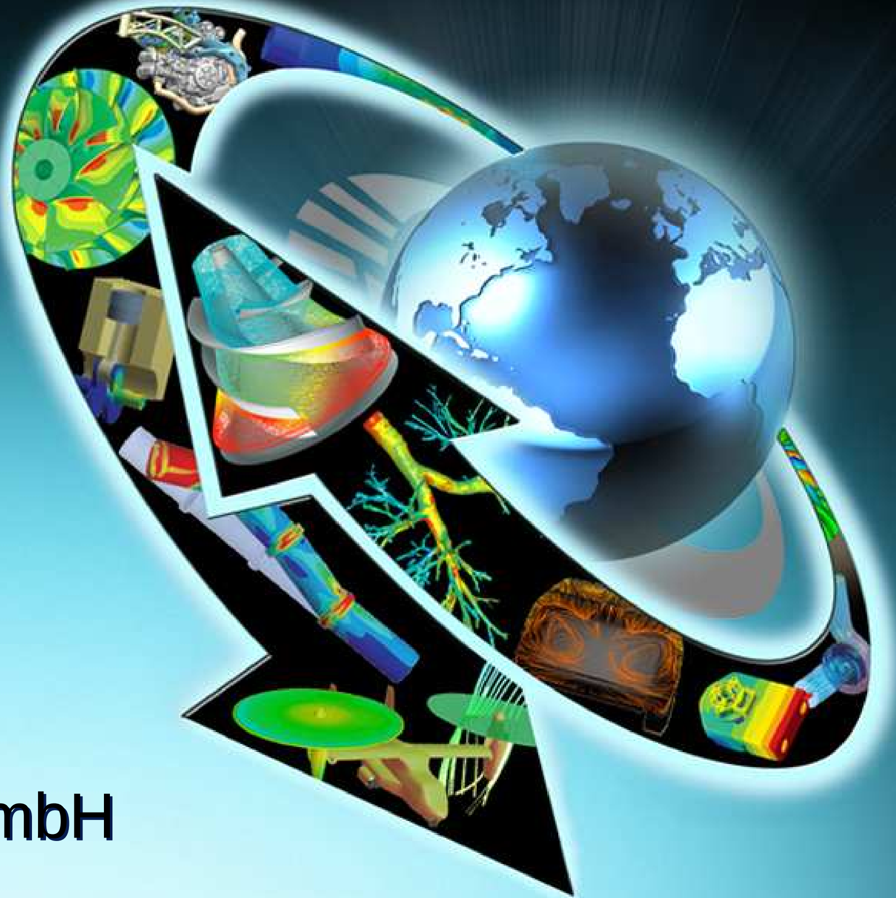
Coupling of Thermodynamic Equilibrium Libraries with a Multidimensional CFD Solver - Application and Potential -



Dr. Stefan Martens
Stefan Kleditzsch
Dr. Markus Braun
ANSYS Fluent Deutschland GmbH

Overview

- Motivation
- Efficient Coupling of CFD-Tools
- Biomass Boiler Simulation
    - Ash Deposition Modeling
    - Implementation into FLUENT
- Summary
- Potential Applications

Motivation

- Process simulation with
  - relevant local thermo-chemical effects
  - relevant convective transport due to hydrodynamics
  - use: **CFD-Tools (like FLUENT)**
- Chemical kinetic of species
  - quite often not known sufficiently
  - but partial equilibrium can be assumed
  - use: **Equilibrium Solvers (like ChemApp)**
- Key to connect both
  - **Efficiency**
    of equilibrium calculations in each CFD grid cell

Key Technology for Efficiency

- In-Situ Adaptive Tabulation of equilibrium calculation results using ISAT (St. Pope)

