

# **Slag Modeling based on Coal-Ash Compositions**

**GTT Workshop**

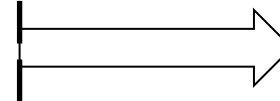
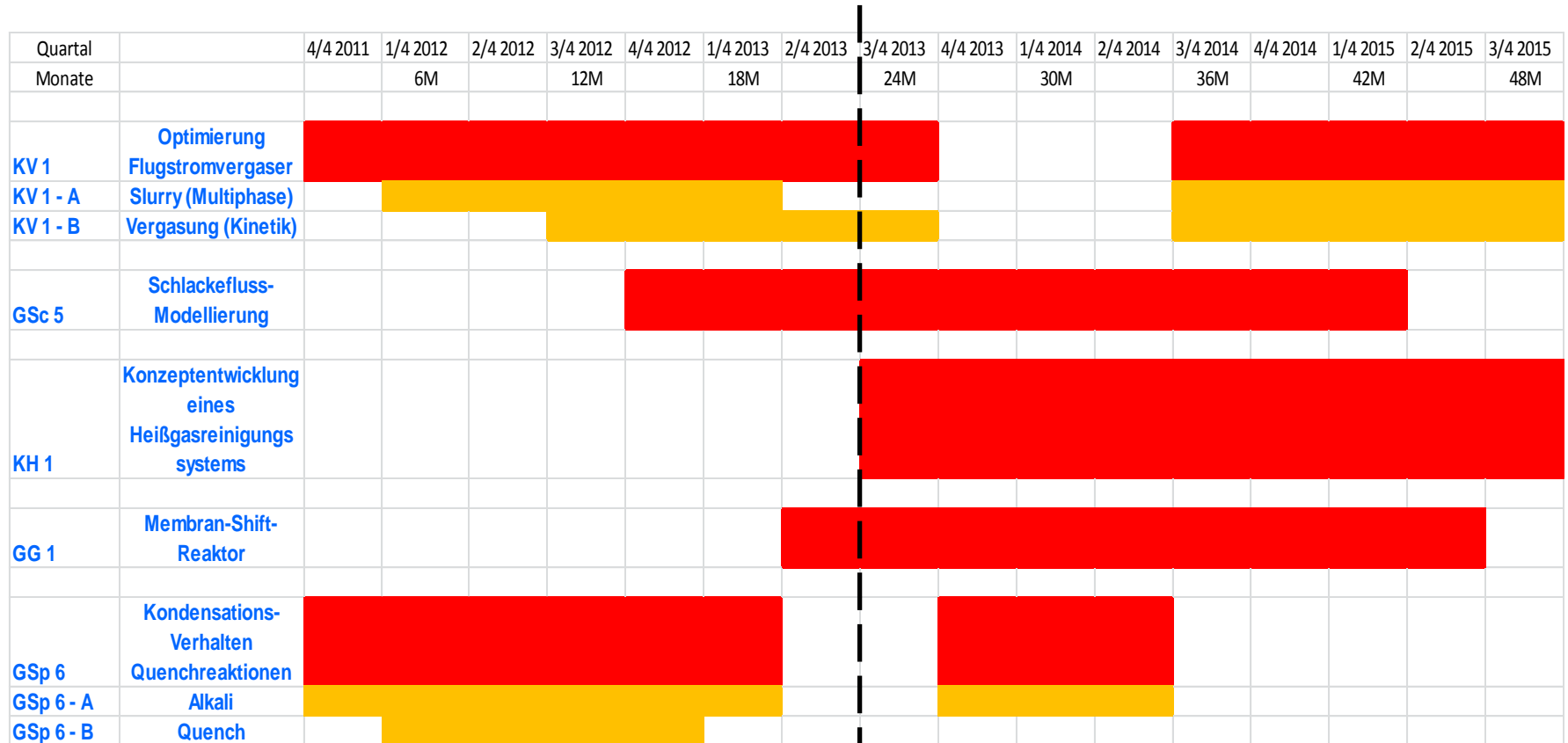
**Philipp Kurowski**

