CFD simulation of chloride-containing flue dust in waste incinerators by coupling ChemApp and CFX

Comparison of calculation and measurements

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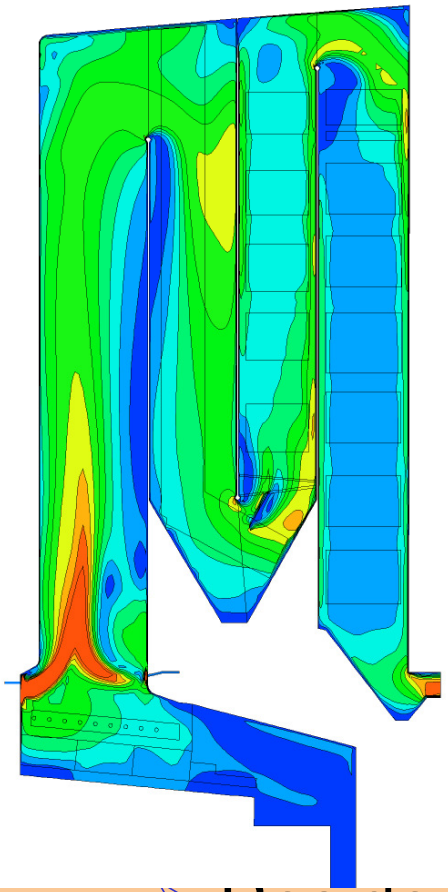
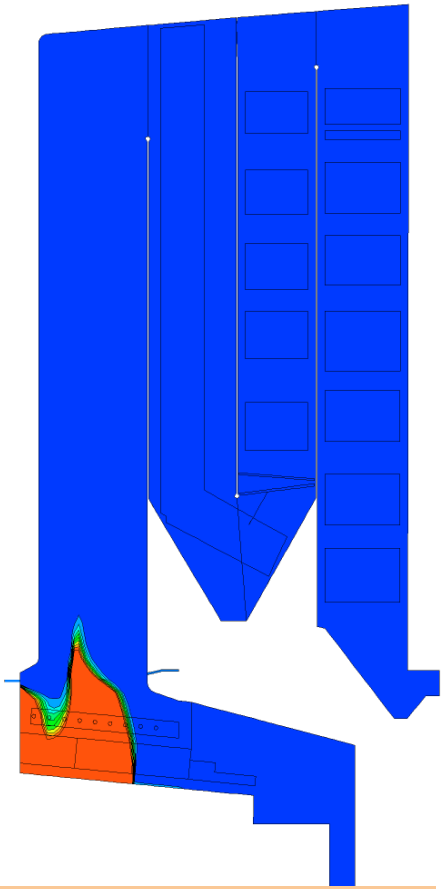
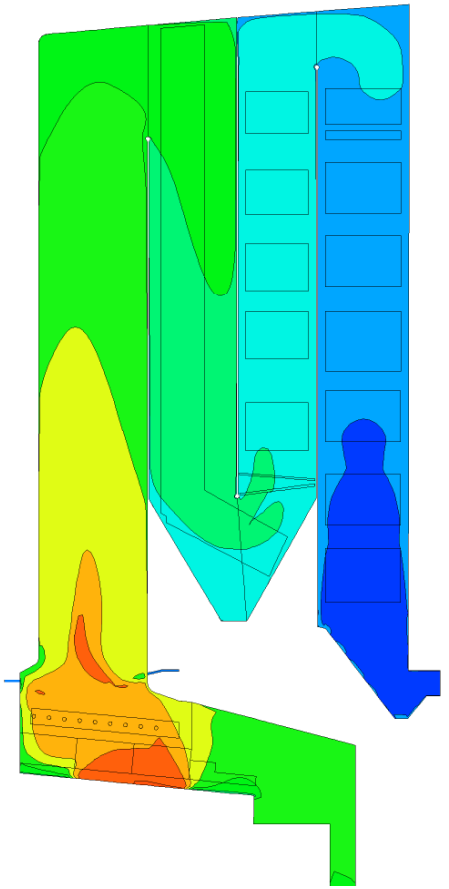
- Introduction
- Methods
- Results of calculation
- Results of measurements
- Comparison
- Summary



Fluid Dynamics)





- Reside

gks weghaus GmbH

Introduction

Combustion

- Combustion models
  - e.g. LUAT-Essen, LEAT-Bochum, Umsicht-Oberhausen, GKS/Cutec Schweinfurt)
- Majority-species
  - C_xH_y, CO, CO_2, H_2O, N_2, N_2, O_2, SO_2, HCl

Introduction

Corrosion

- Minority-species
  - Alkali- / alkalineearth- / heavy metals
- Variety of possible compounds
- Limited knowledge of „Product forming models“
- Lacking of material data
- Complicate validation

Methods

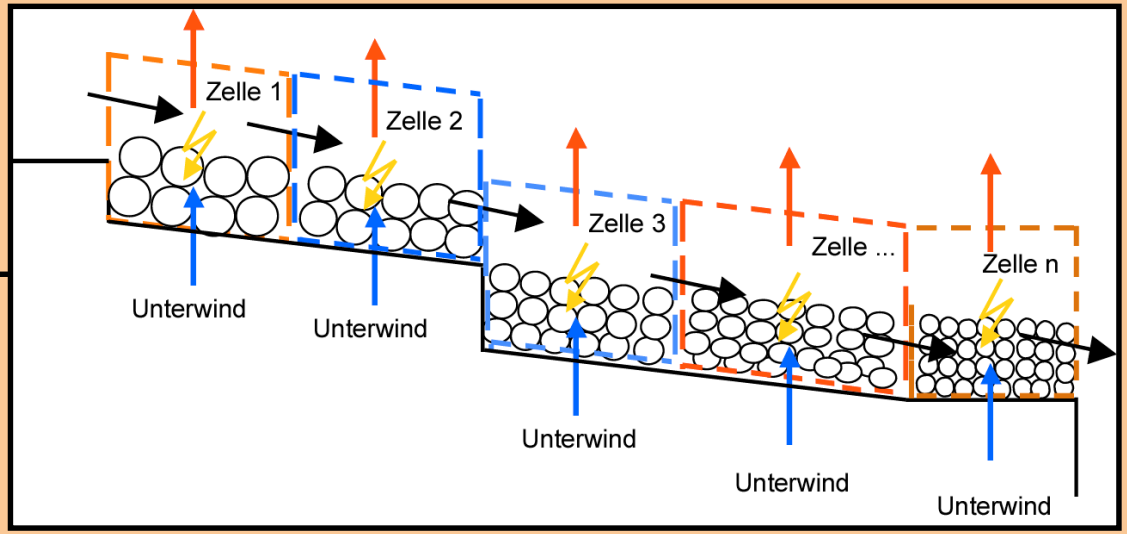
Ansys-CFX

- One of the 3 great CFD-Codes
- Robust solver
- Good performance (parallel , multigrid-solver)
- Good models for radiation and combustion
- Comprehensive wall-functions

Methods

CFD-Simulation

- Grate model
- Species
- Combustion
- Heat exchange
- Further sources / sinks
  - Secondary air, SNCR ...



Methods

Validation

- Continous validation with implemented plants

CFD-Studies of waste incinerations

- Brüssel
- Gamsen
- Horgen
- Ningbo
- Lippendorf
- Schweinfurt
- Würzburg
- Kirklees
- Isle of Man
- Neapel/Calabrien
- Palermo/Casteltermini
- Moerdijk
- Halmstadt
- Södertälje
- Joenkoeping
- ...

Methods

FactSage / ChemApp

- Unification of FACT-Win and ChemSage in 2001
- One of the largest databases for chemical thermodynamics in the world

Methods

ChemApp

- Libraries for intergration into own programs
- Communication over standarised interfaces
- High calculation speed

Methods

Coupling ChemApp to CFX

- Additional transported species / elements
  - Al, Br, Ca, Cl, Cr, Cu, Fe, K, Mg, Mn, Na, Ni, P, Pb, S, Si, Ti, V, Zn
- Implementation of 300 additional variables
  - For storing the results of ChemApp-calculation

Methods

Wall treatment

- Radiation and convection
  - Complete wall structure with fouling, refractory, piping
- No usable mechanism for aerosol-deposition
  - Not implemented
- Depositon in the boiler < 2% of total aerosol
  - Acceptable failure

Methods

Calculation time

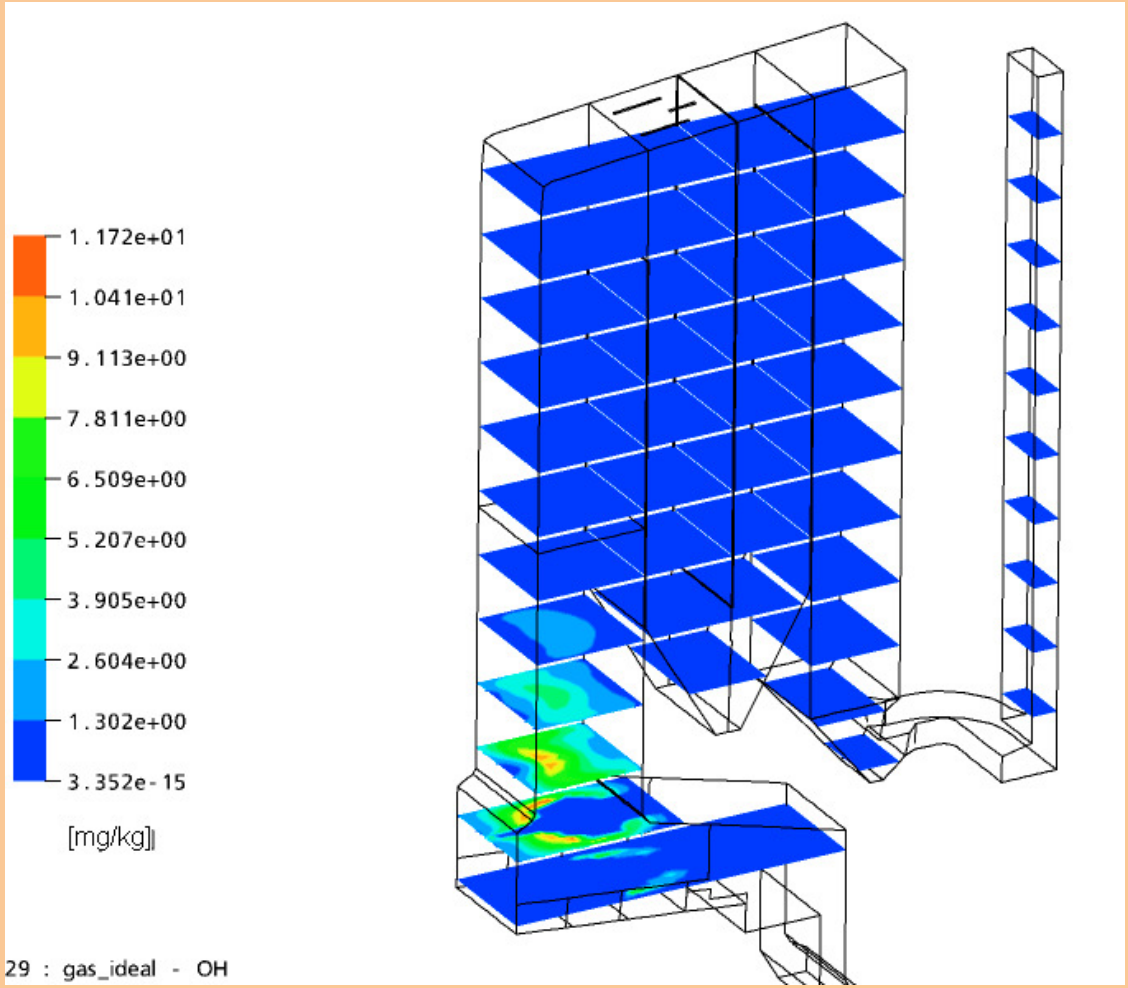
- Net size ca, 1.000.000 cells
- 1 equilibrium calculation ca. 3 -10 s
  - Separate coupled nets for CFD and ChemApp calculation
- Total computation time 4 - 5 days

Methods

Relevant Species

- 1473 possible species
- Reducing for meaningful species
  - Massfraction
  - Temperature range
  - Not meaningfull (e.g. hydride)
  - Not probable (e.g. intermetallic)

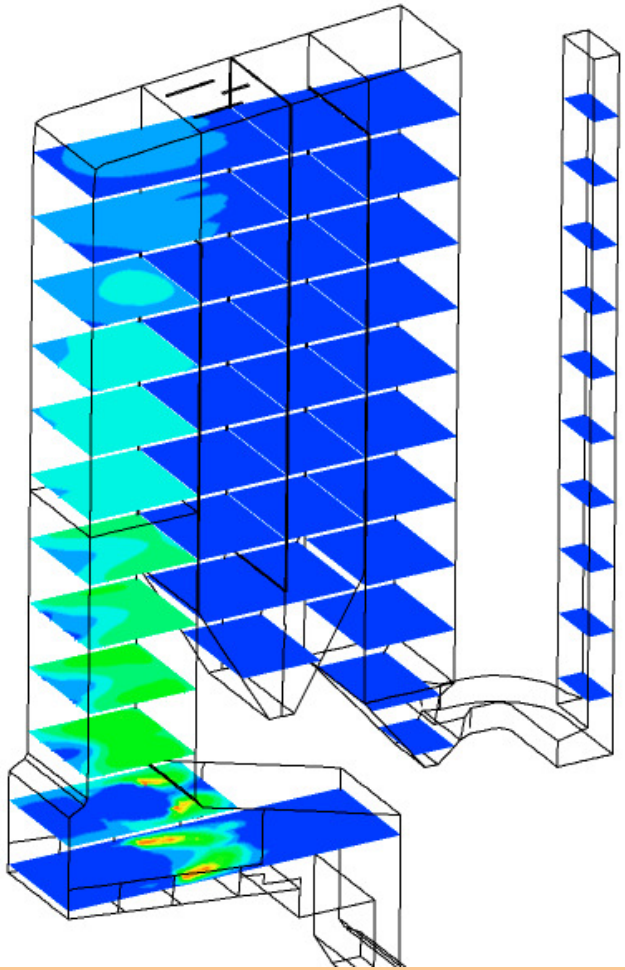
Results



OH-Radicals

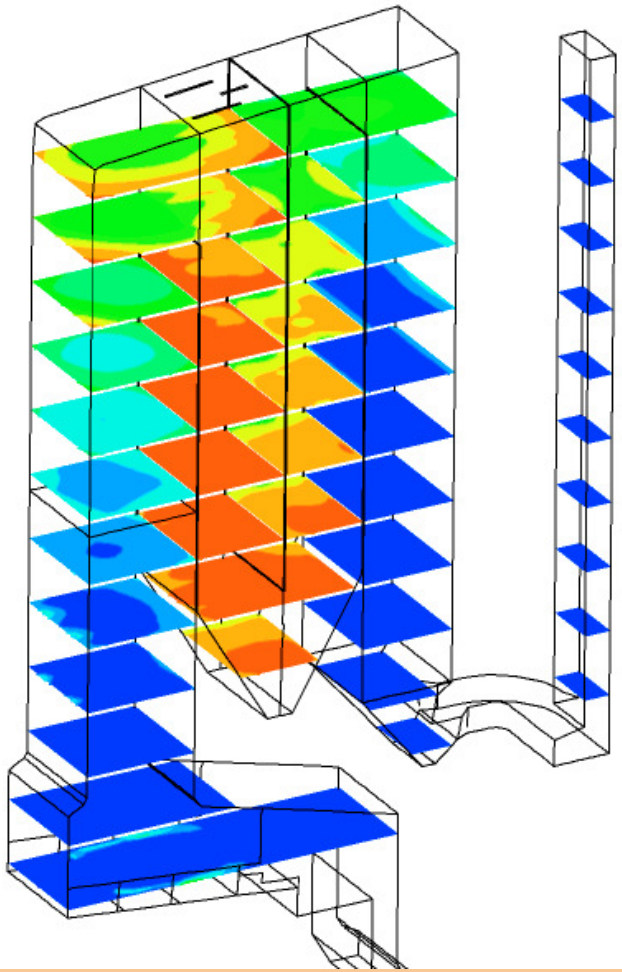
- Important reaction partner for combustion
- Stable at high temperature