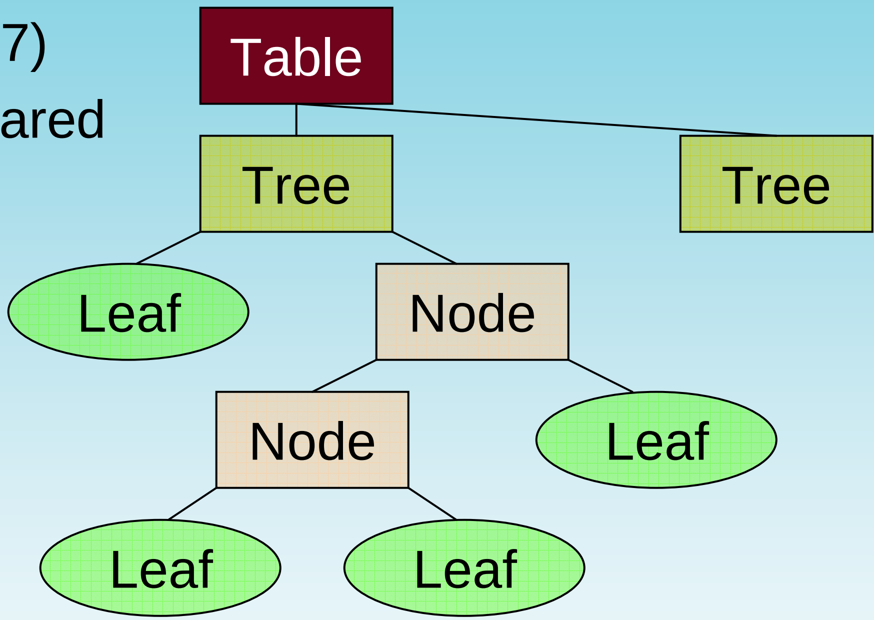
- Possible speedup for complex systems:
  factor 10 – 100

- Tabulated function f:

  mass of phase constituents = f(mass of elements)
  (ChemApp) (FLUENT)