**Institute for Energy Systems  
TU München**

## Inhalt

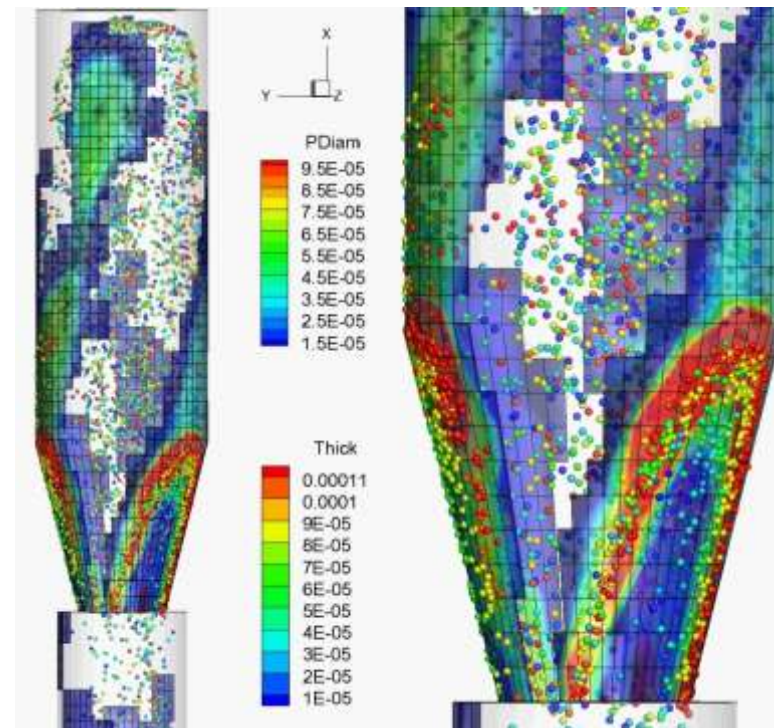
- HotVeGas Project
- P<sup>3</sup> - Particle Post Processor
- Slag Modeling
  - Overview
  - Models
  - Performance

# HotVeGas Project (Computational Fluid Dynamics)



## P<sup>3</sup> - Particle Post Processor

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



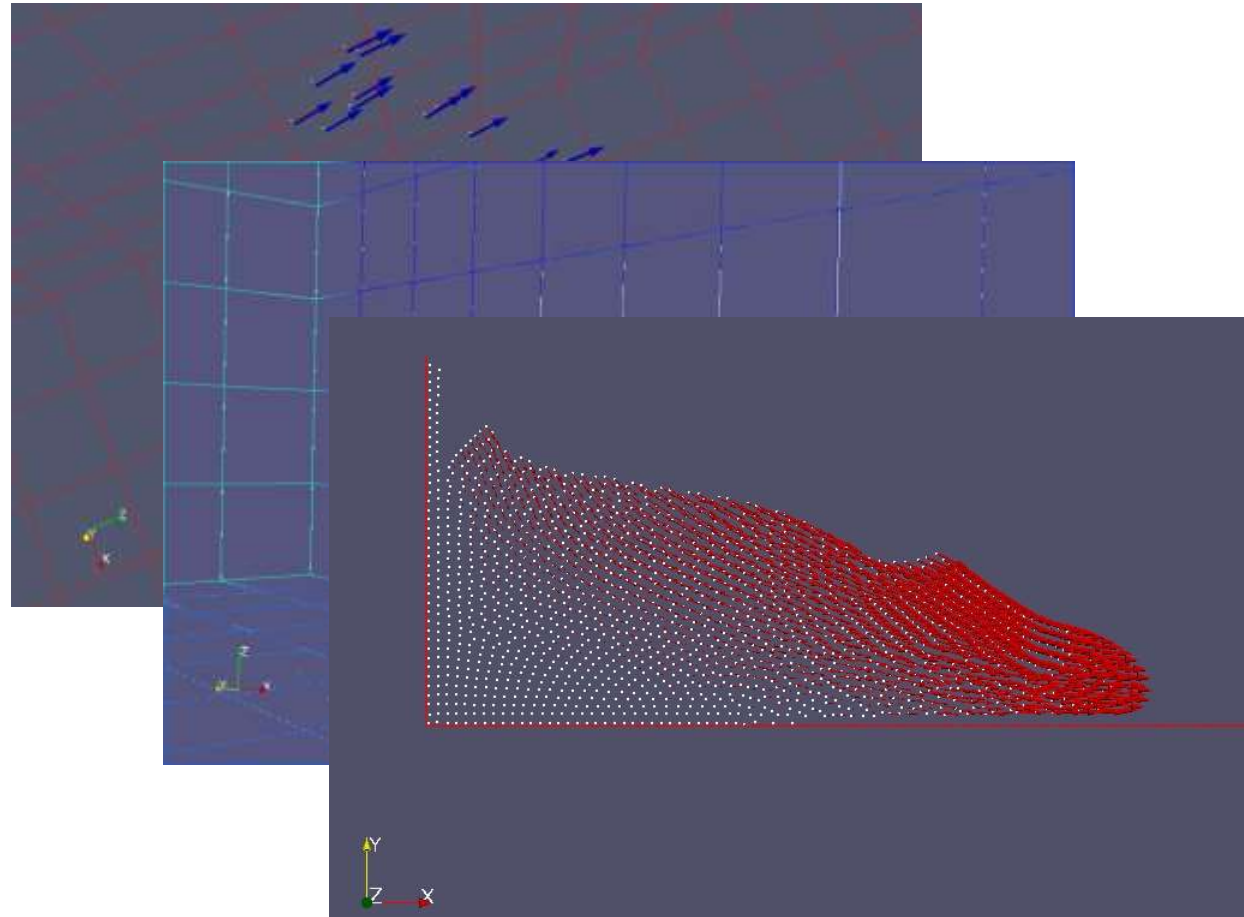
Particle Deposition and Slag Flow in a generic Gasifier

