AACHENER VERFAHRENSTECHNIK

General Considerations for Process Modelling on a Thermochemical Basis

GTT-Workshop 4. - 6.6.2008

Tobias Ginsberg, Michael Modigell

AVT, Turmstraße 46, D-52056 Aachen

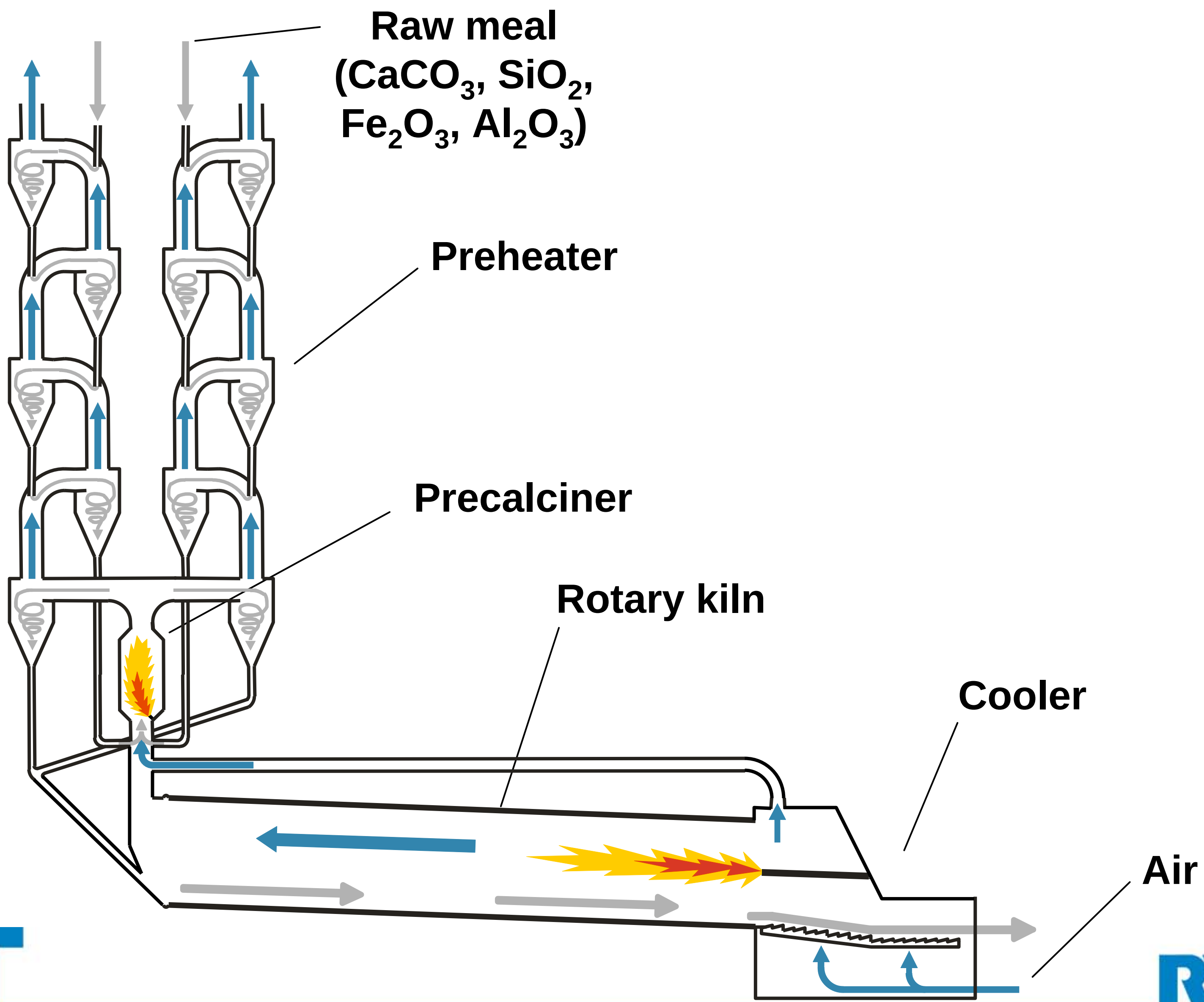
RWTH

Introduction

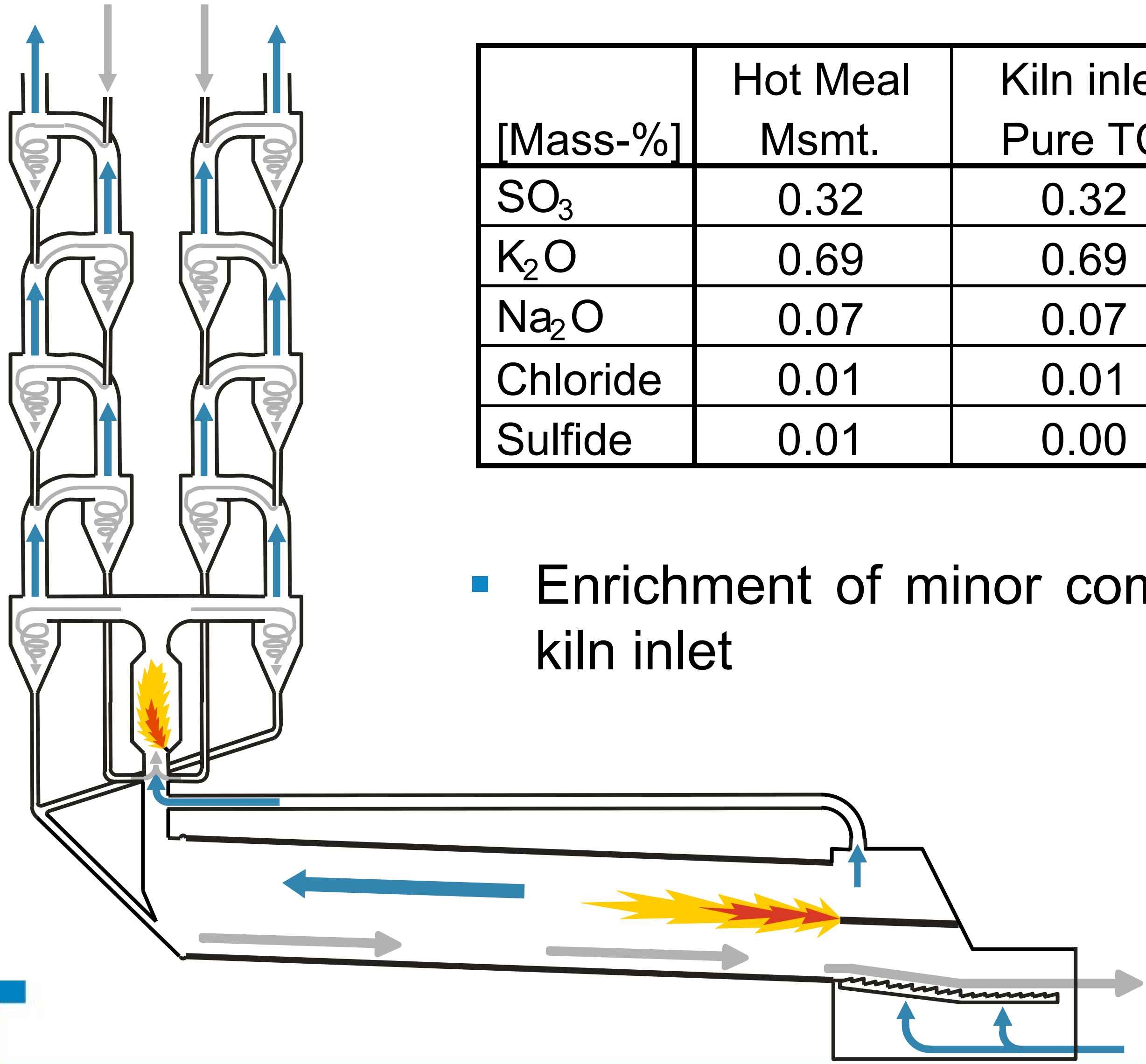
- Computational thermochemistry is a strong tool to simulate the behaviour of complex chemical Systems
- Restricted in pure form to ideal conditions
  - homogeneous mixing
  - no reaction kinetic inhibitions
- However, many technical processes involve both, complex chemistry and incomplete mixing or kinetic inhibitions

⇨ Improve pure thermochemical model by process analysis and choice of a proper model structure