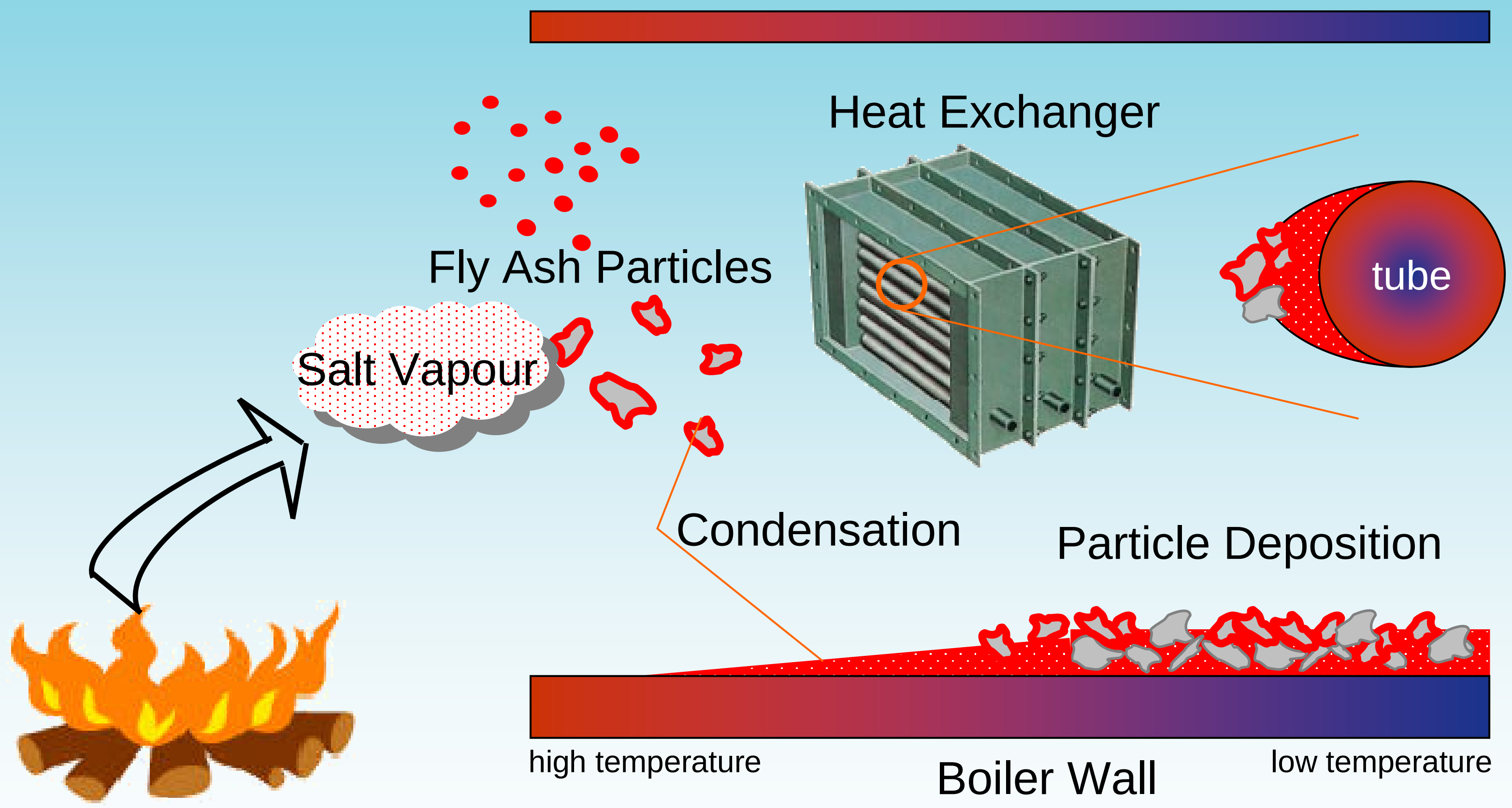
ISAT: Tree Structure

- developed by S.Pope (1997)
- searching a tree fast compared to function evaluation
- currently using version 5



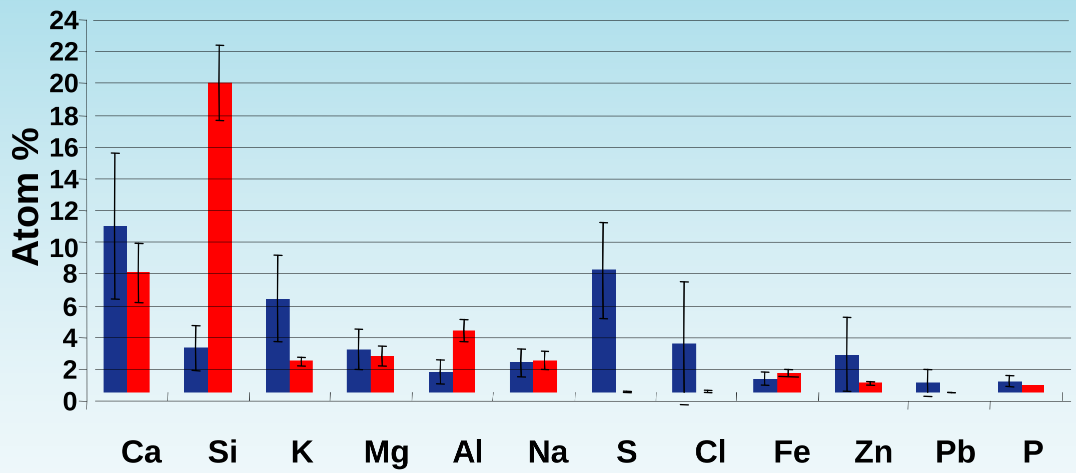
Node	=	two half rooms separated with plane (x,p)
Leaf	=	stores the coordinate (x), function (f) and first derivative (g = df/dx)