## P<sup>3</sup> - Particle Post Processor

CFD Post-Processing:

Based on Flow Field Simulation:

- 1) Particle Tracking
- 2) Deposition
- 3) Slag Flow



## P<sup>3</sup> - 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

## P<sup>3</sup> - Particle Post Processor

### Grid-based methods

- Eulerian
- Lagrangian
- Hybrid



- Finite Difference
- Finite Element
- Finite Volume

### Meshfree methods

- Lagrangian

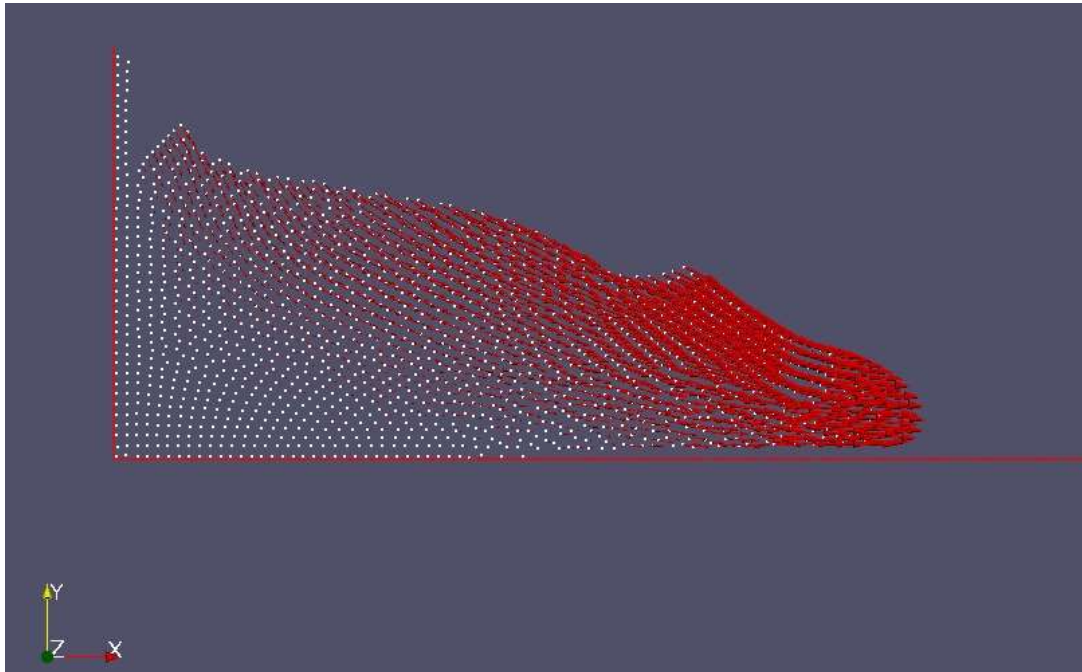


- Molecular Dynamics
- Discrete Element Method
- Smoothed Particle Hydrodynamics

# Smoothed Particle Slagdynamics

## Why SPH?

- Free Surfaces
- Large Deformation and Separation
- No Meshing



Freie Oberfläche

0.0	0.0	0.0	0.0	0.0
0.0	?	?	0.0	0.0
?	1.0	?	?	?
1.0	1.0	1.0	?	?
1.0	1.0	1.0	1.0	1.0