Results

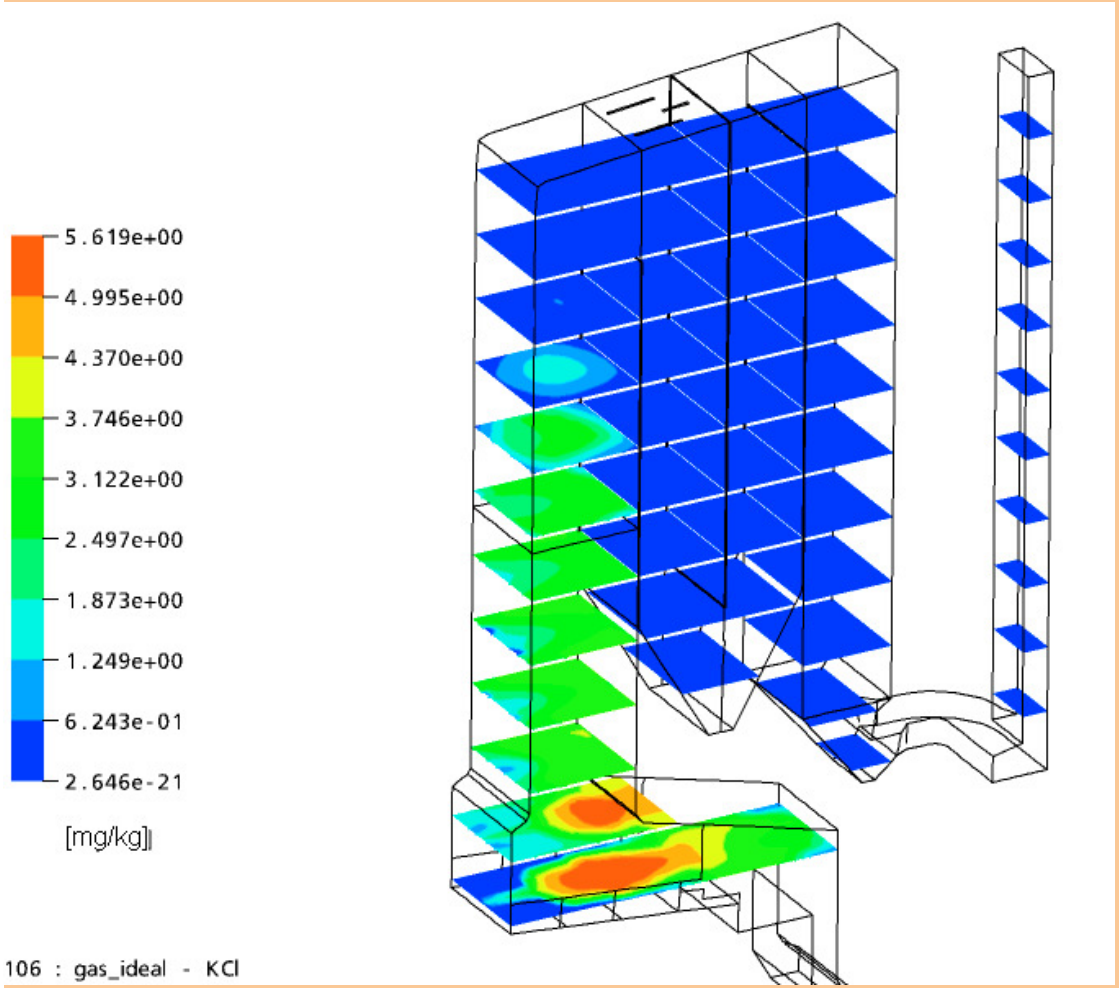


SO_2 - SO_3

- Transition from SO_2 to SO_3 with falling temperature
- Later sulfuric acid and Sulfate