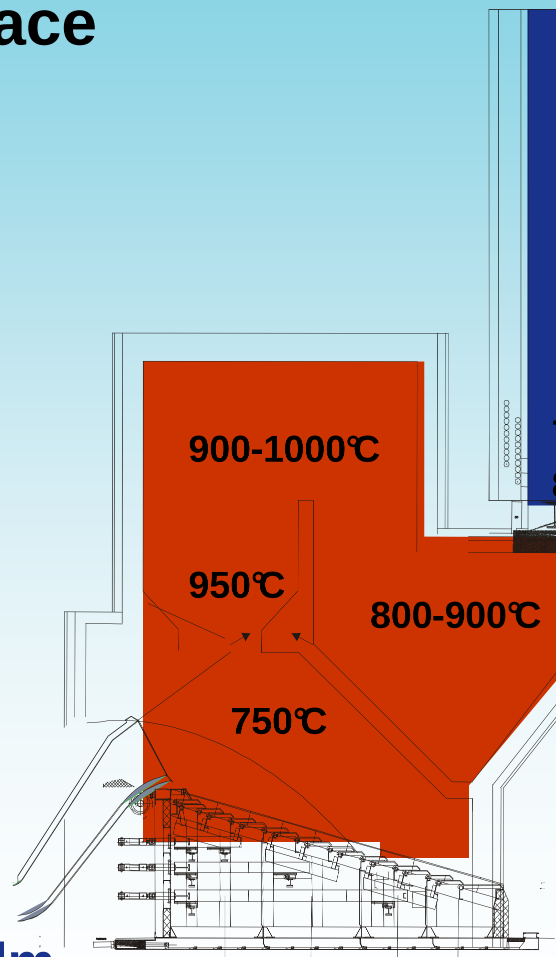
Deposition in Biomass Furnaces



Ash Deposit Chemistry

Comparison of deposits in the furnace and in the boiler section





Furnace => deposition of silicate particles

Boiler => condensation of salt vapour and sticking of particles on the liquid salt film

Source: Jonas Dahl (BIOS Graz)

Ash Deposit Chemistry

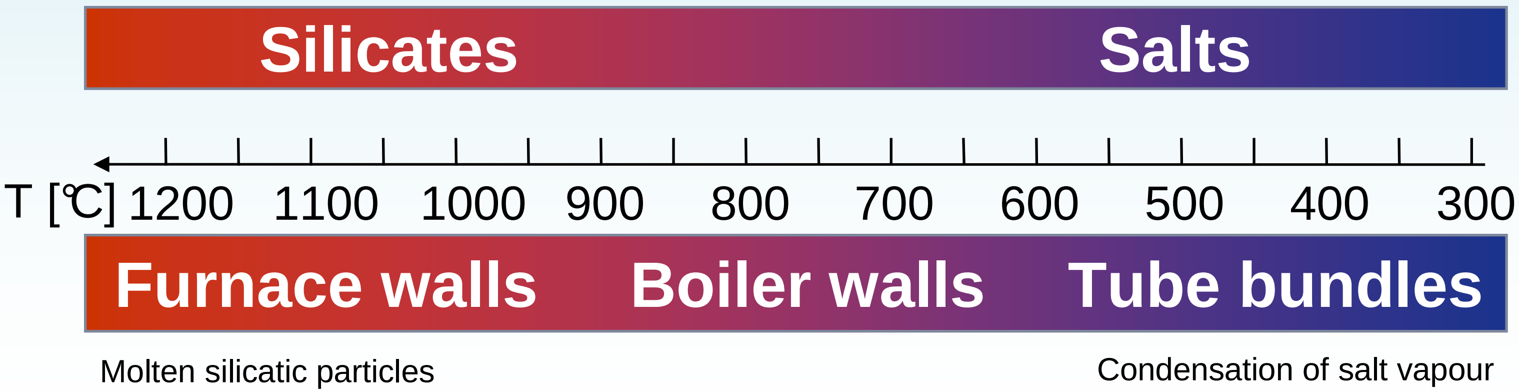
ANSYS

Volatile components (Salts)

- K_2SO_4, K_2CO_3, KCl, Na_2SO_4, Na_2CO_3, NaCl, $CaSO_4$, $CaCO_3$,
- additional: $ZnSO_4$, $ZnCl_2$, $PbSO_4$, $PbCl_2$, $CaCl_2$

Particle only components (Silicates)

- SiO_2, CaO, MgO, Al_2O_3, Na_2O, K_2O, ZnO, P_2O_5



Ash Vapour Transport Modeling

- Many salt anion/cation combinations possible
- Do not participate in combustion processes nor affect fluid flow.