Cement production plant



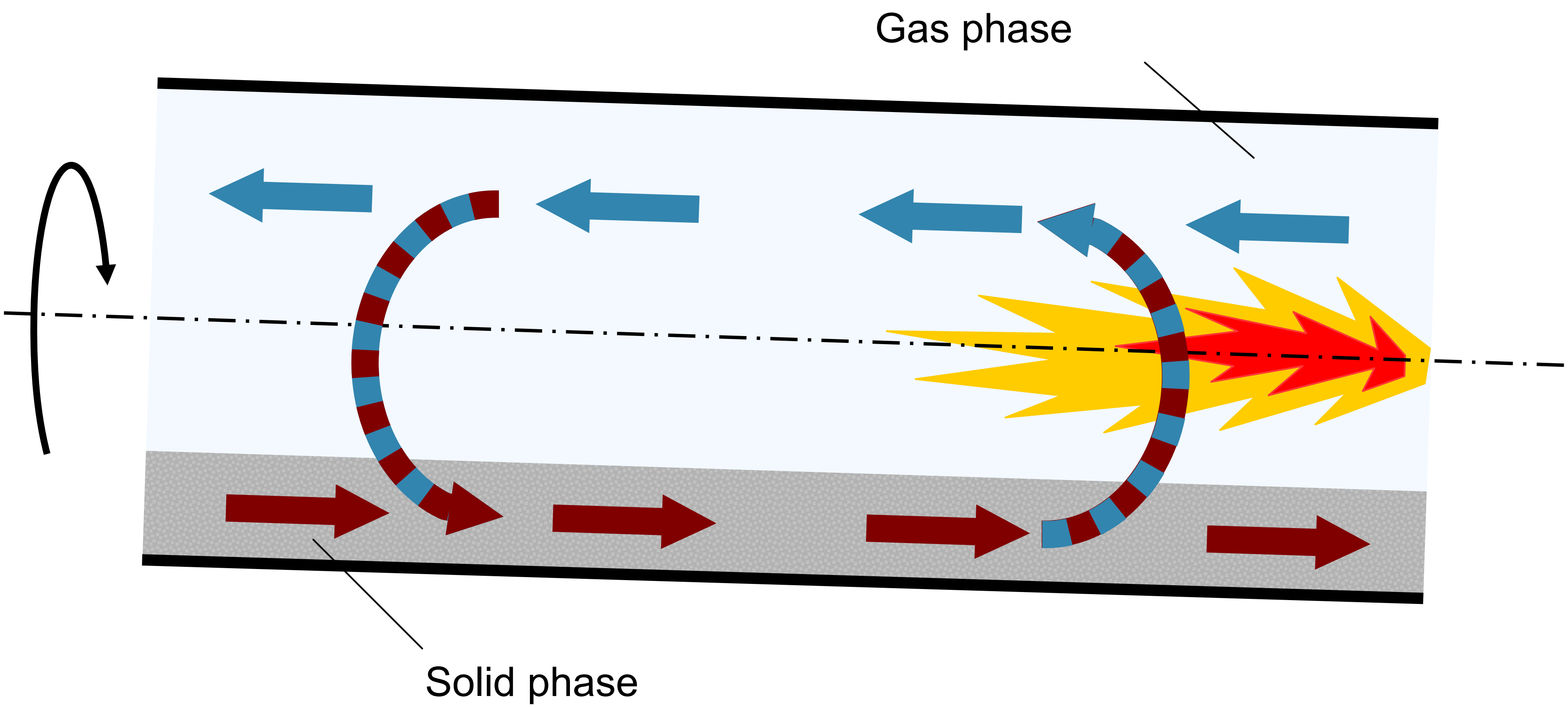
Minor components – Pure TC



[Mass-%]	Hot Meal Msmt.	Kiln inlet Pure TC	Kiln Inlet Msmt.
SO_3	0.32	0.32	1.19
K_2O	0.69	0.69	5.20
Na_2O	0.07	0.07	0.11
Chloride	0.01	0.01	3.56
Sulfide	0.01	0.00	0.01

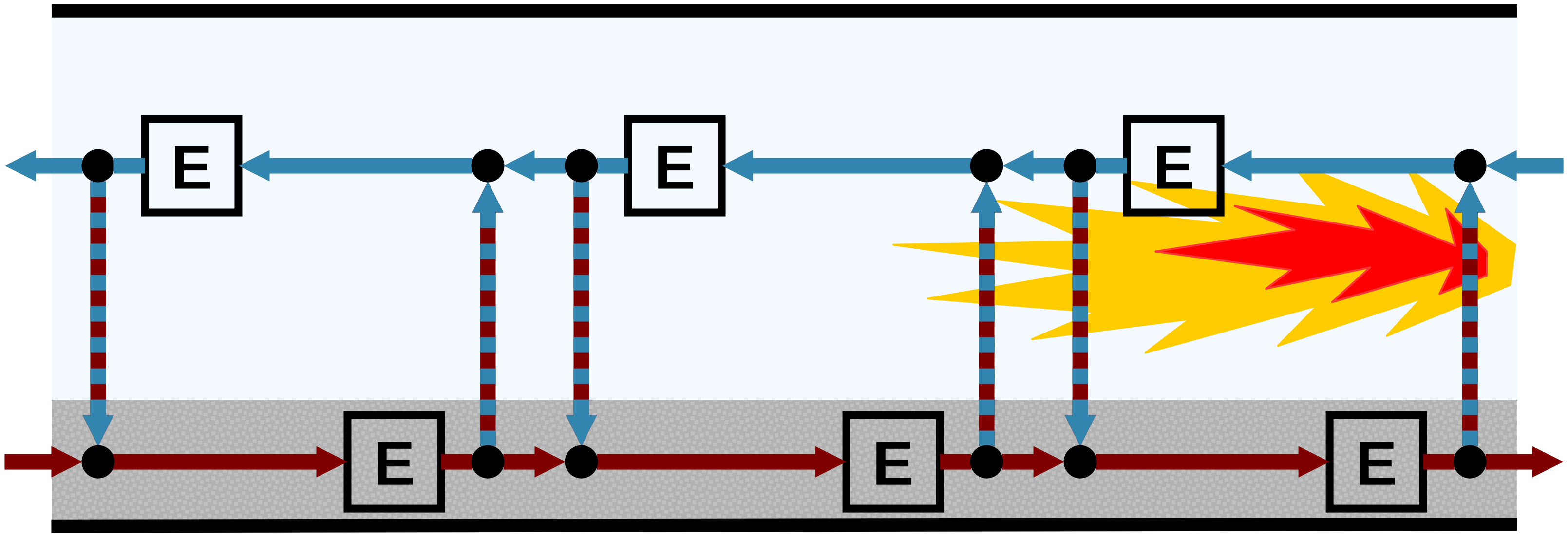
- Enrichment of minor components at kiln inlet