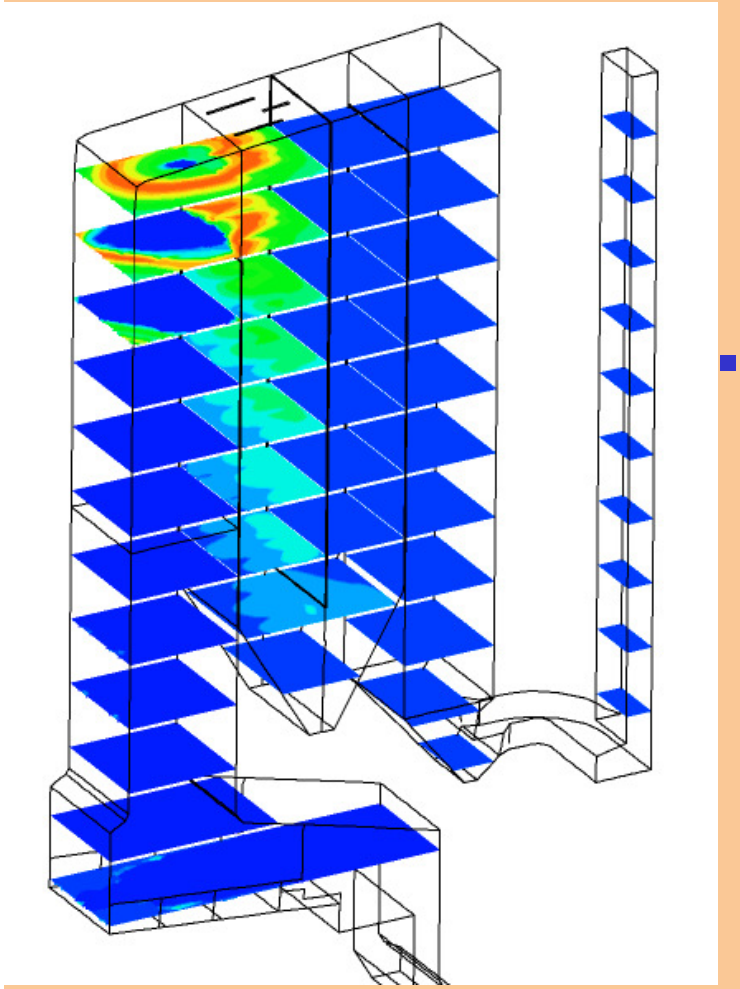
Results



KCl

- Stable up to middle of 1. pass

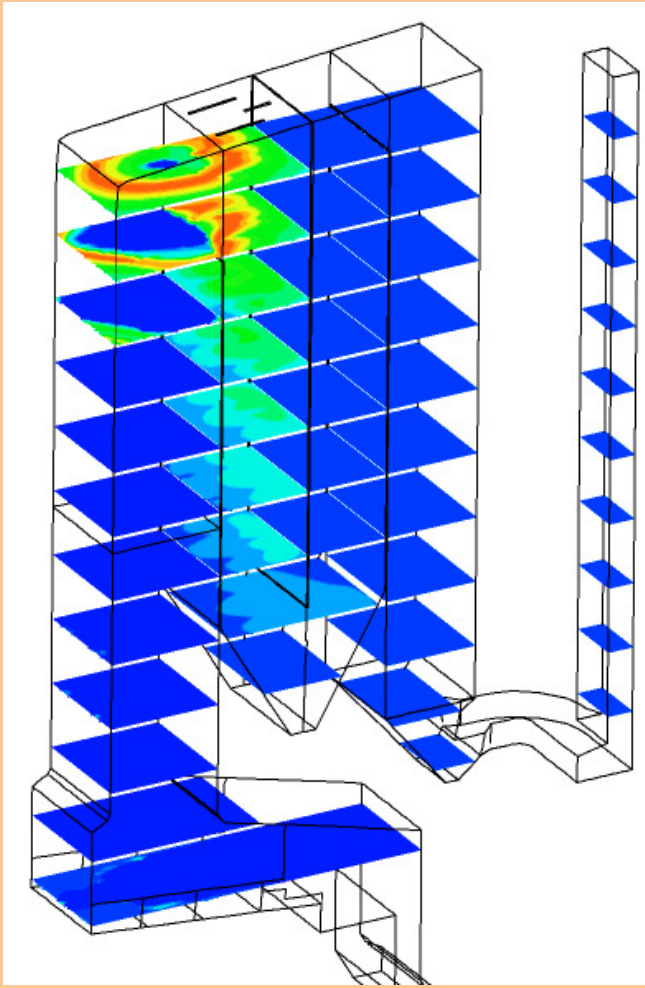
Results



Liquid

$KCl - K_2SO_4$

- Little amound at transition 1. / 2. pass

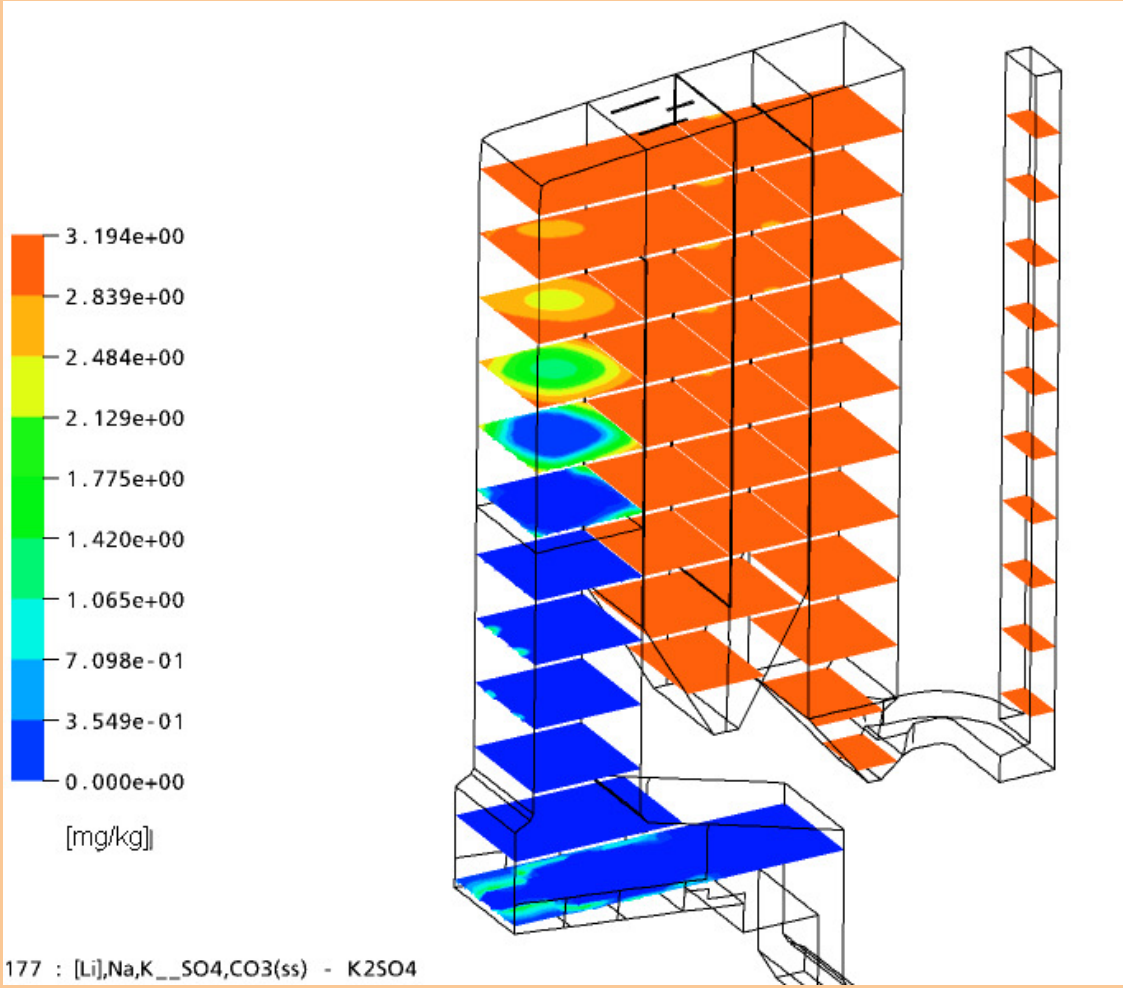


Results

Solid

K_2SO_4

- As mixed phase
- From 2. pass to end

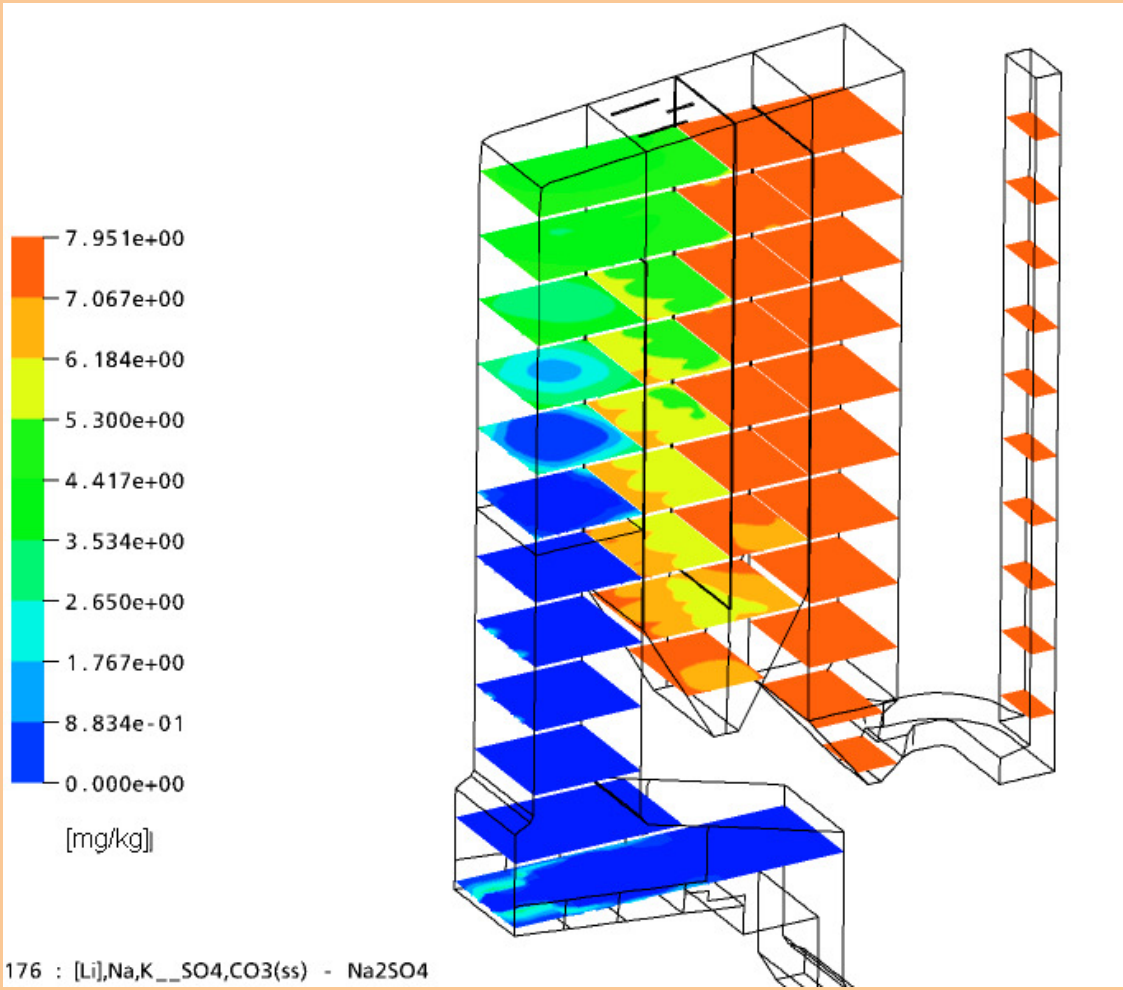


Results

Solid

Na_2SO_4

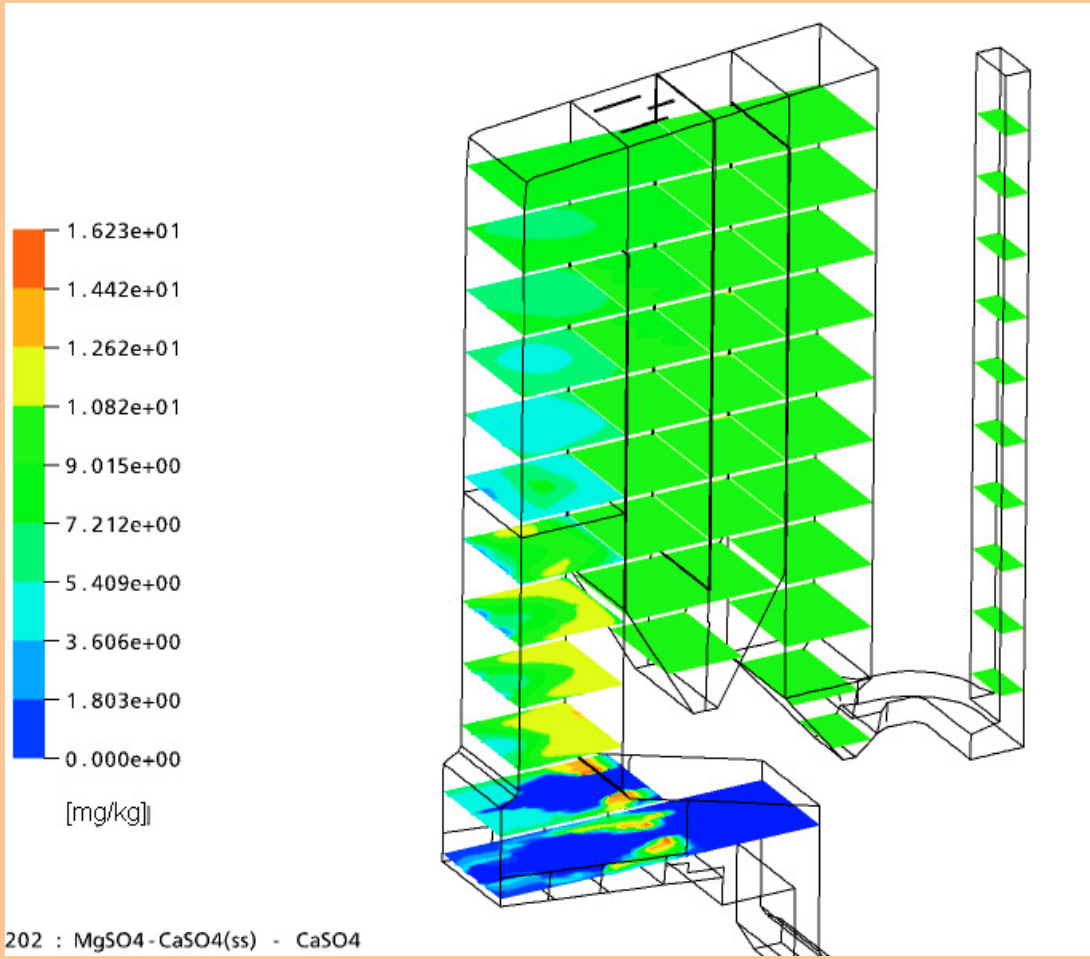
- As mixed phase
- From 2. pass to end



Results

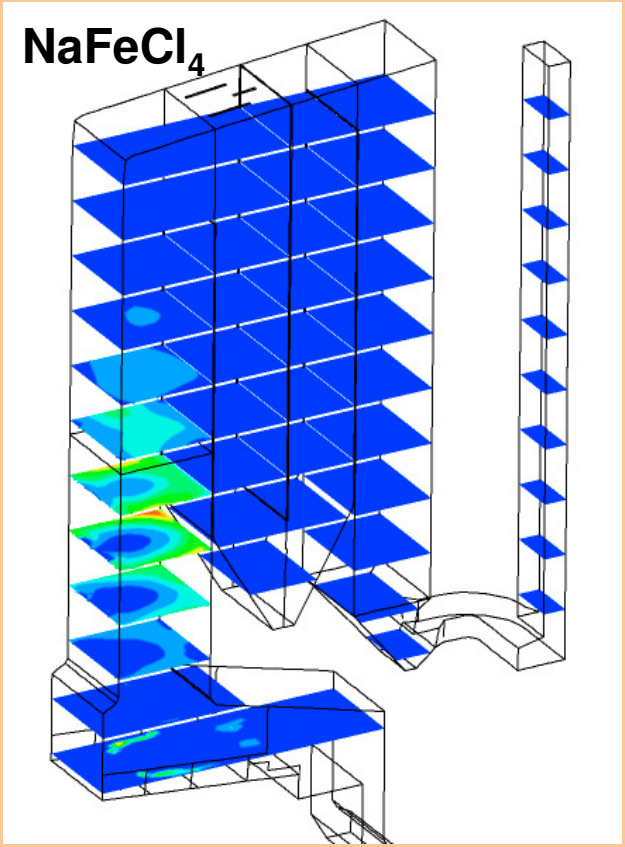
Solid $CaSO_4$

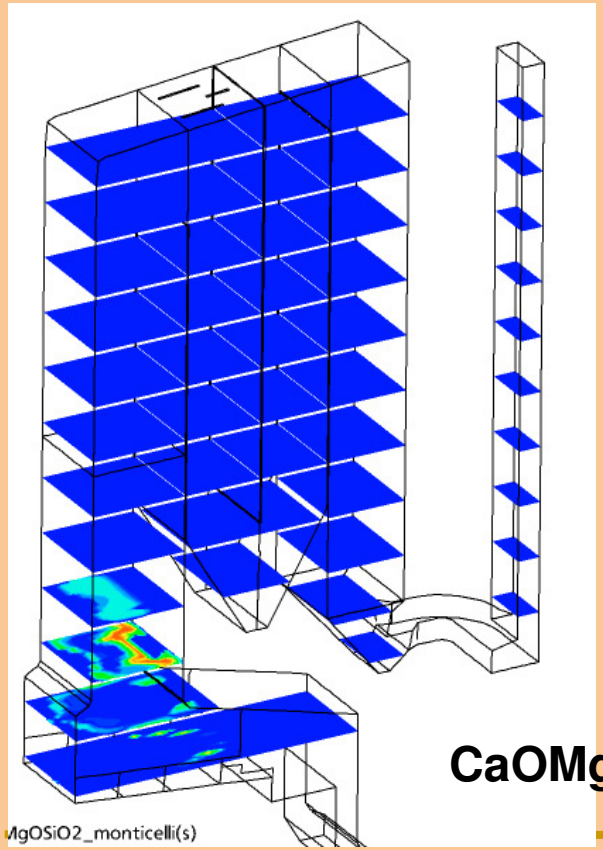
- As mixed phase



Results

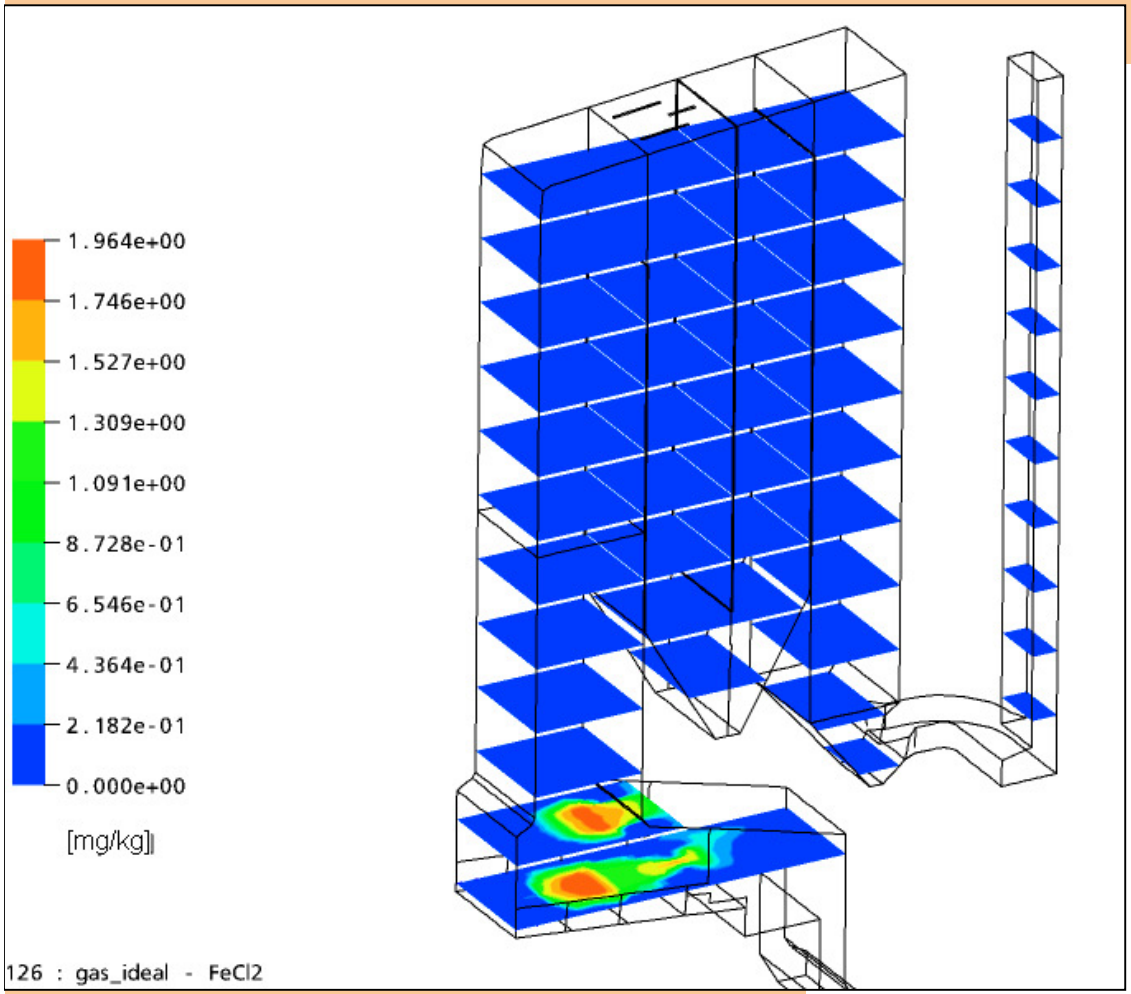
There are various compounds in the combusiton chamber