  ➔ Gaseous transport of ash vapour elements

- Evaluating of local multiphase equilibrium (ChemApp) to compute constituents of phases
  - gaseous, solid and/or liquid
- Simulation predicts:
  - gas condensation rates in each finite volume cell that has a wall

Ash Vapour Deposition (Condensation)

- Wall condensation mass flux [mol/m²s]

$$\dot{N}_{cond} = \beta \cdot \left(c_{\infty} - c_{w} \right)$$

- β ... mass transfer coefficient [m/s] from convective heat transfer coefficient (Lewis analogy)
- c_{∞} ... species free gas concentration [mol/m³]
- c_{w} ... species saturation concentration at the wall [mol/m³]

Computed with local equilibrium (ChemApp)

Equili. calc. necessary for each wall face and each neighboured fluid cell.
For particle condensation this is necessary even in each fluid cell.

Ash Particle Transport Modeling

- Lagrange approach for particle transport
- sticking probability of a particle on a surface:

$$P_{stick} = P_p + P_s - P_p P_s - k_c (1 - P_p)(1 - P_s)$$

Erosion by non-sticky particles

P_s = Ash Stickiness of Surface

P_p = Ash Stickiness of Particle

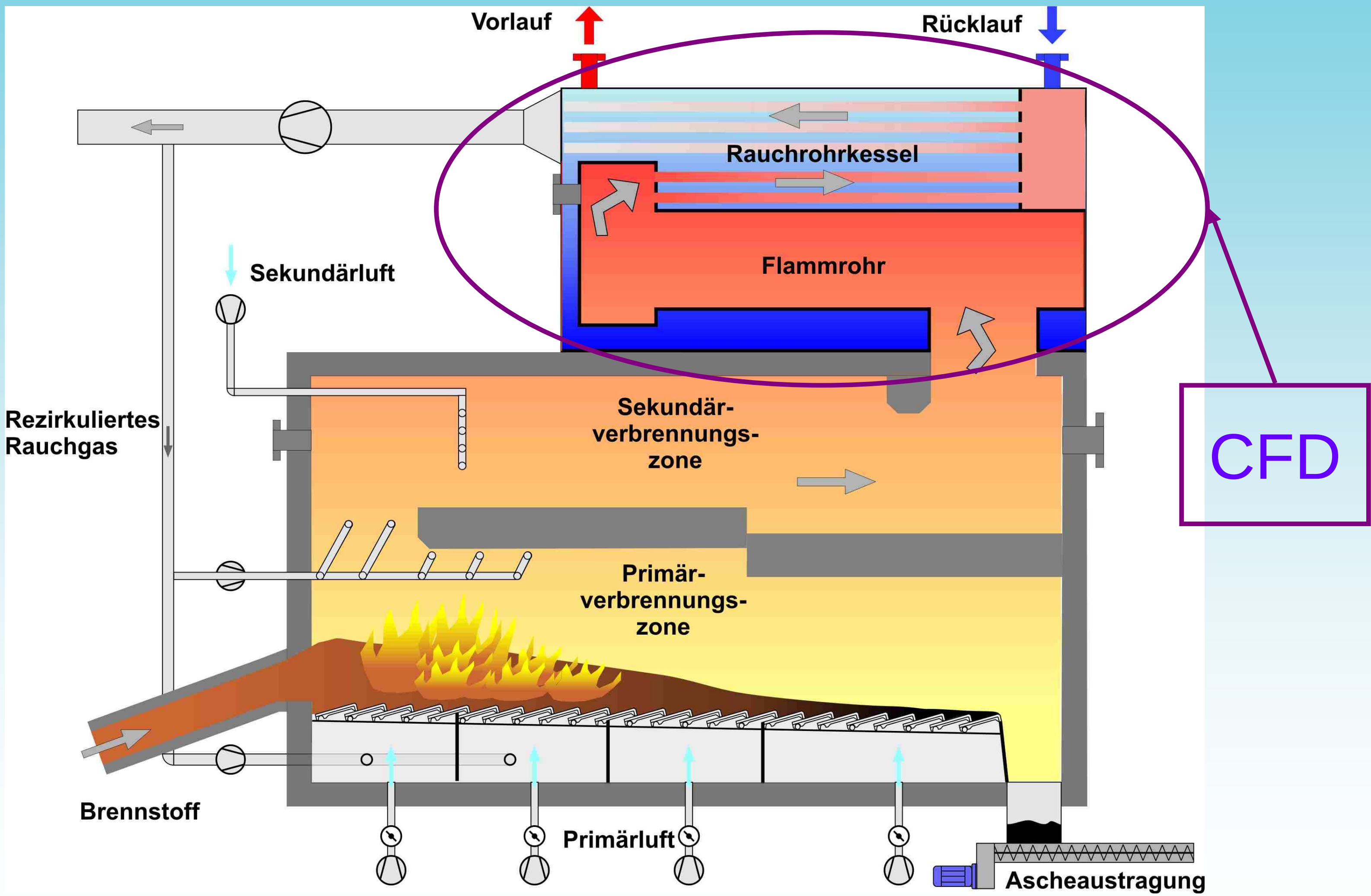
Ash Stickiness

- Salts:
  - P_{Salt} = function of molten phase amount (10%-70%)
    - P = 1 (> 70%) calculated from multiphase chemical equilibrium (ChemApp)
- Silicates:
  - Urbain model (1981): $P_{Sili} = \min(1, \eta_{ref} / \eta)$
    - viscosity depending on composition
    - reference viscosity estimated from particle kinetic energy

Volume averaged stickiness for salt/silicate mixtures:

$$P = \frac{V_{Sili}P_{Sili} + V_{Salt}P_{Salt}}{V_{Sili} + V_{Salt}}$$

Boiler Simulation (400kW$_{thermal}$)

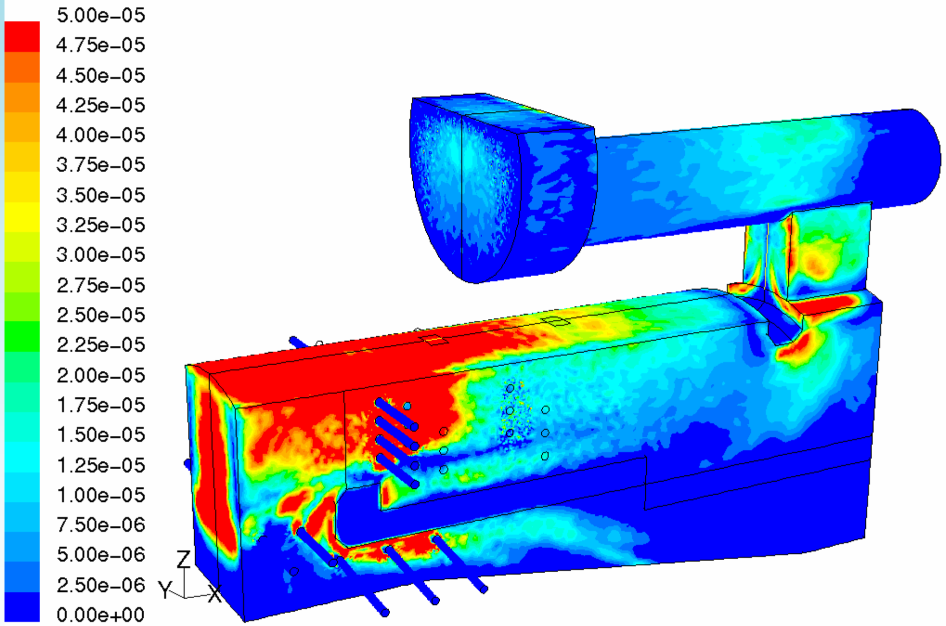


Source: R. Scharler (BIOS Graz)