Pugachev – Numerische Berechnung  
Energetischer Systeme

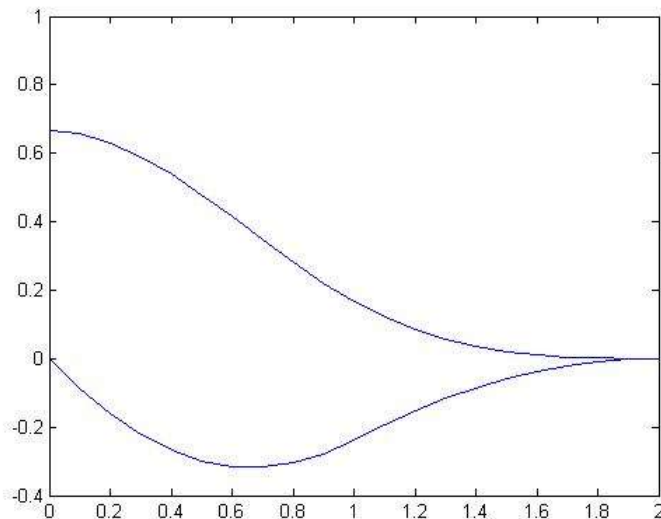
Dam break scenario  
with a viscous fluid in SPH



# Smoothed Particle Slagdynamics

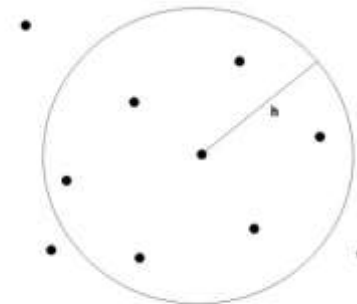
## SPH Basics

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

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

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

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

# 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

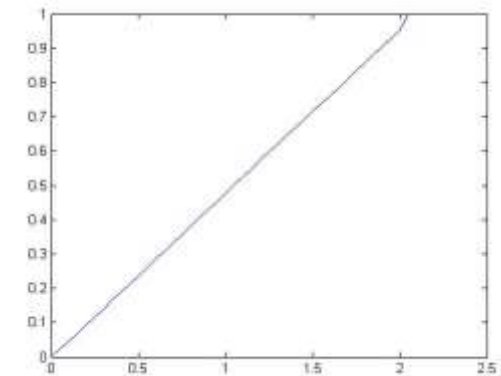
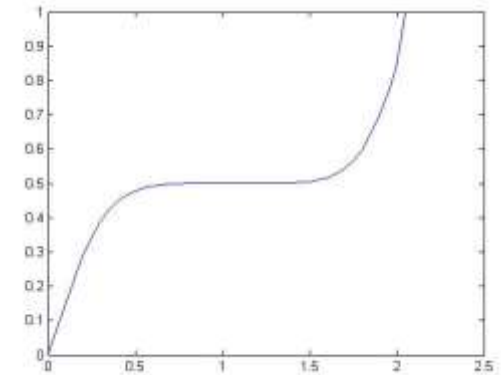
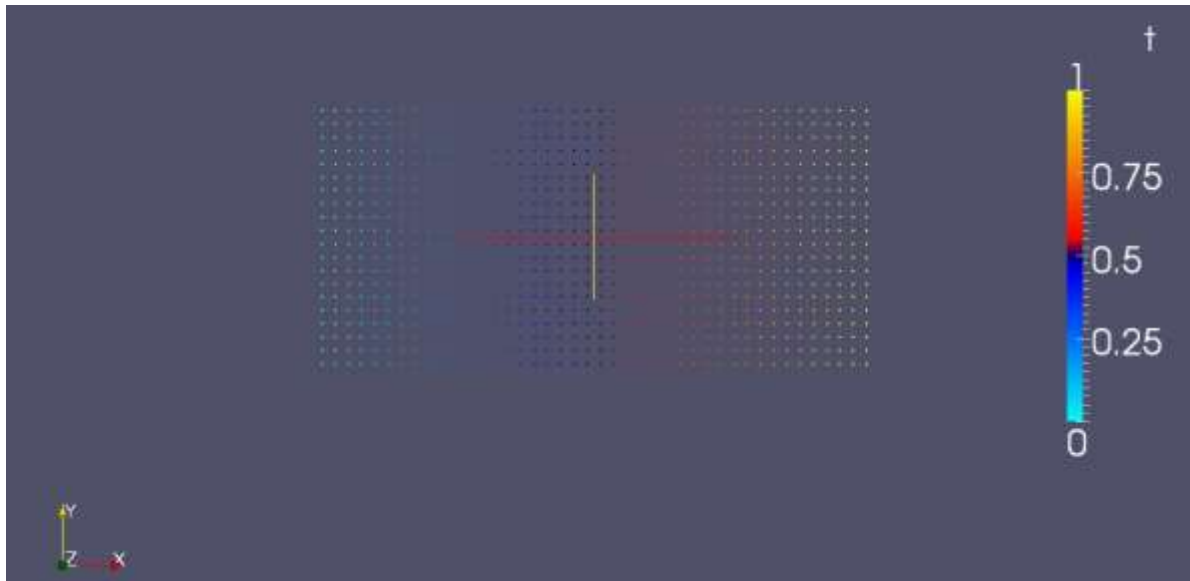
$$\frac{De_i}{Dt} = \frac{1}{2} \sum_{j=1}^N m_j \frac{p_i + p_j}{\rho_i \rho_j} v_{ij}^\beta \frac{\partial W_{ij}}{\partial x_i^\beta} + \frac{\mu_i}{2\rho_i} \epsilon_i^{\alpha\beta} \epsilon_i^{\alpha\beta}$$