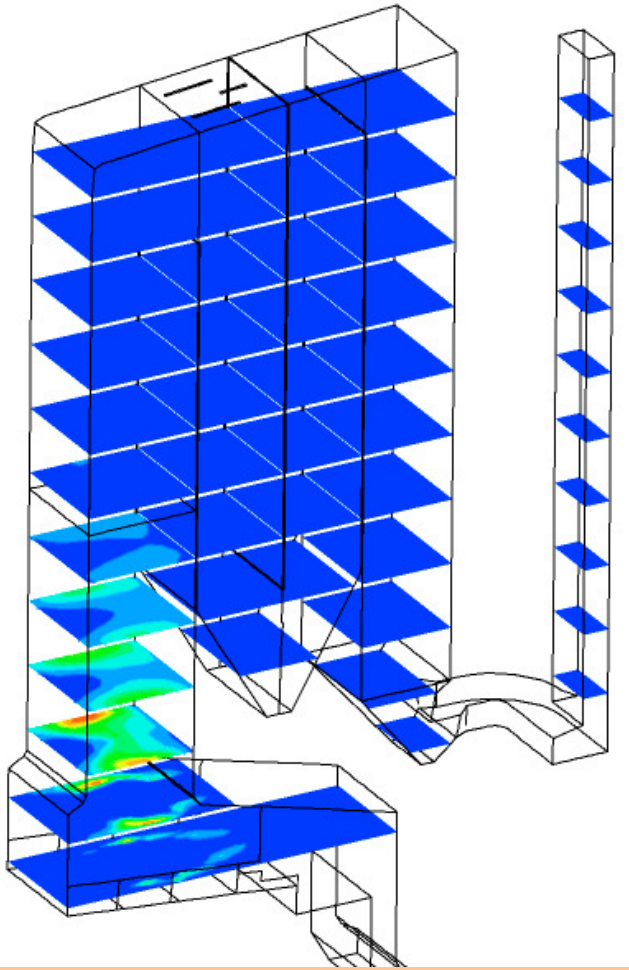




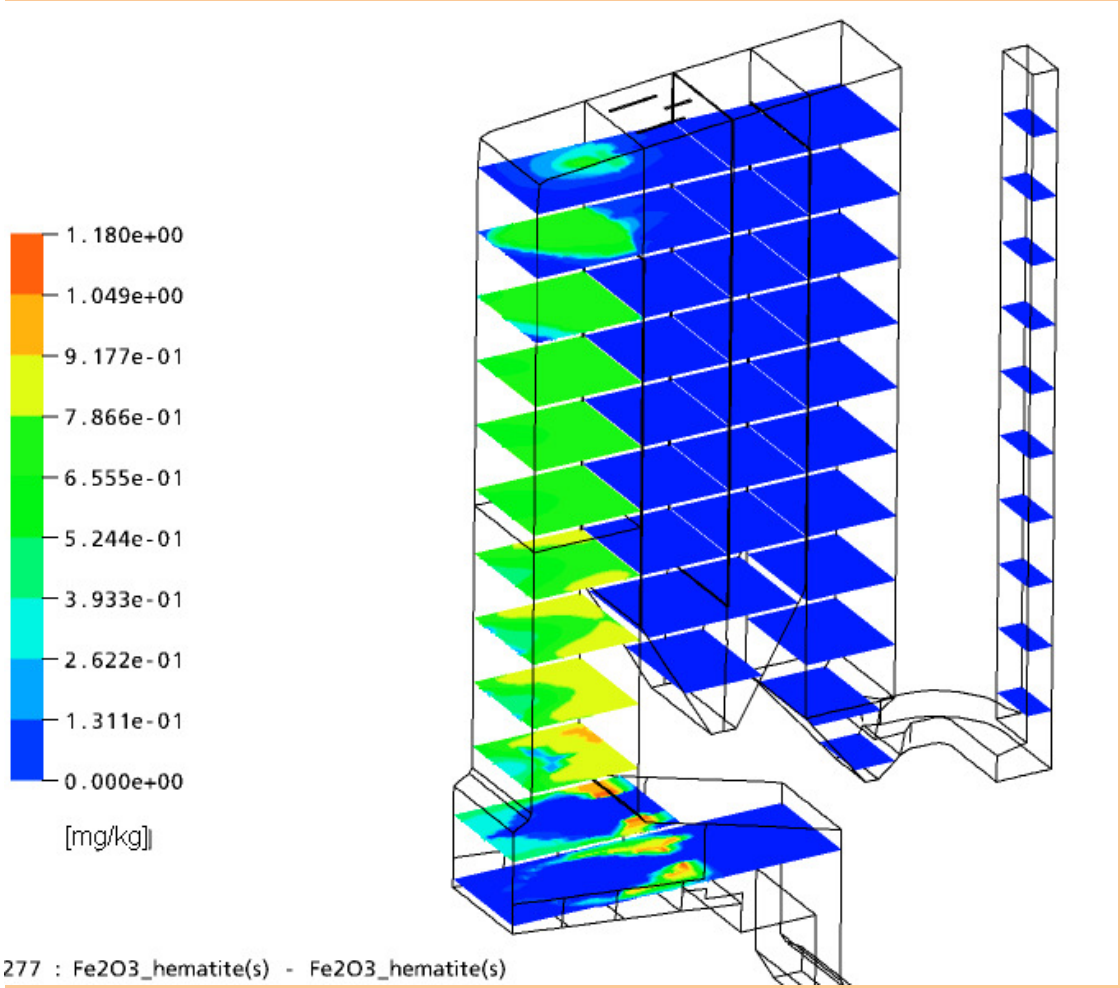
$CaOMgOSiO_2$

Results


1.964e+00
1.746e+00
1.527e+00
1.309e+00
1.091e+00
8.728e-01
6.546e-01
4.364e-01
2.182e-01
0.000e+00
[mg/kg]
126 : gas_ideal - FeCl2


127 : gas_ideal - FeCl3

Results

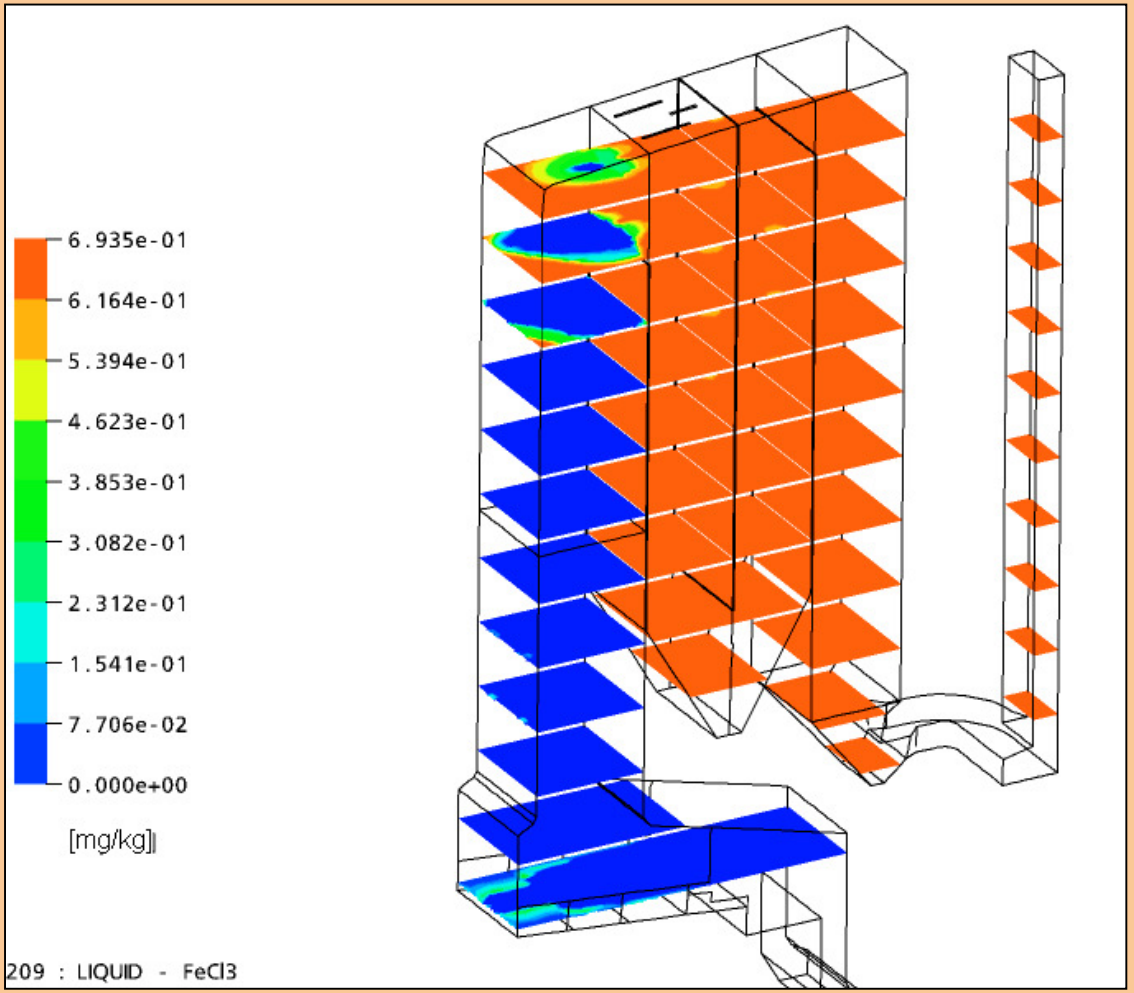


Fe_2O_3

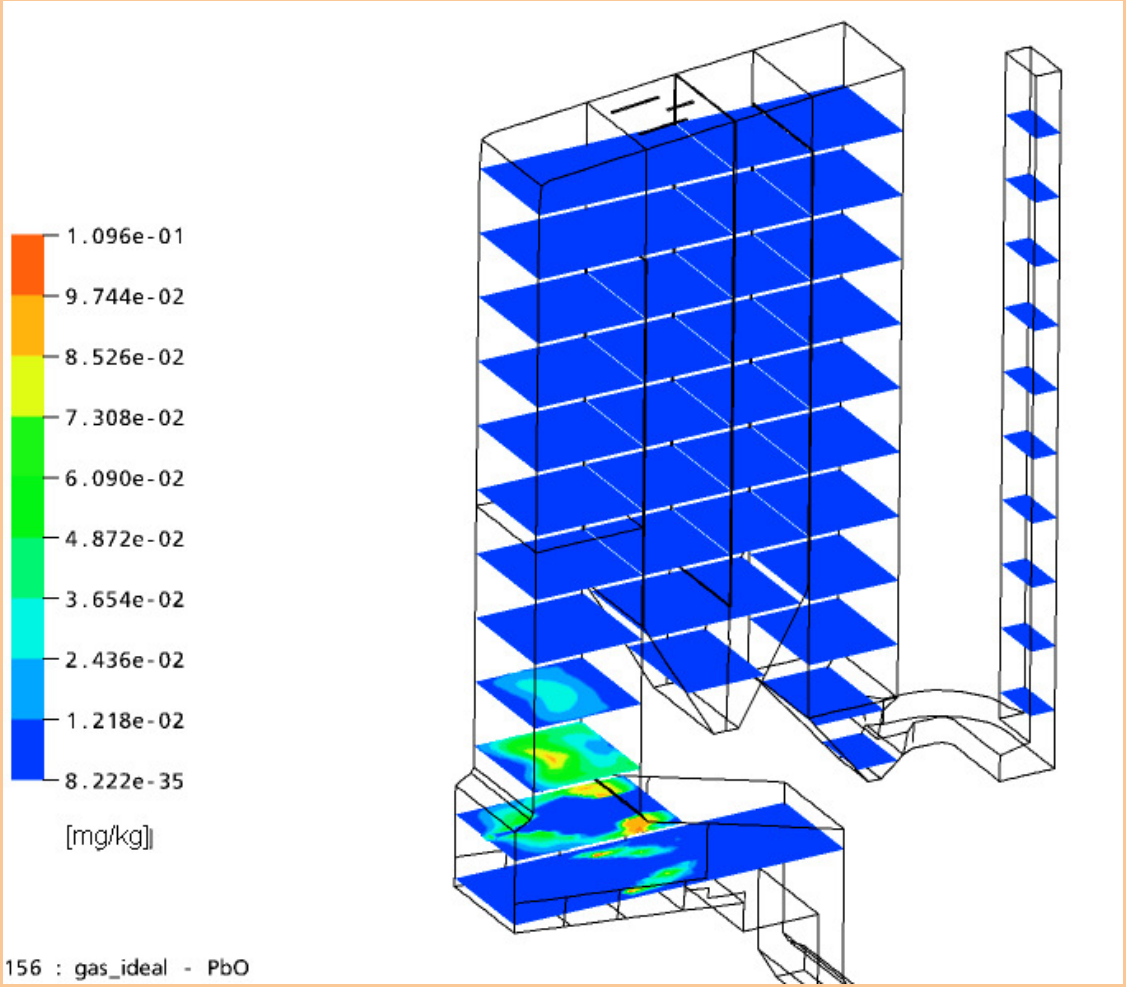
- Main component of ferrous species in 1. pass