Transport conditions within a rotary kiln



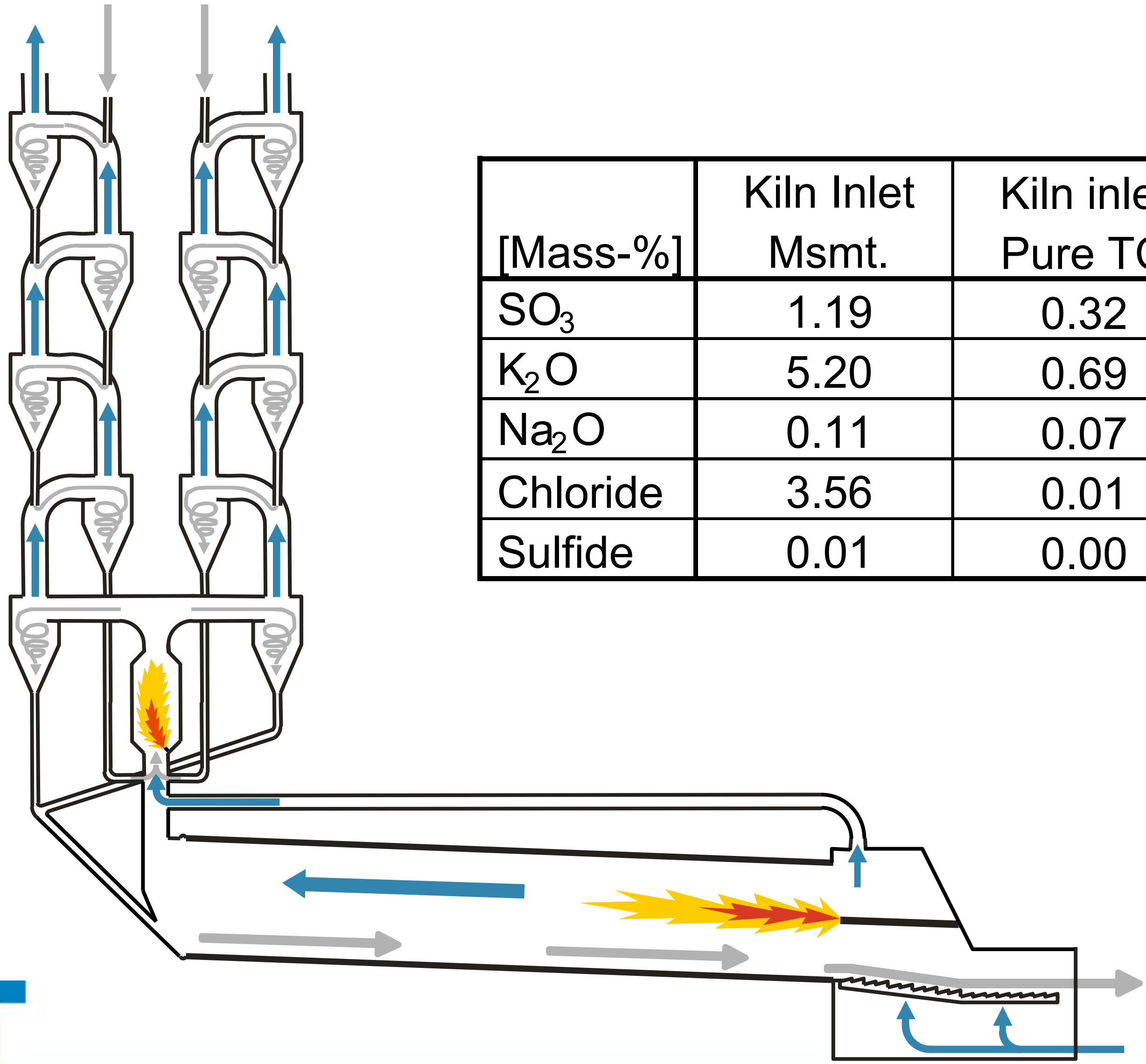
- Mass exchange by
  - Rising and depositing dust
  - Vaporizing and precipitating volatile components

Process model



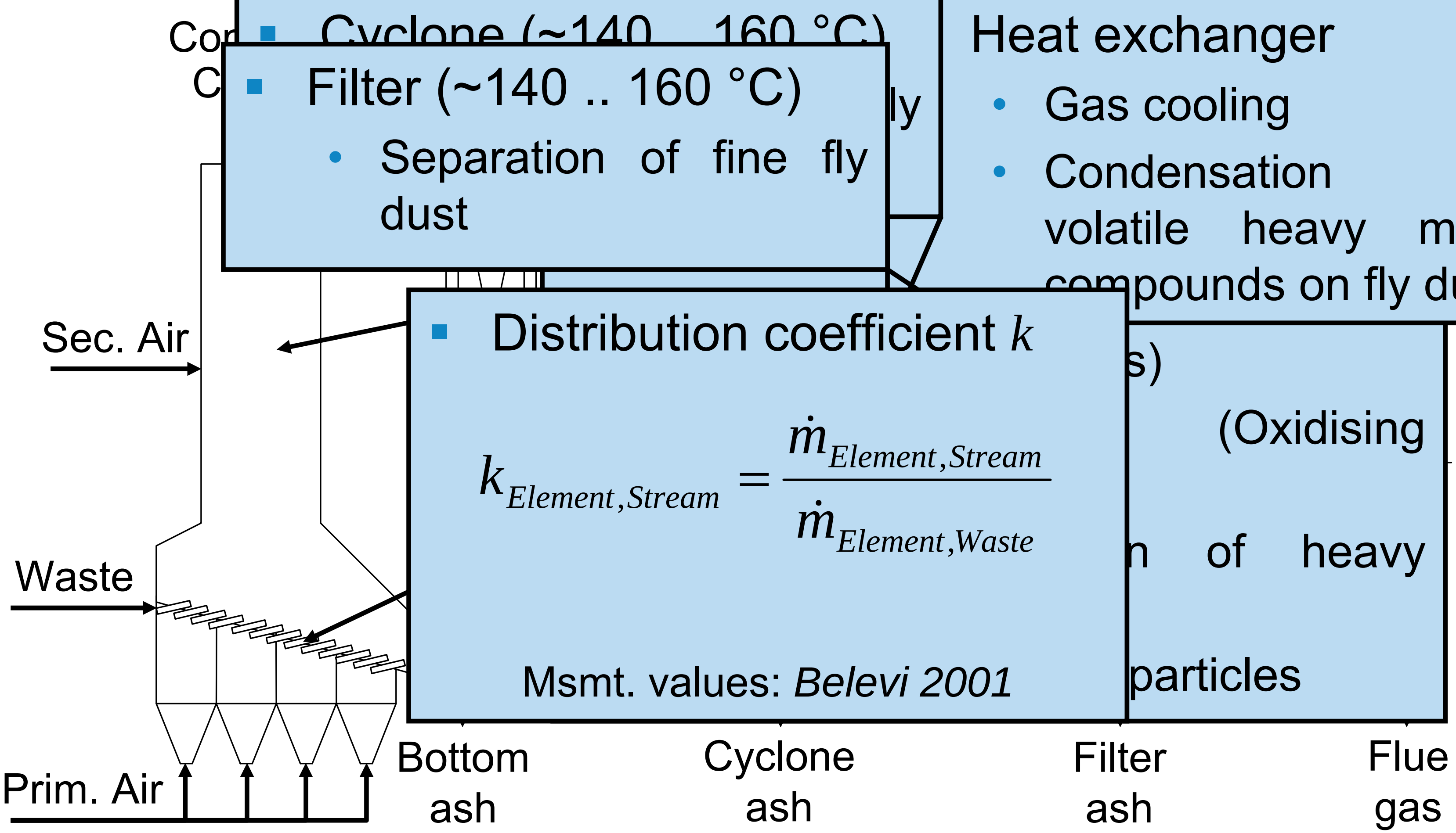
- Dust loading of gas phase — y_S = 0,2 kg Dust / kg Gas
- Gas in between solid particles (Frisch, 1983 / Brauers, 1971) — y_G = 10-4 kg Gas / kg Solid