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

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

$$\rho v(\dot{\gamma}) = v_{\infty} + \frac{v_0 - v_{\infty}}{(1 + (K \dot{\gamma})^m)}$$


# 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

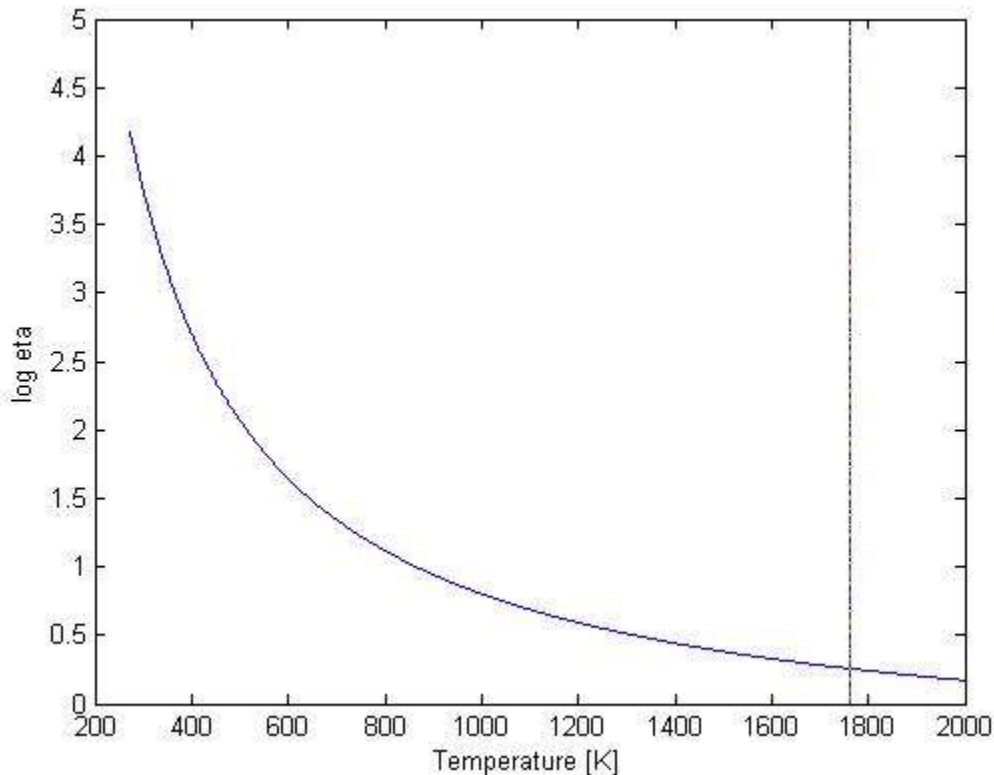
2)

