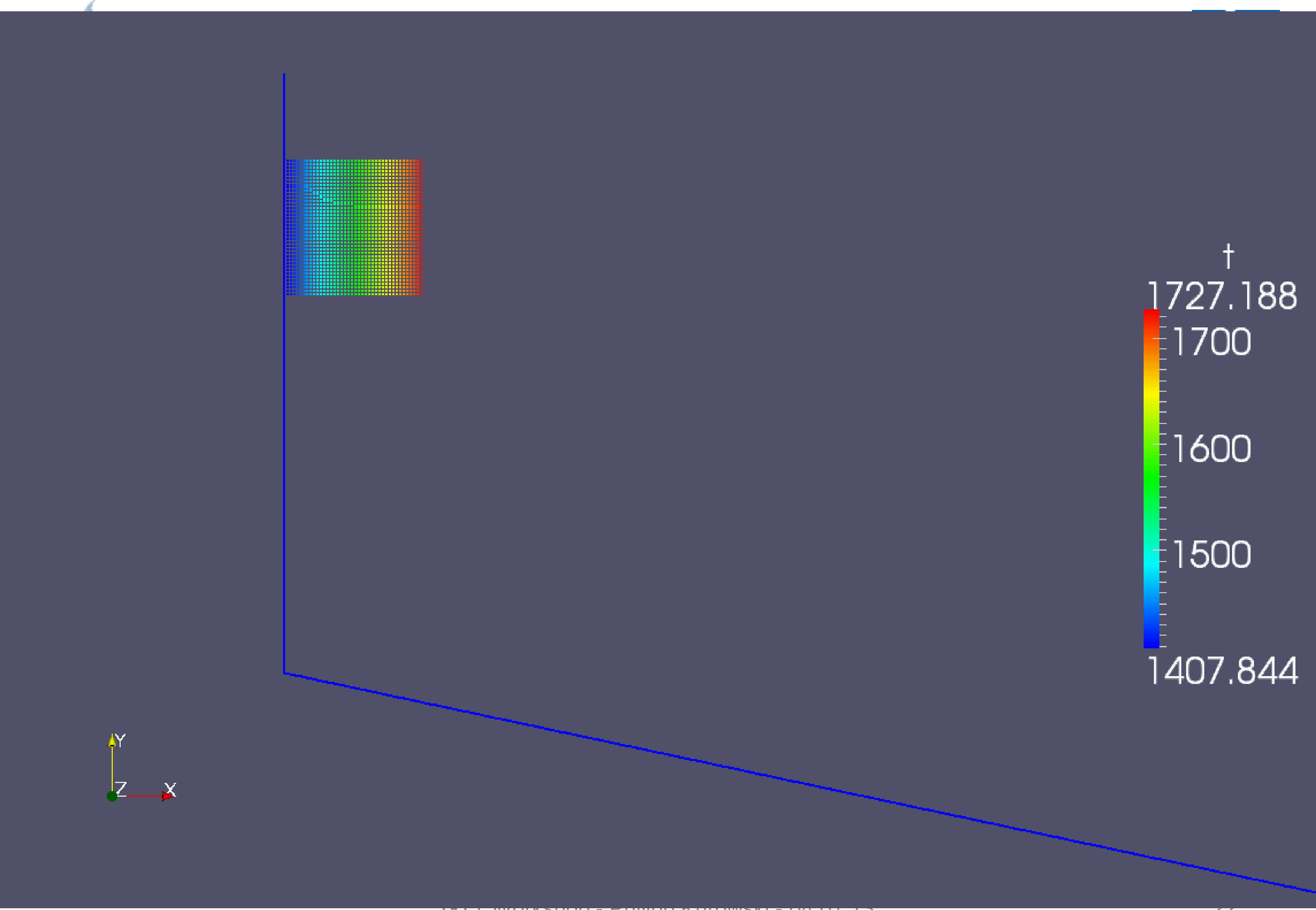
Simulation

- 1 Particle per millimeter
- $T_{wall} = 1200$ K
- $T_{slag} = 1400$ K – 1720 K
- $T_{cv} = 1762.15$ K
- $\varrho = 2759.35$ kg/m^3

- Coal-ash composition:

SiO_2	53.37 wt%
Al_2O_3	27.88 wt%
TiO_2	0.65 wt%
Fe_2O_3	5.36 wt%
CaO	6.94 wt%
MgO	1.30 wt%
Na_2O	0.33 wt%
K_2O	2.18 wt%
P2O5	0.10 wt%
SO3	1.89 wt%




t
1727.188
1700
1600
1500
1407.844
Y
Z
X

Smoothed Particle Slagdynamics

Goals

- Coupling Fluent/Particle-Tracking/SPH
- Implementing Deposition Rate as Starting Condition
- Tool Development for Deposition Predicition depending on Slag Flow

Thank you for your Attention