Results – Minor components at kiln inlet



[Mass-%]	Kiln Inlet Msmt.	Kiln inlet Pure TC	Kiln inlet TC-Model
SO_3	1.19	0.32	1.40
K_2O	5.20	0.69	1.87
Na_2O	0.11	0.07	0.10
Chloride	3.56	0.01	0.92
Sulfide	0.01	0.00	0.00

Waste incineration plant



- Cyclone (~140 .. 160 °C)
  ... ly

- Filter (~140 .. 160 °C)
  - Separation of fine fly dust

Heat exchanger

- Gas cooling
- Condensation of volatile heavy metal compounds on fly dust

... s)

(Oxidising

... n of heavy

particles

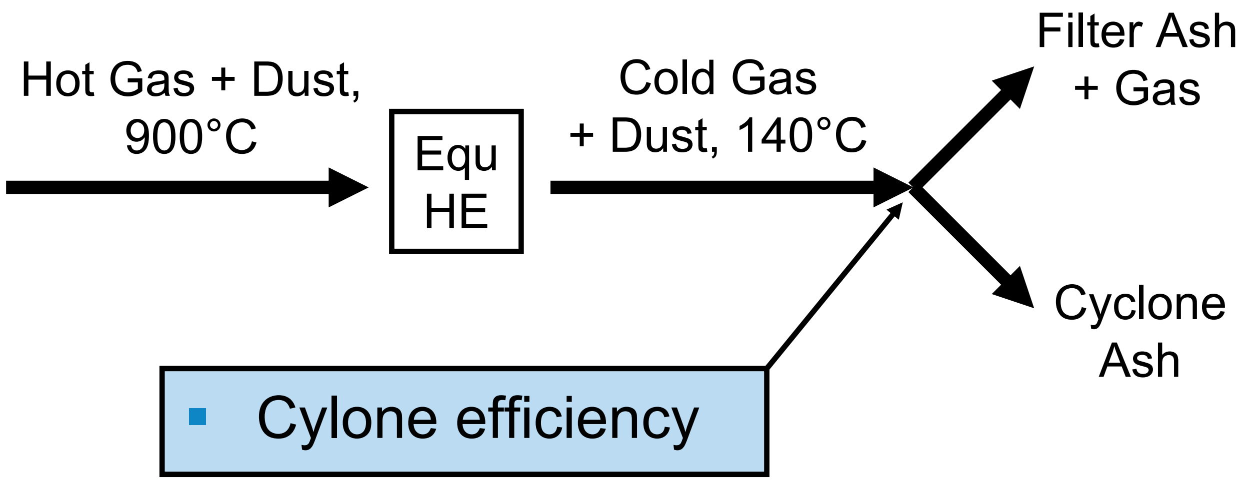
- Distribution coefficient k

$$k_{Element,Stream} = \frac{\dot{m}_{Element,Stream}}{\dot{m}_{Element,Waste}}$$