- Solid behavior below  $T_{cv}$

# Smoothed Particle Slagdynamics

SiO <sub>2</sub>	53.37 wt%
Al <sub>2</sub> O <sub>3</sub>	27.88 wt%
TiO <sub>2</sub>	0.65 wt%
Fe <sub>2</sub> O <sub>3</sub>	5.36 wt%
CaO	6.94 wt%
MgO	1.30 wt%
Na <sub>2</sub> O	0.33 wt%
K <sub>2</sub> O	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):

$$\eta_s = \eta_L (1 - V_s)^{-2.5}$$

$V_s$  : Volume Fraction of Solids



# Smoothed Particle Slagdynamics

## Solid Fraction of Slag with FactSage

Brennstoff		Luft		Brennstoff/Luft/Asche		Asche	
C	63,99%	O2	76,40%	C	639,9	Fe2O3	5,36%
			9,50%	H	45,204755	SiO2	53,37%
			3,20%	O	941,93285	Al2O3	27,88%
			10,90%	N	112,664	CaO	6,94%
				S	36,39258	MgO	1,30%
				Cl	0,2	Na2O	0,33%
				Ar	32,9984	K2O	2,18%
				Fe2	8,3819673	TiO2	0,65%
				Si	55,777197	P2O5	0,10%
				Al2	32,994297	SO3	1,89%
				Ca	11,089943		
				Mg	1,7526612	Summe	100,00%
				Na2	0,5473979		
				K2	4,0454044		
				Ti	0,8707121		
				P2	0,0976082		

Menu - Equilib: last system

File Units Parameters Help

T(C) P(atm) Energy(J) Mass(g) Vol(litre)

**Reactants (16)**

(gram) 36.392 S + 0.2 Cl + 32.99 Ar + 8.382 Fe2 + 55.777 Si + 32.994 Al2 + 11.089 Ca + 1.753 Mg

**Products**

Compound species

- gas  ideal  real 310
- aqueous 0
- pure liquids 69
- pure solids 147
- custom selection species: 526

Transitions - temperature

Number of transitions: All

**Solution species**

*	+	Base-Phase	Full Name
<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	FToxid-SLAGA	ASlag-liq all oxides + S
<input type="checkbox"/>	<input type="checkbox"/>	FToxid-SLAGB	BSlag-liq with SO4
<input type="checkbox"/>	<input type="checkbox"/>	FToxid-SLAGC	CSlag-liq with PO4
<input type="checkbox"/>	<input type="checkbox"/>	FToxid-SLAGD	DSlag-liq with CO3
<input type="checkbox"/>	<input type="checkbox"/>	FToxid-SLAGE	ESlag-liq with H2O/OH
<input type="checkbox"/>	<input type="checkbox"/>	FToxid-SLAGH	HSlag-liq with F/Cl
<input type="checkbox"/>	<input type="checkbox"/>	FToxid-SLAG?	?Slag-liq
<input type="checkbox"/>	<input type="checkbox"/>	FToxid-SPINA	ASpinel

Legend

immiscible 1

Show  all  selected

species: 44 Select

solutions: 2

**Custom Solutions**

- fixed activities
- ideal solutions
- activity coefficients

Pseudonyms

apply  List ...

include molar volumes

paraequilibrium & Gmin edit

Total Species (max 3000) 570

Total Solutions (max 40) 2

Total Phases (max 1500) 219

**Final Conditions**

<A> <B> T(C) P(atm) Product H(J)

10 steps Table 151+ calculations

**Equilibrium**

- normal
- normal + transitions
- transitions only
- open

Calculate >>

FactSage 6.4

# Smoothed Particle Slagdynamics

## Density

SiO <sub>2</sub>	53.37 wt%
Al <sub>2</sub> O <sub>3</sub>	27.88 wt%
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K <sub>2</sub> O	2.18 wt%

- With Partial Molar Volumes approach (Mills, Rhine)

$$V = (M_1 x_1 + M_2 x_2 + M_3 x_3 \dots) / \rho$$

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

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

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

# Smoothed Particle Slagdynamics

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## Heat Capacity and Thermal Conductivity