Results

Ferrous mixed phase in rest of the boiler



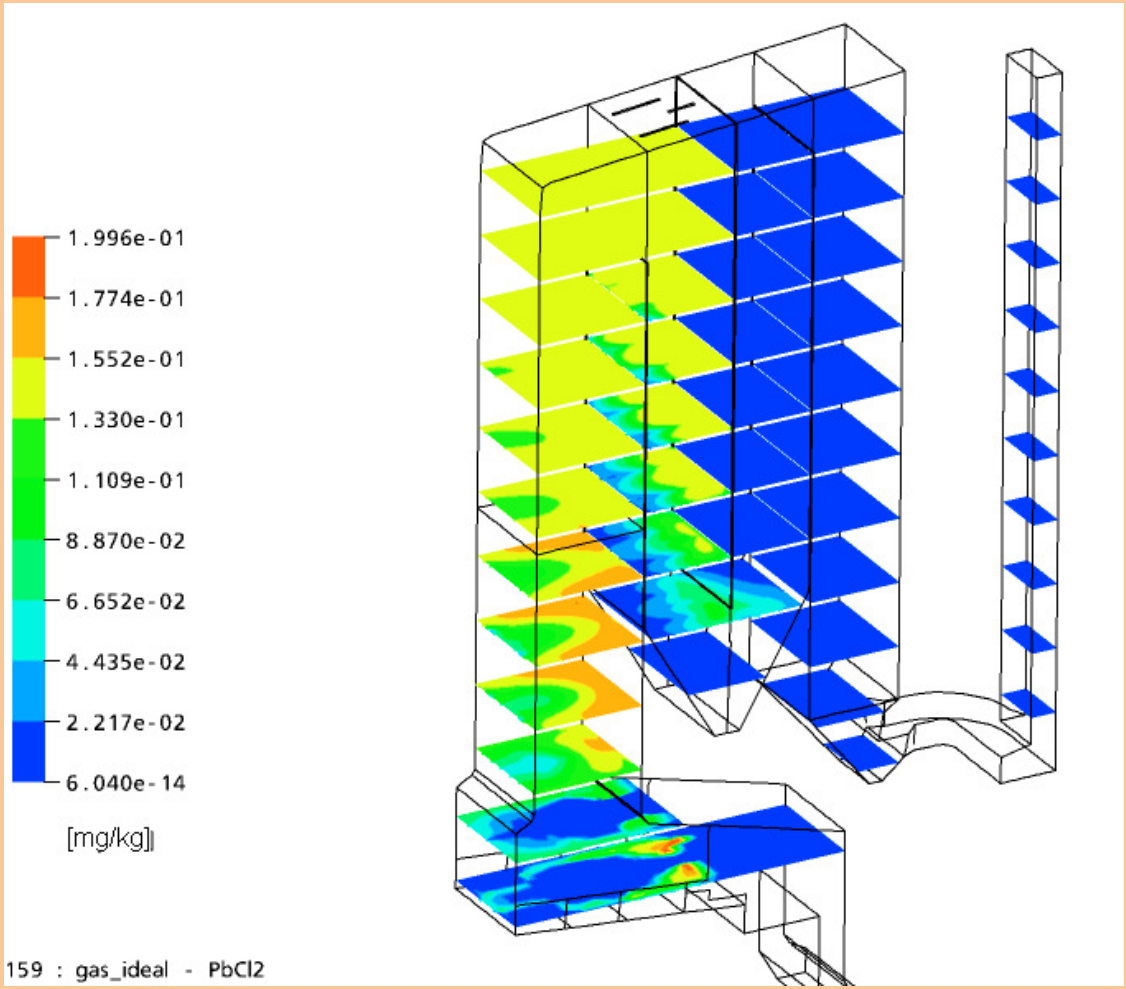
Rsults



PbO

- Combustion chamber

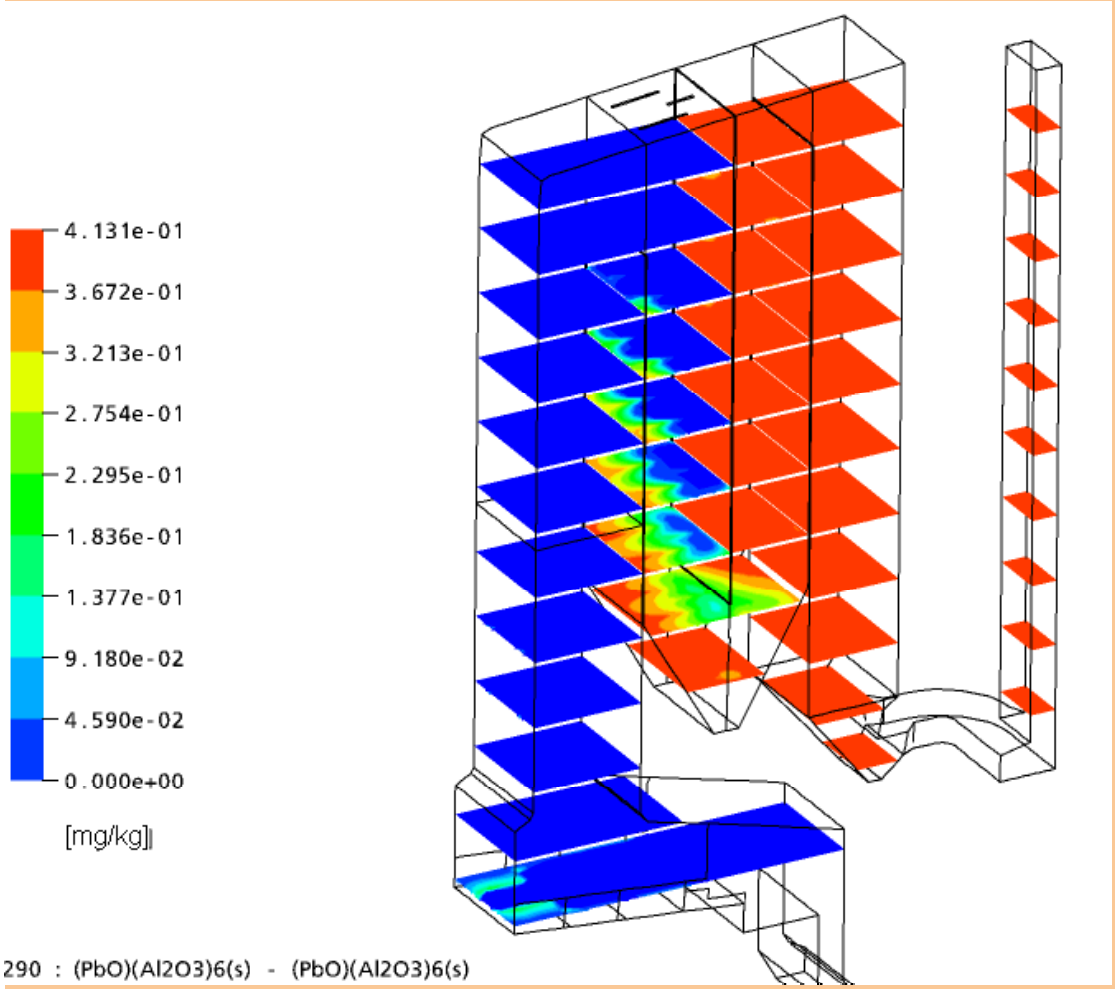
Results



PbCl2

- 1. - 2. pass

Results



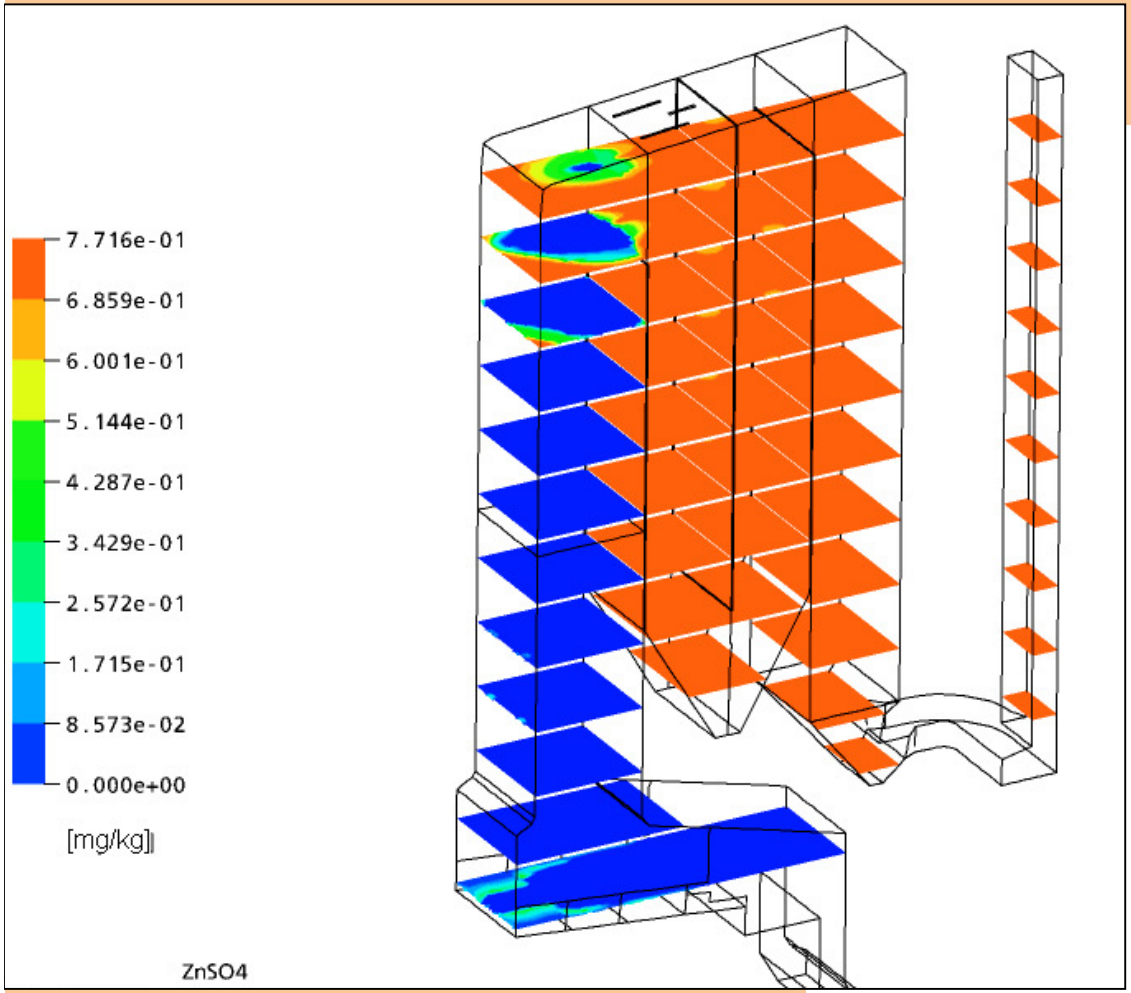
Lead-Aluminium mixed phase

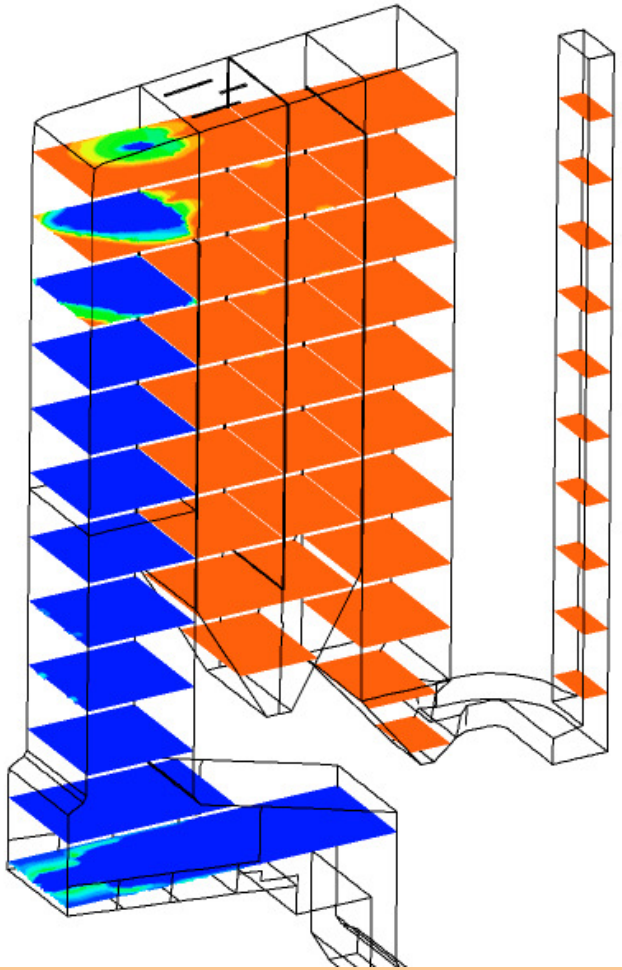
- Up to boiler end

Results

- Zinc and lead
  - Important factor for corrosion
    - Low melting eutektika
  - In the front area stable as aluminat
  - In the back area sulfatic and chloridic mixing phases

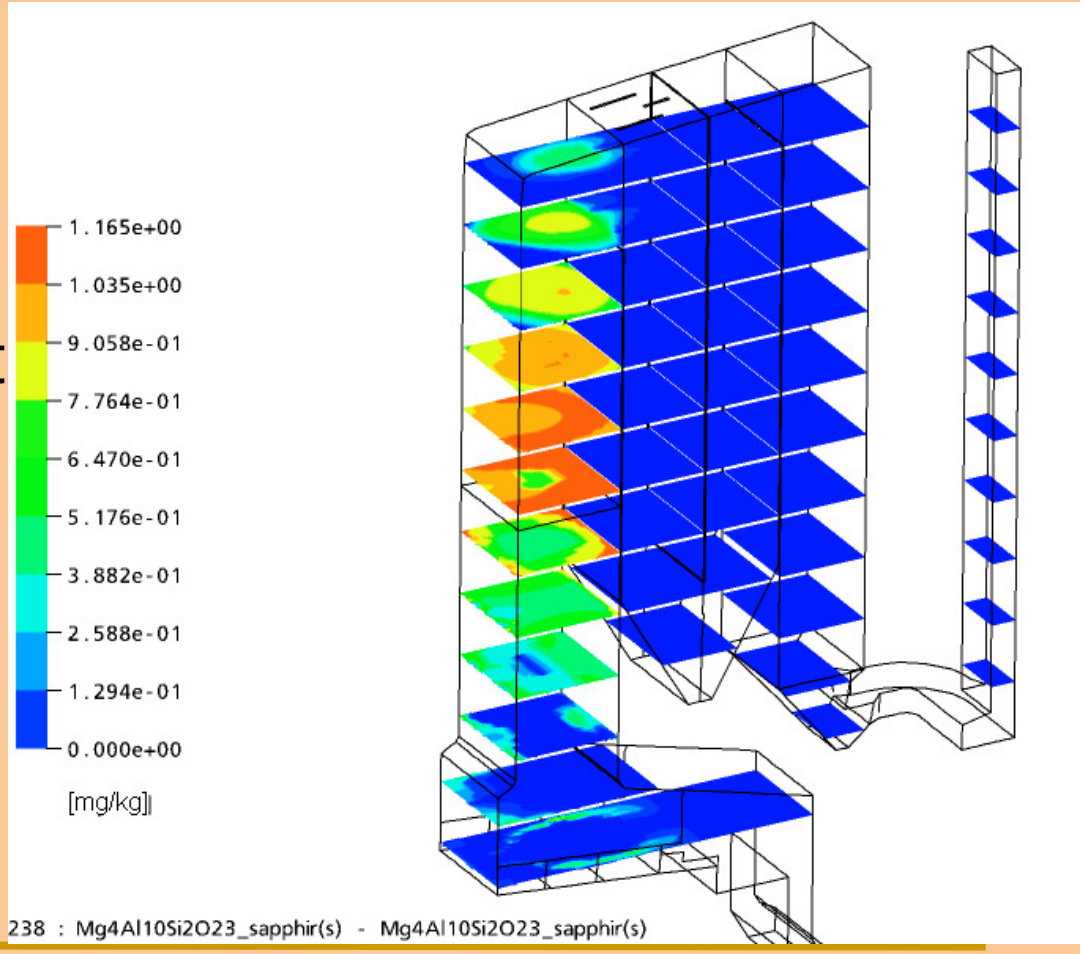
Results


7.716e-01
6.859e-01
6.001e-01
5.144e-01
4.287e-01
3.429e-01
2.572e-01
1.715e-01
8.573e-02
0.000e+00
[mg/kg]
ZnSO4