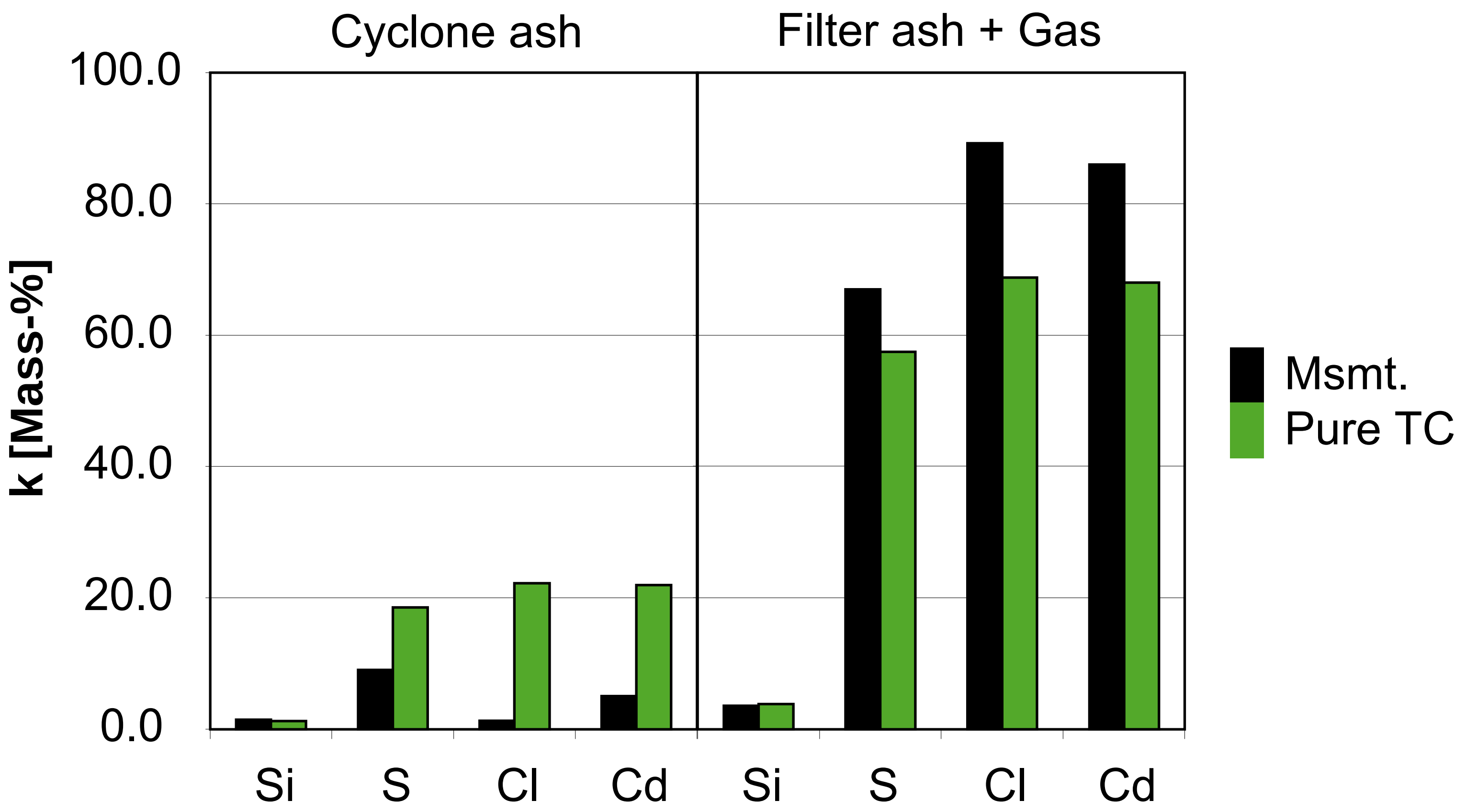
Msmt. values: *Belevi 2001*

Fly ash composition – Pure TC

- Condensation of volatile heavy metals in the heat exchanger section



Fly ash composition – Pure TC

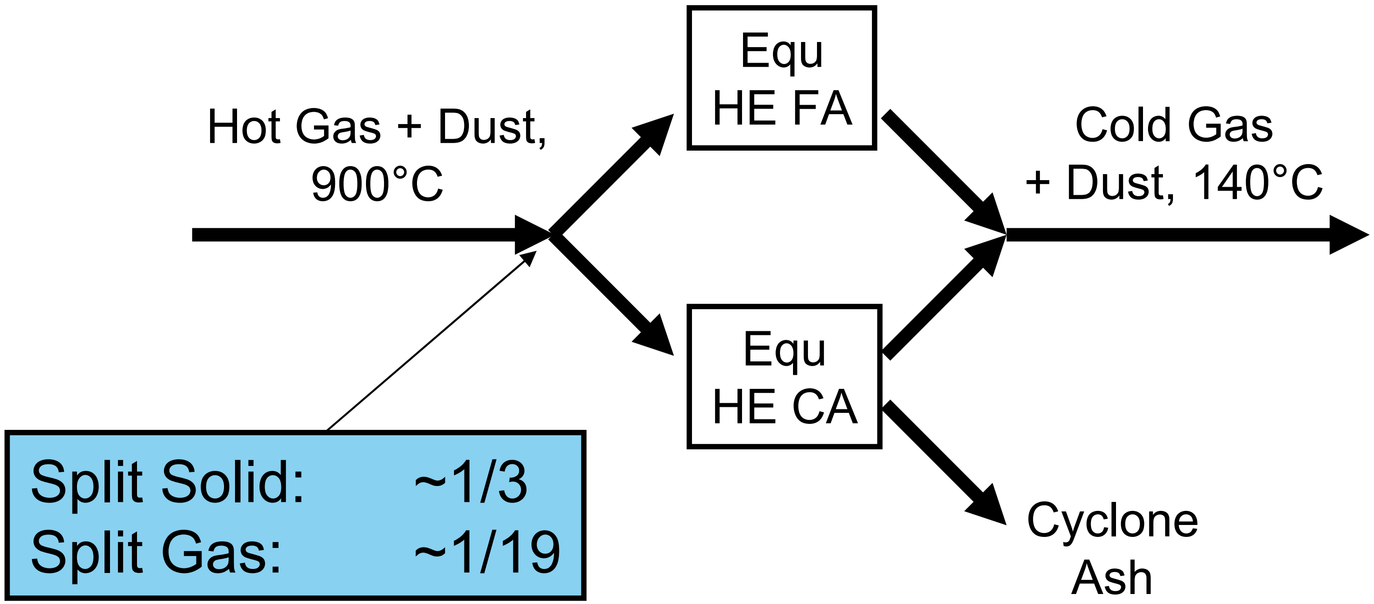


- Combustion chamber temperature: 900 °C

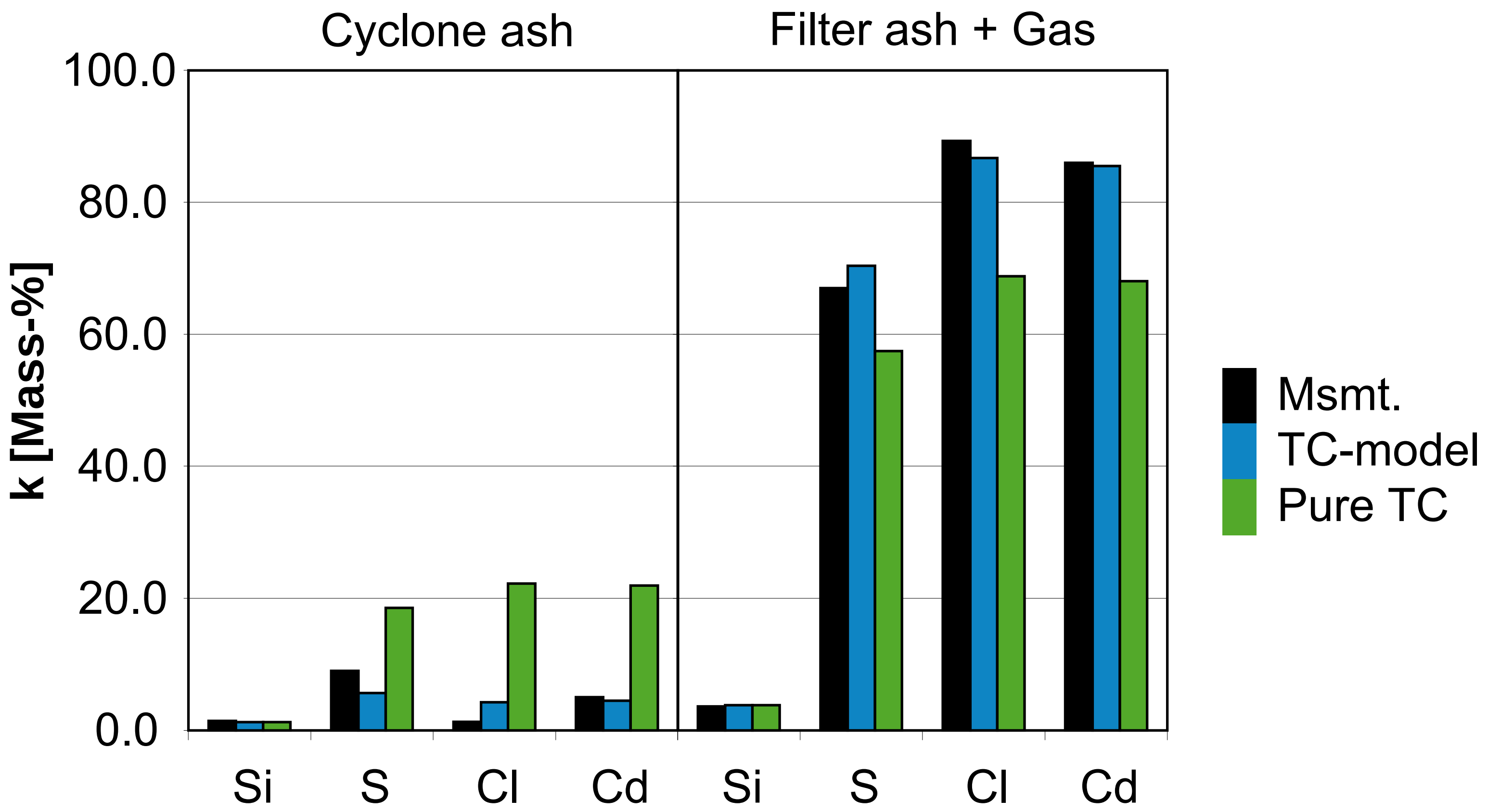
Heavy metal condensation on fly ash

- Gaseous heavy metals condense on the surface of fly dust particles
  - $$\frac{\dot{m}_{Cyclone\ ash}}{\dot{m}_{Filter\ ash}} \approx \frac{25\%}{75\%} = \frac{1}{3}$$
  - $$\frac{S_{Cyclone\ ash}}{S_{Filter\ ash}} \approx \frac{5\%}{95\%} = \frac{1}{19}$$
- Separation of heavy metal compounds
  - Solid: By mass (~ 1/3)
  - Gaseous: By specific surface area (~ 1/19)