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

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

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

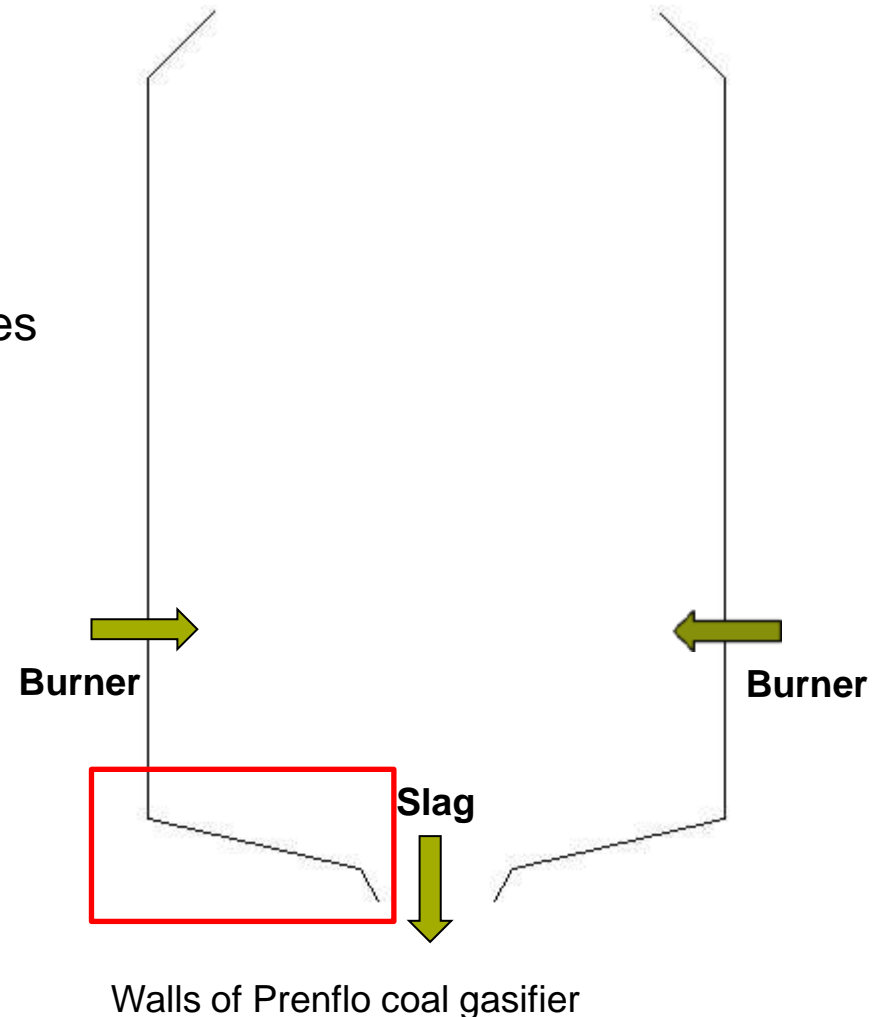
$$\lambda = \alpha C_p \rho$$

C<sub>p</sub>: partial molar heat capacity  
X: mole fraction

# Smoothed Particle Slagdynamics

## Performance

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



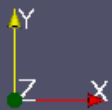
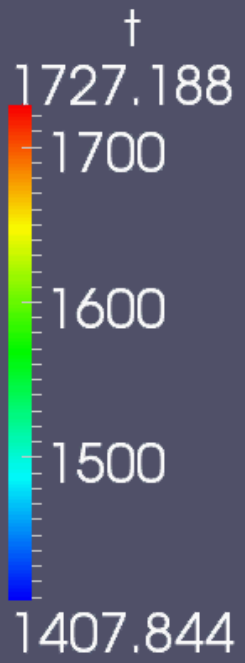
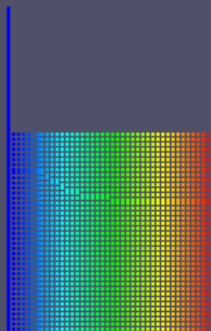
# Smoothed Particle Slagdynamics

## Simulation

- 1 Particle per millimeter
- $T_{\text{wall}} = 1200 \text{ K}$
- $T_{\text{slag}} = 1400 \text{ K} - 1720 \text{ K}$
- $T_{\text{cv}} = 1762.15 \text{ K}$
- $\rho = 2759.35 \text{ kg/m}^3$
- Coal-ash composition:

SiO <sub>2</sub>	53.37 wt%
Al <sub>2</sub> O <sub>3</sub>	27.88 wt%
TiO <sub>2</sub>	0.65 wt%
Fe <sub>2</sub> O <sub>3</sub>	5.36 wt%
CaO	6.94 wt%
MgO	1.30 wt%
Na <sub>2</sub> O	0.33 wt%
K <sub>2</sub> O	2.18 wt%
P <sub>2</sub> O <sub>5</sub>	0.10 wt%
SO <sub>3</sub>	1.89 wt%





# Smoothed Particle Slagdynamics

## Goals

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

Thank you for your Attention