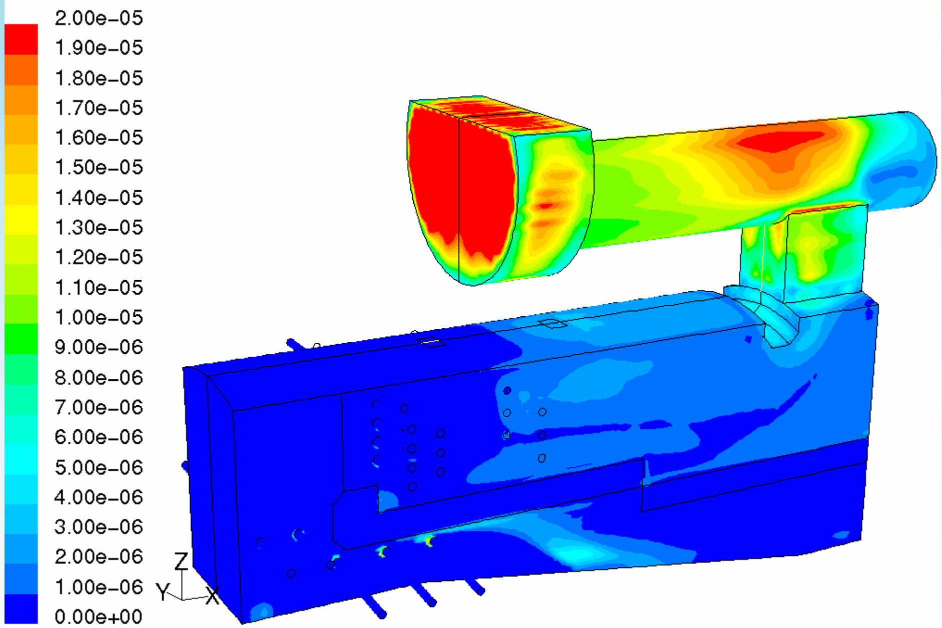
Ash Deposition Simulation

Deposition Mass Flux [kg/m^{2}s]

Ash Particle Deposition (Silicates)



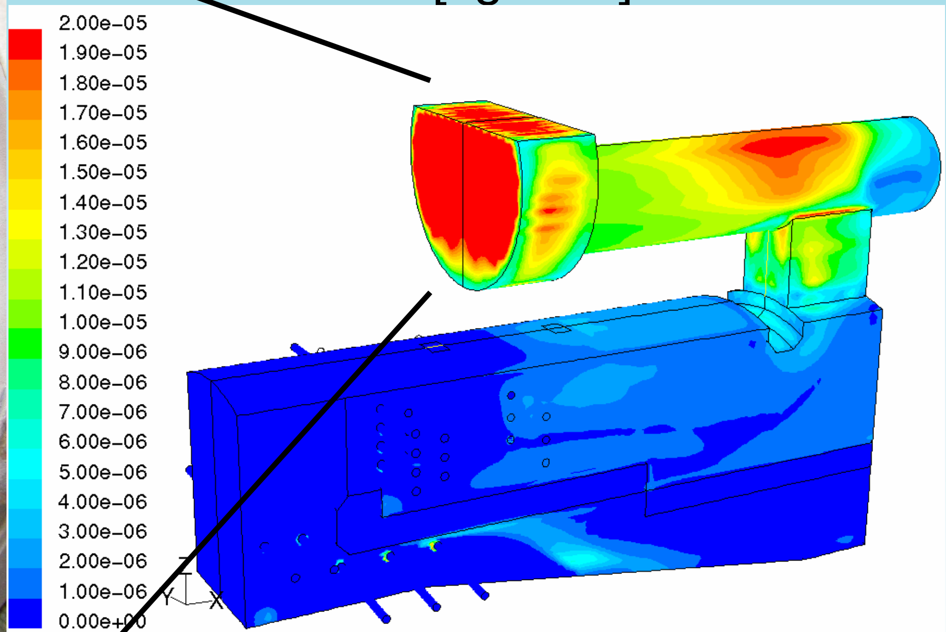
Vapour Condensation (Salts)



Source: R. Scharler (BIOS Graz)

Ash Deposition Simulation

Vapor Condensation Mass Flux
[kg/m2s]



Source: R. Scharler (BIOS Graz)

Summary

- We heavily use local equilibrium calculations to reduce the number of transported species during the deposition of fly ash in biomass furnaces
- We consider the influence of salt and silicate components to the particle wall interaction
- Reduction of calculation time using ISAT, enables highly sophisticated chemical equilibrium calculations within a CFD environment

➔ Bringing science to engineering business

Potential Applications

Tabulation technology enables
all CFD simulations using

- equilibrium calculations
- or any complex function evaluation
  in each CFD grid cell.

Examples:

- Segregation of molten metal phases (steel industry)
- Local material property lookup (glass industry)
- ...