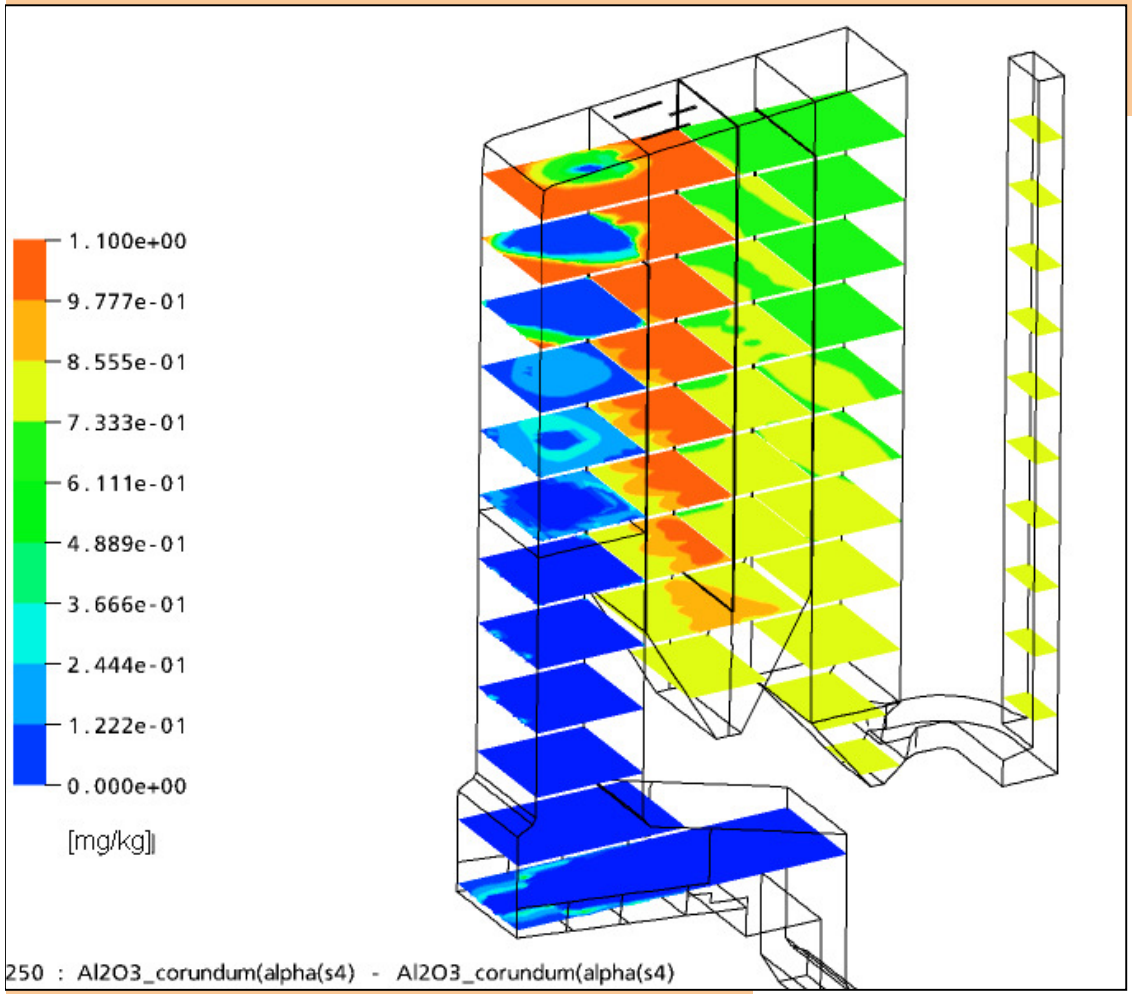

ZnCl2

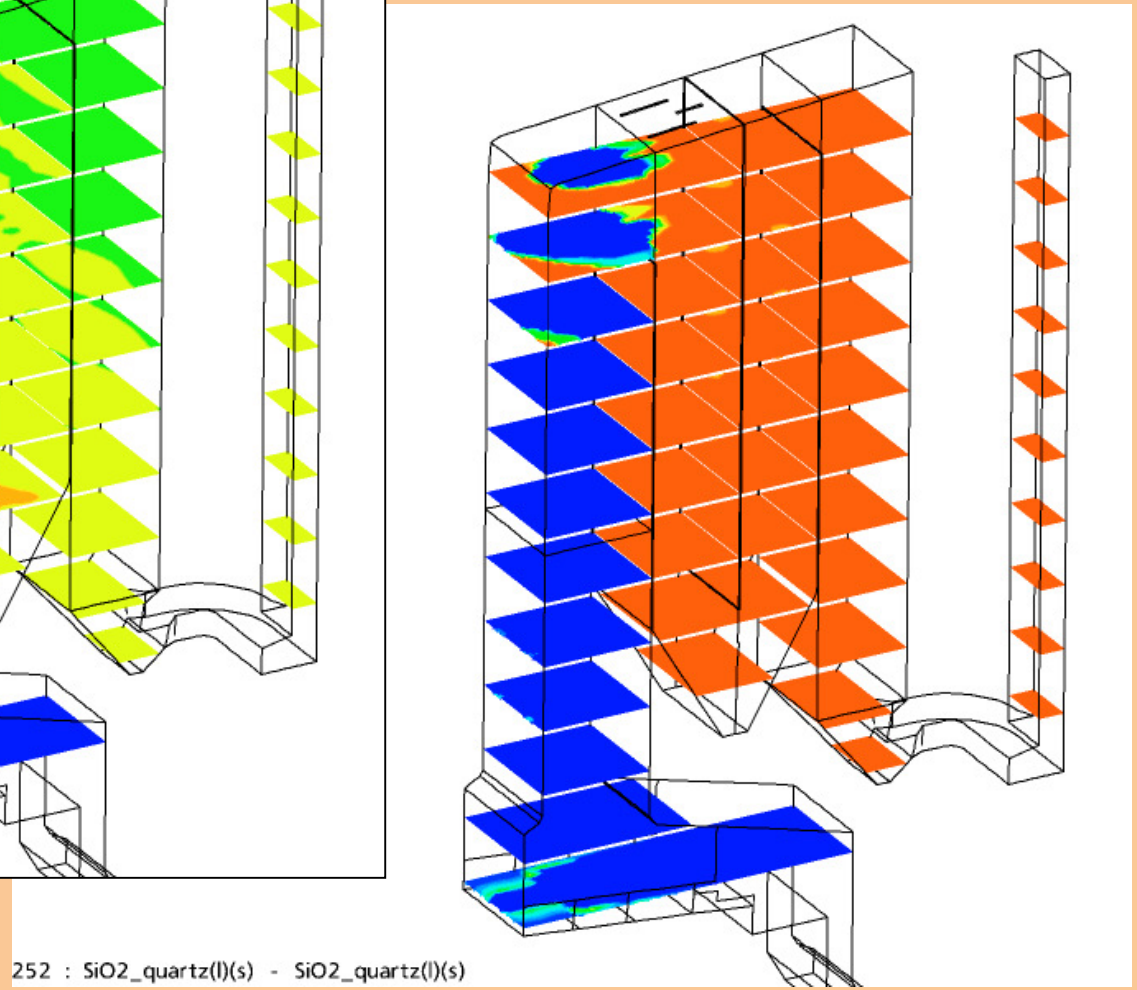
Results

- Alumina und Aluminium Silicate
  - Delimited stability
  - Stable final product
    - Aluminiumoxide
    - Siliciumdioxide



Results


1.100e+00
9.777e-01
8.555e-01
7.333e-01
6.111e-01
4.889e-01
3.666e-01
2.444e-01
1.222e-01
0.000e+00
[mg/kg]
250 : Al2O3_corundum(alpha(s4)) - Al2O3_corundum(alpha(s4))

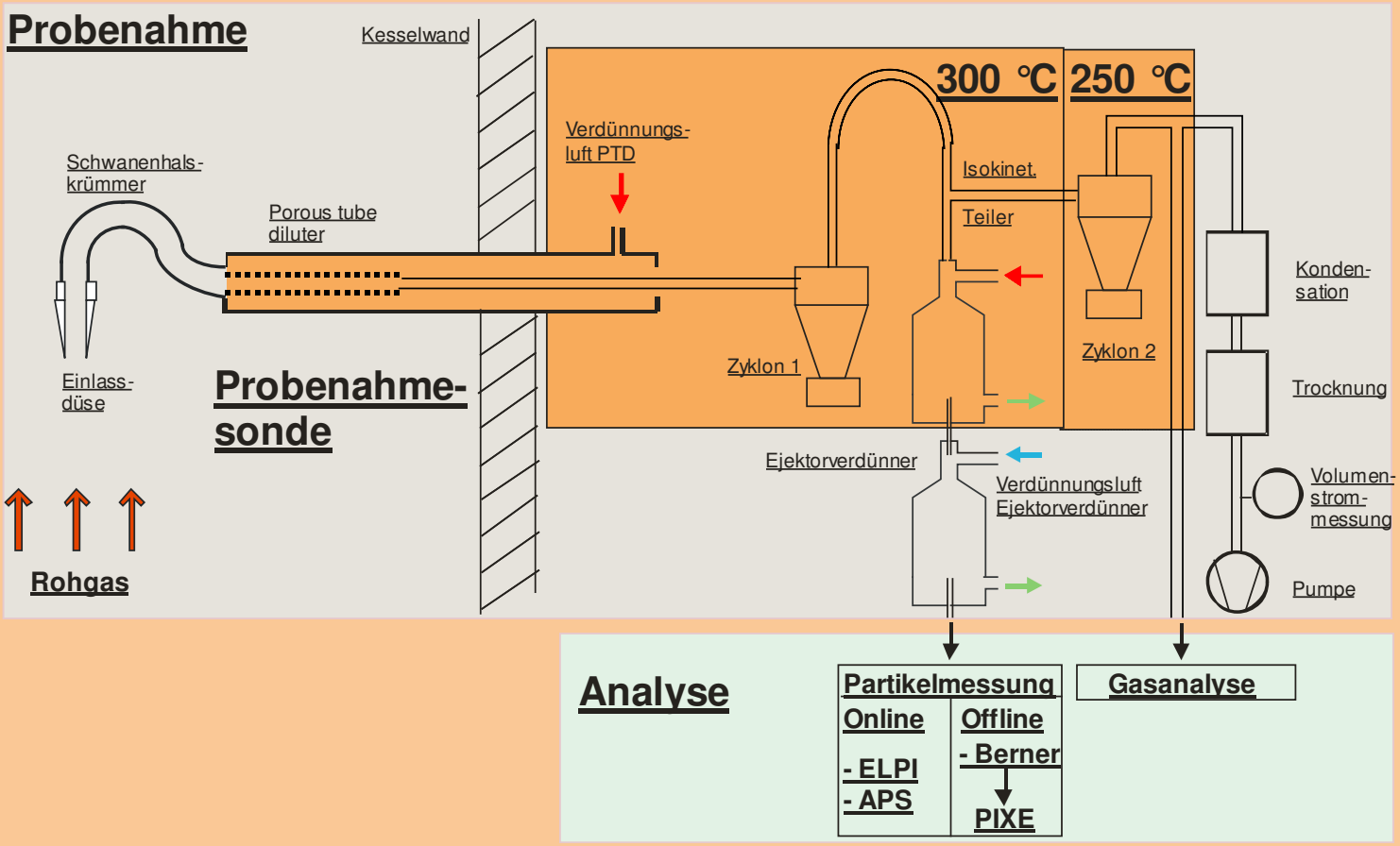

252 : SiO2_quartz(l)(s) - SiO2_quartz(l)(s)

Results

- Boundary Conditions
  - The total content of species will react
    no deposition
- Plausible results for many species
- A lot of surprises
  - Complex states in the combustion chamber
    cannot be reproduced by „simple“ calculations
    without CFD

Results of Measurements

- Particle and Gas sampling



Results of Measurements

- Particle-Analysis
  - Impactor-samples with PIXE
    - Element distribution
  - Dust / Aerosol samples
    - Transmissionsröntgendiffraktogramm
      - Mineral phases

Results of Measurements

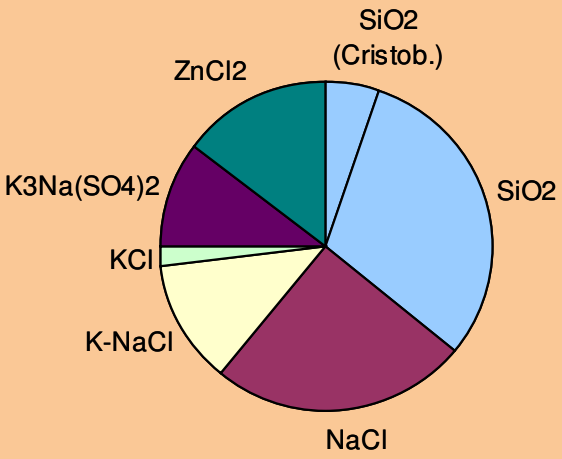
	Z2_ 0,25-1 µm	Z2_ 5-20 µm	Z3_ 5-20 µm
P	0,1%	0,3%	0,3%
S	5,8%	4,2%	4,9%
Zn	3,3%	3,9%	3,7%
Pb	0,8%	1,8%	2,2%
Si	1,8%	6,8%	4,8%
Fe	0,3%	1,5%	1,6%
Mg	0,1%	0,5%	0,4%
Ca	0,8%	5,1%	3,3%
Al	0,4%	0,6%	0,6%
Na	14,3%	11,2%	11,2%
K	22,6%	15,4%	13,9%
Cl	33,7%	5,2%	5,1%
Br	n.b.	0,4%	0,3%

Results of Measurements

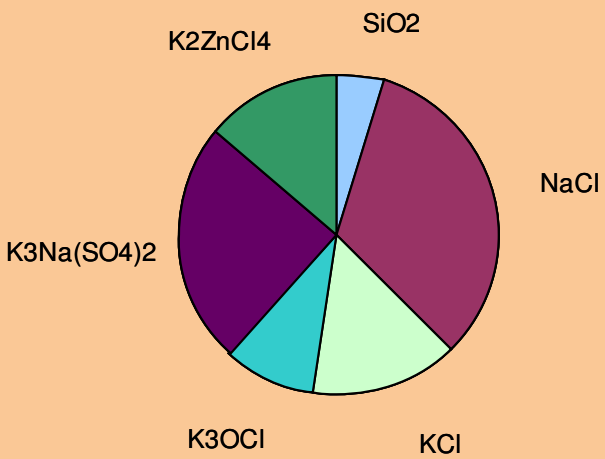
Fractions of identifiable phases

Röntgendiffraktometrie

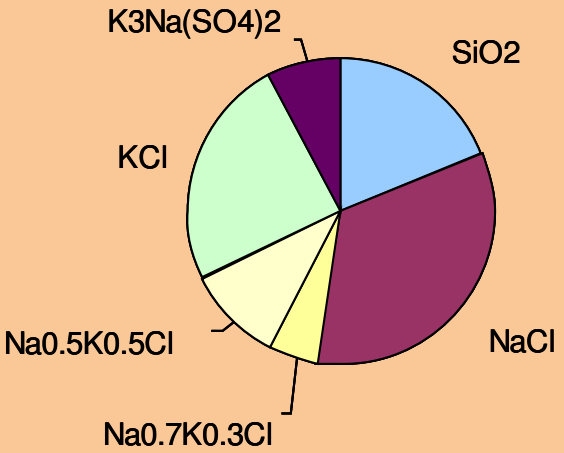
Z2 0,25 - 1µm



Z2 5 – 20 µm

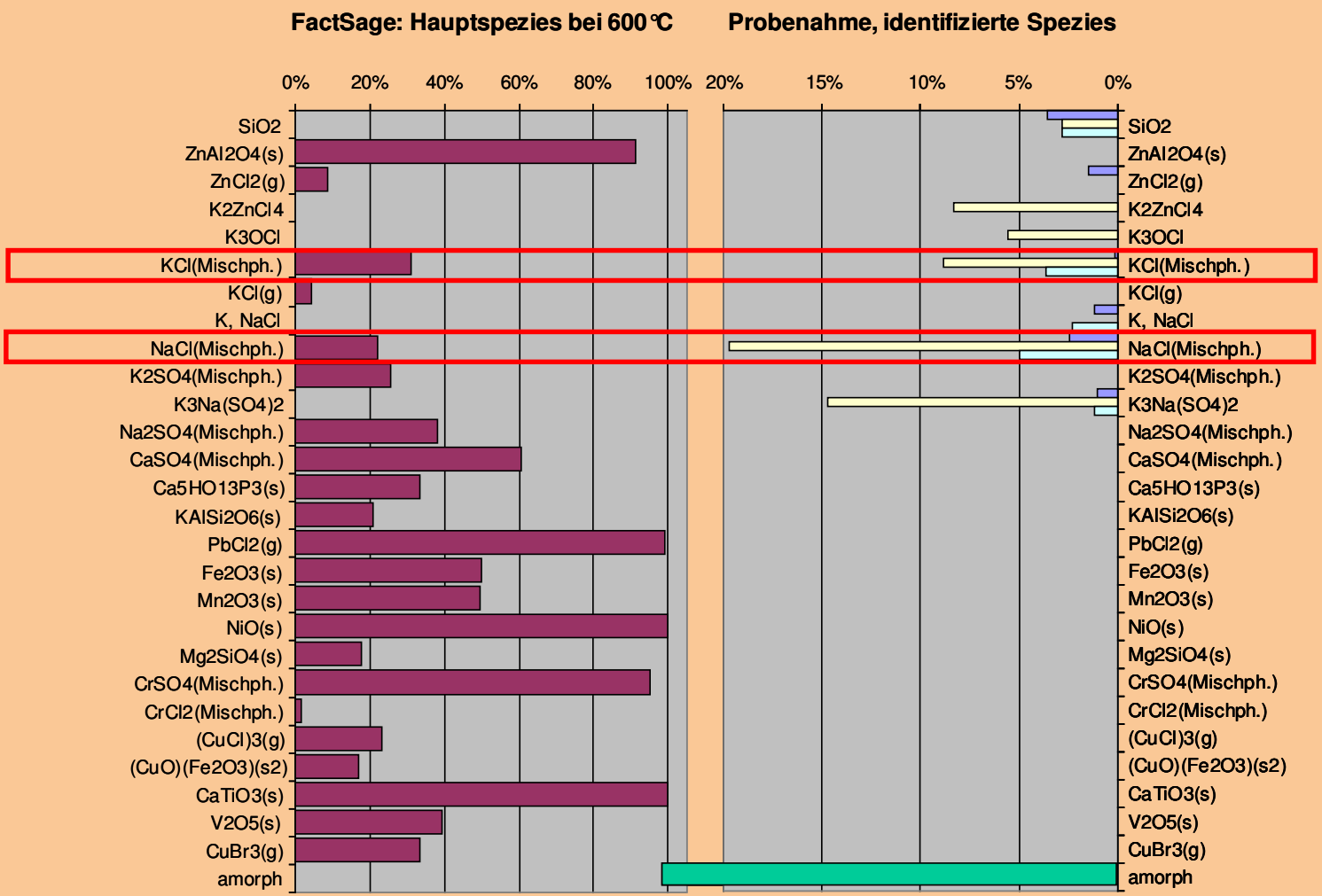


Z3 5 – 20 µm

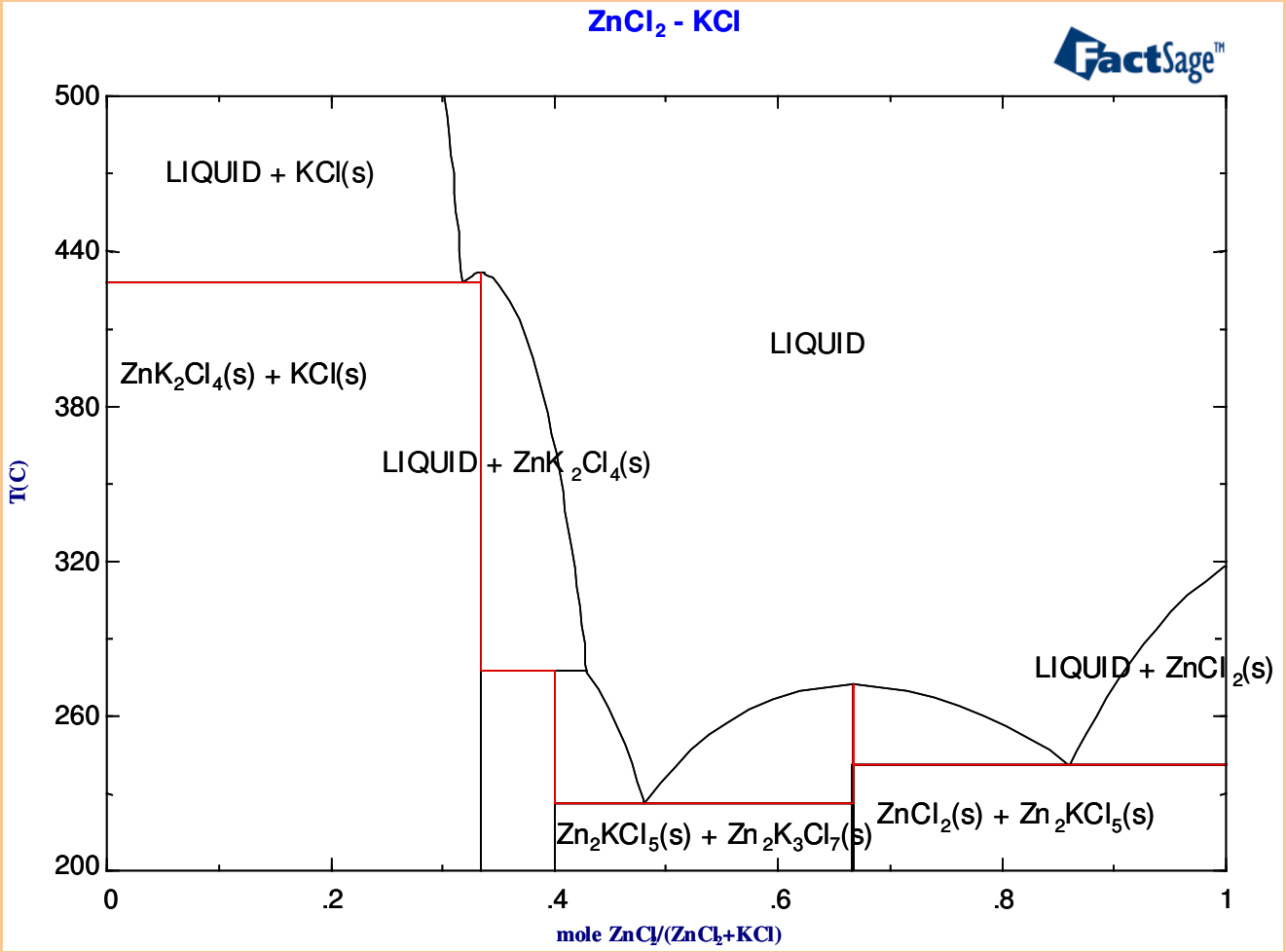


High SiO2-fraction -> great part of salts is not well crystallised

Compartison of Results



Comparison of Results

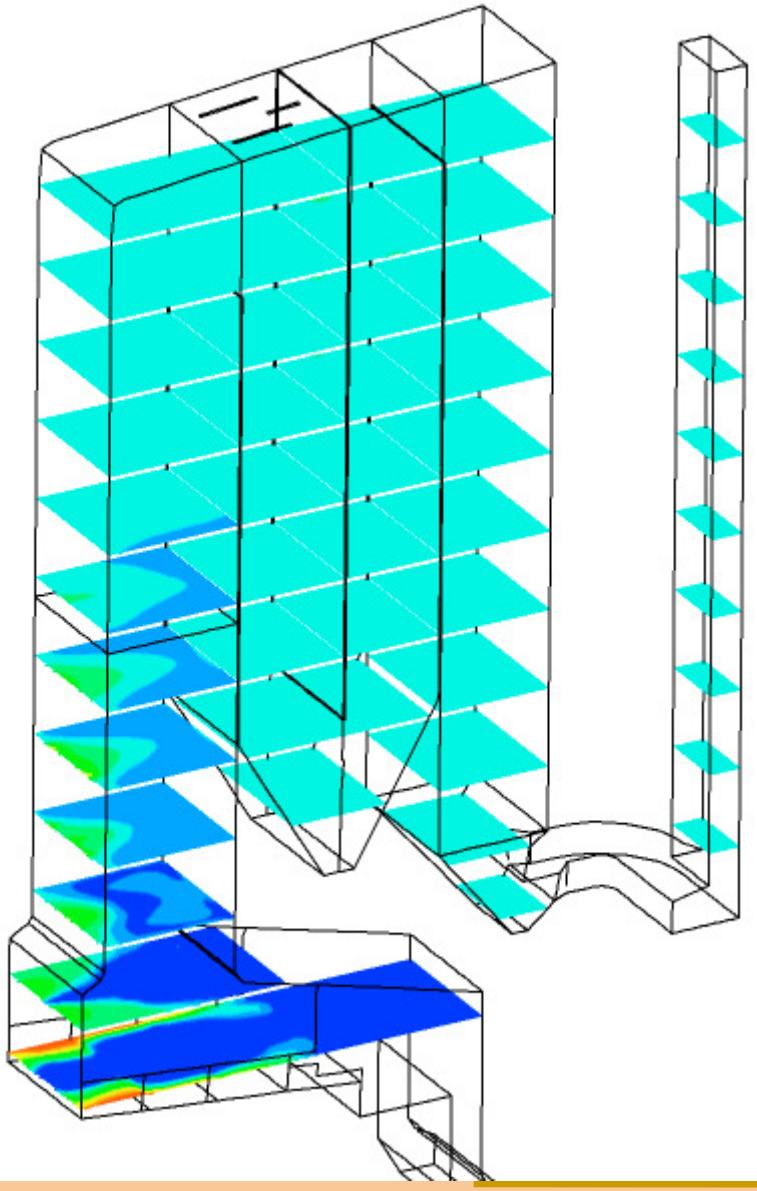


Summary

- Coupling of ChemApp and CFX
  - Fluid-mechanical view of minority compounds
- Reduced Variety of Species
- Results are plausible
  - Conclusions for stability ranges
- Validation of Relevance with Measuring-Results

Summary

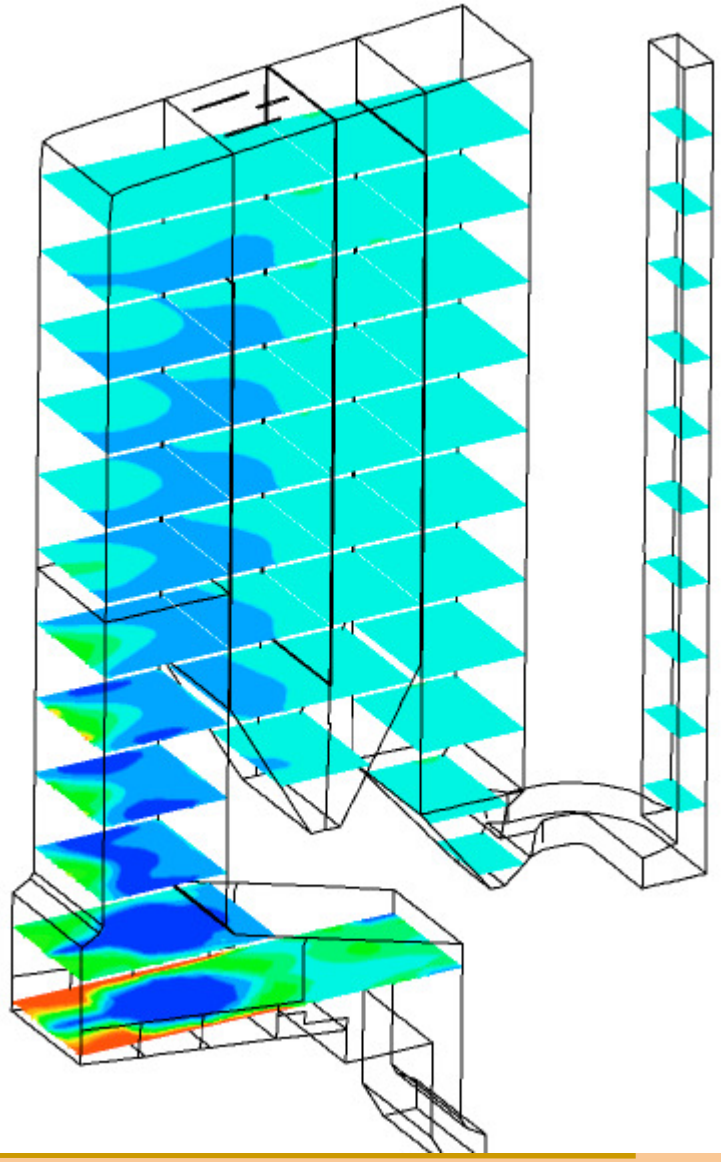
- SO2/SO3/H2SO4 shows the expected deviation
- Cristal phases show slight correlation
  - Inhibited acchivement of equilibrium in the gas phases
  - Interesting for the aerosol deposit on walls and tubes

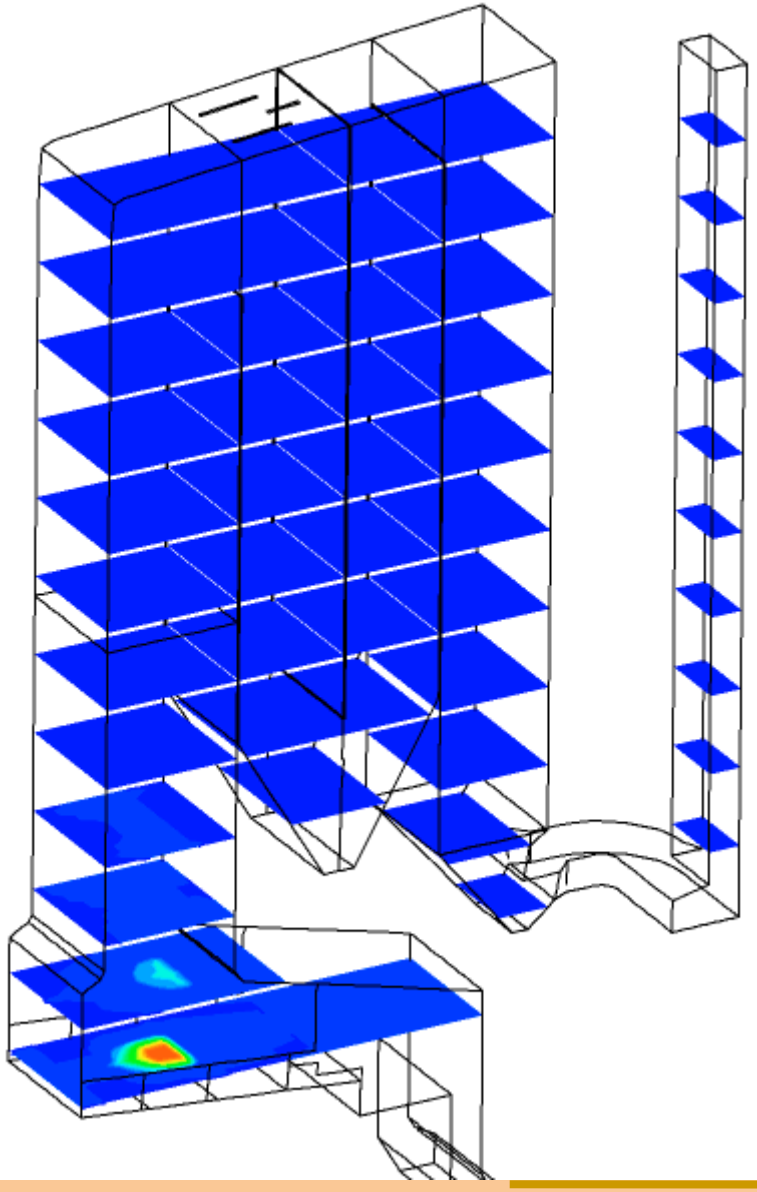


← ChemApp

CFX →

O_2

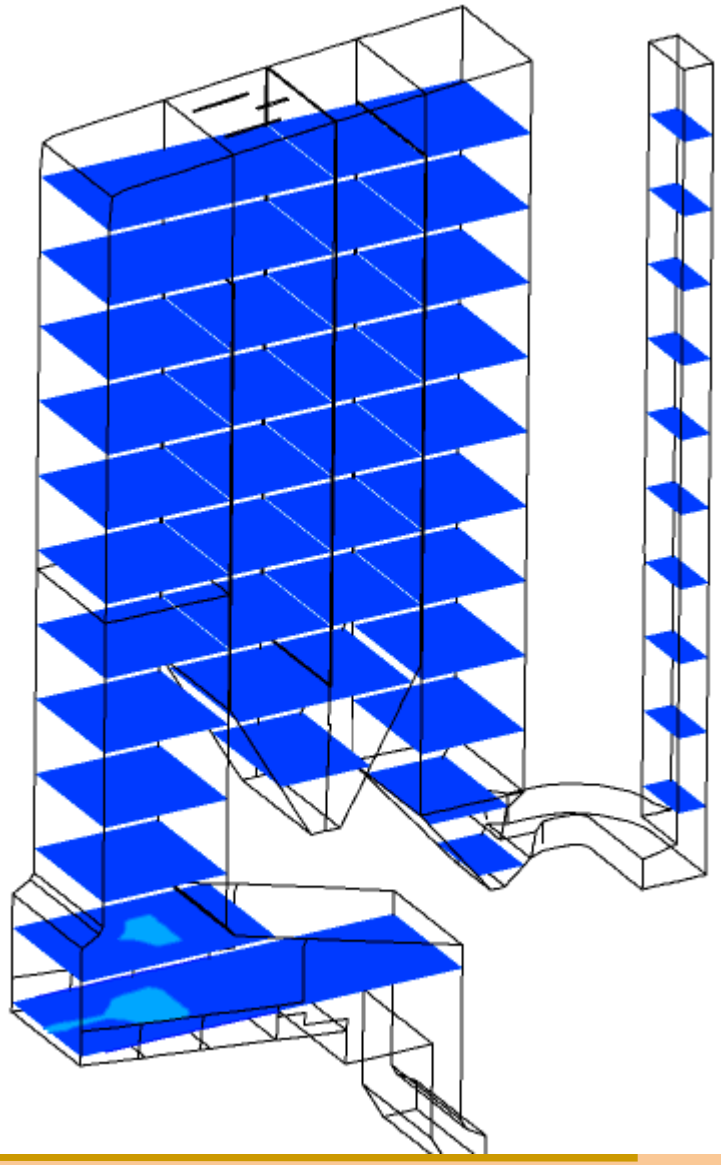


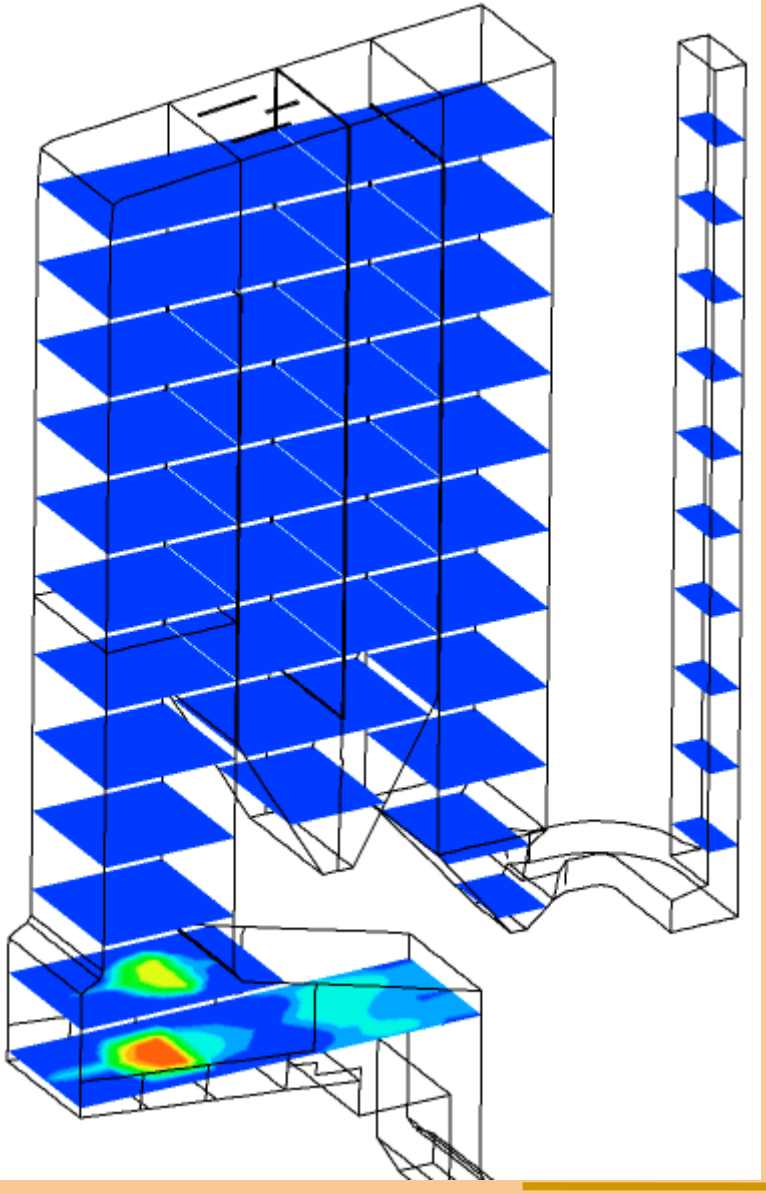


← ChemApp

CFX →

Organic

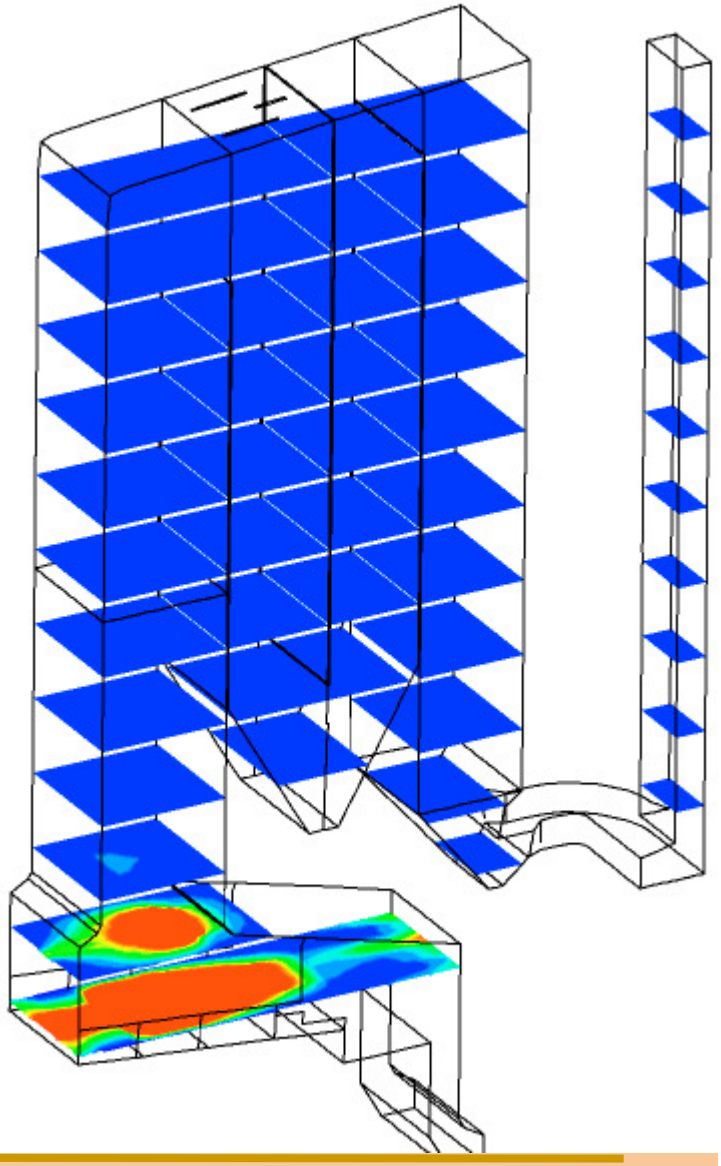


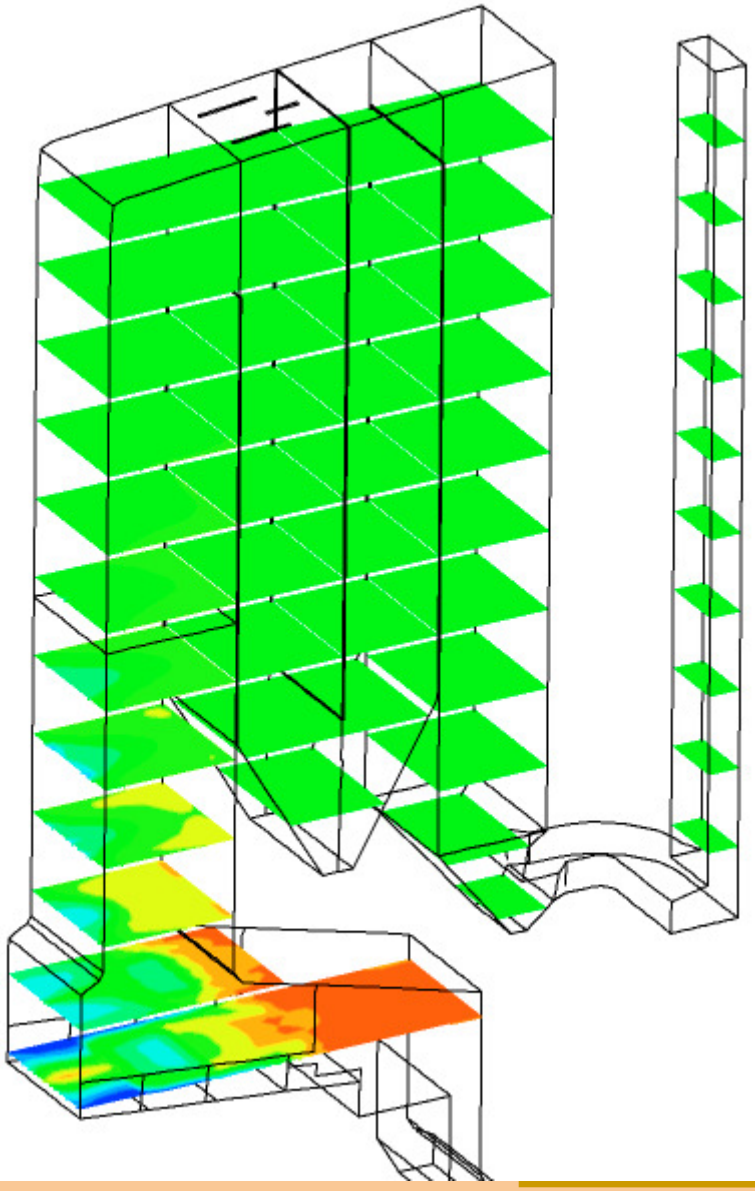


← ChemApp

CFX →

CO





← ChemApp

CFX →

CO_2