Heavy metal condensation on fly ash

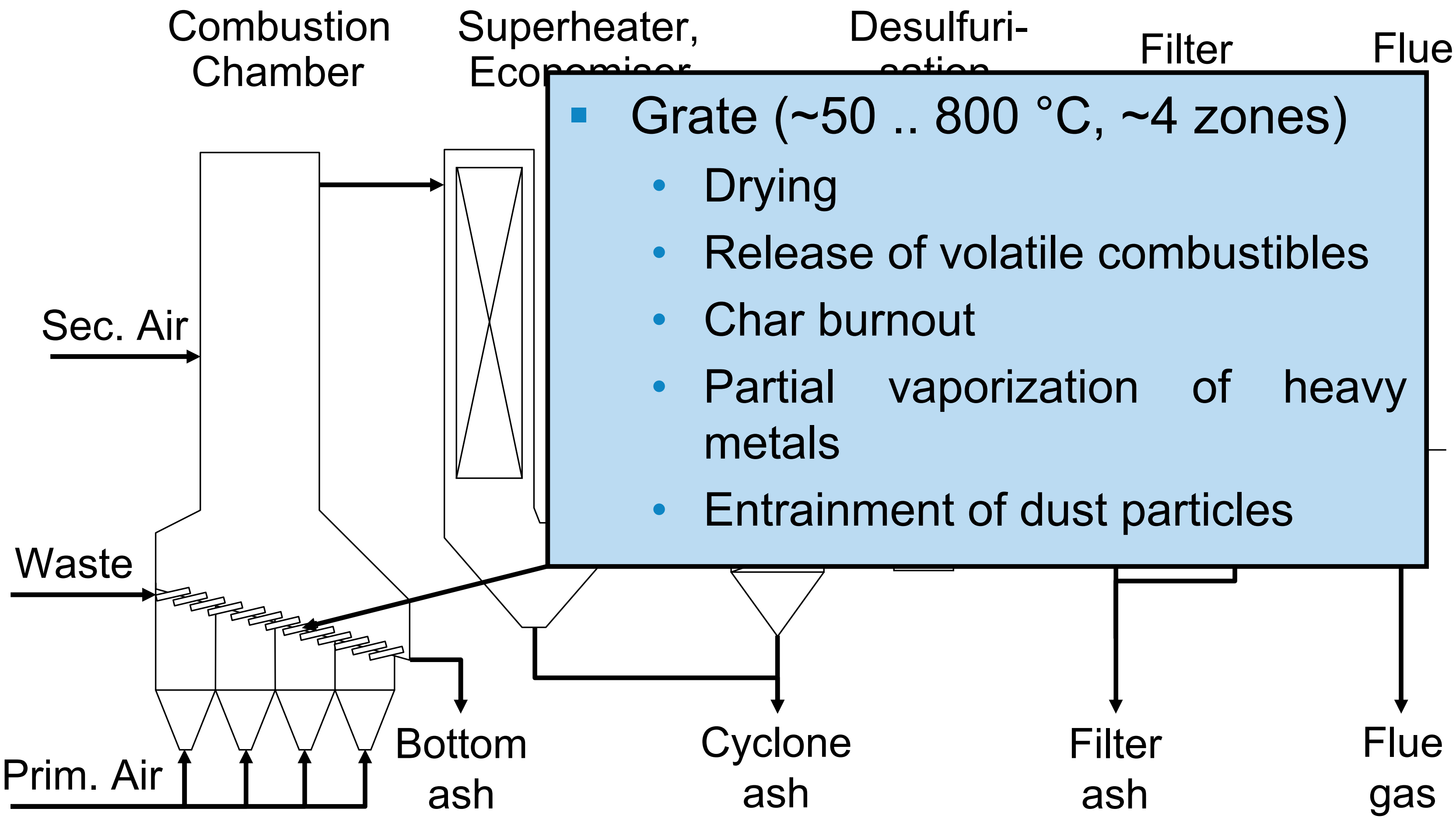


Results - Heavy metal condensation



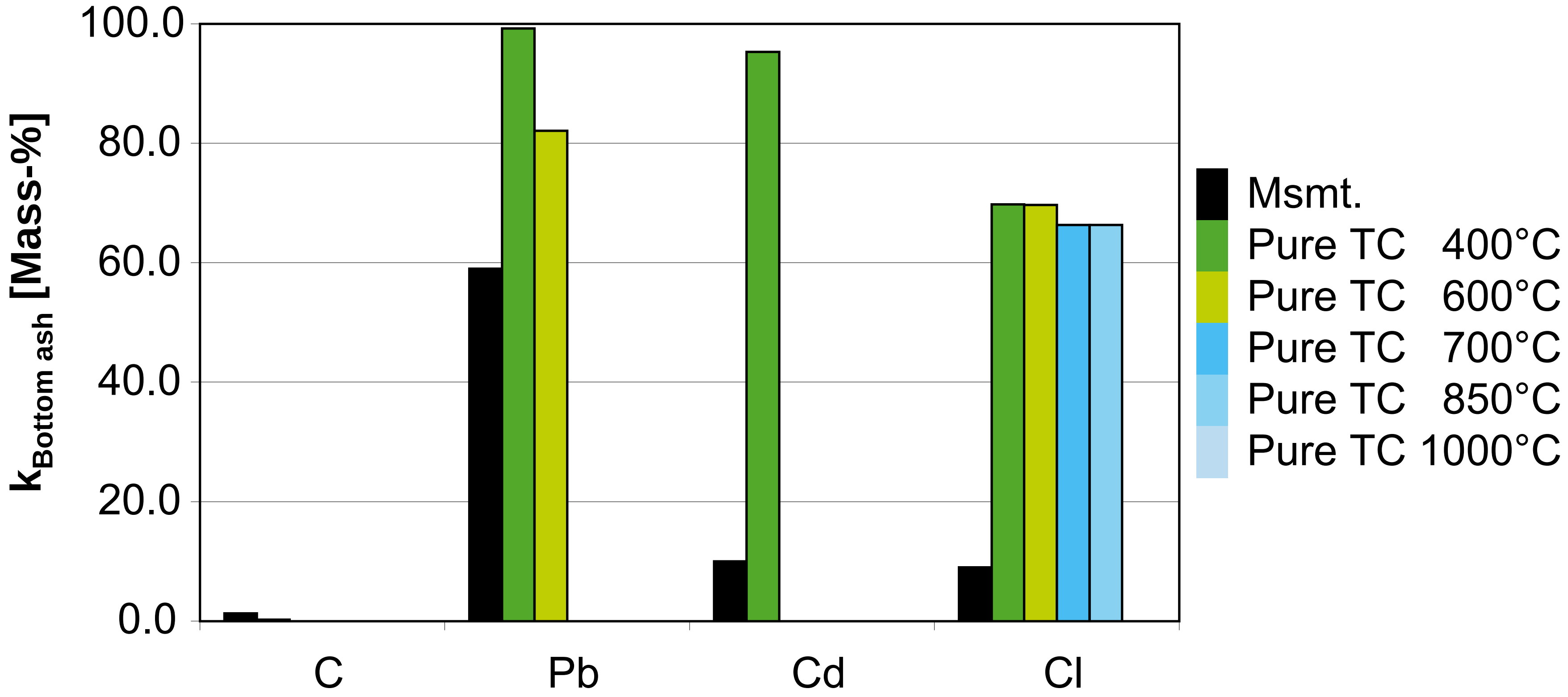
Mean Errors		Split gas phase	1/19
Pure TC	14.9 Mass-%	Split solid phases	1/3
TC-Model	6.5 Mass-%	T comb. chamb.	900°C

Grate Combustion



- Grate (~50 .. 800 °C, ~4 zones)
  - Drying
  - Release of volatile combustibles
  - Char burnout
  - Partial vaporization of heavy metals
  - Entrainment of dust particles

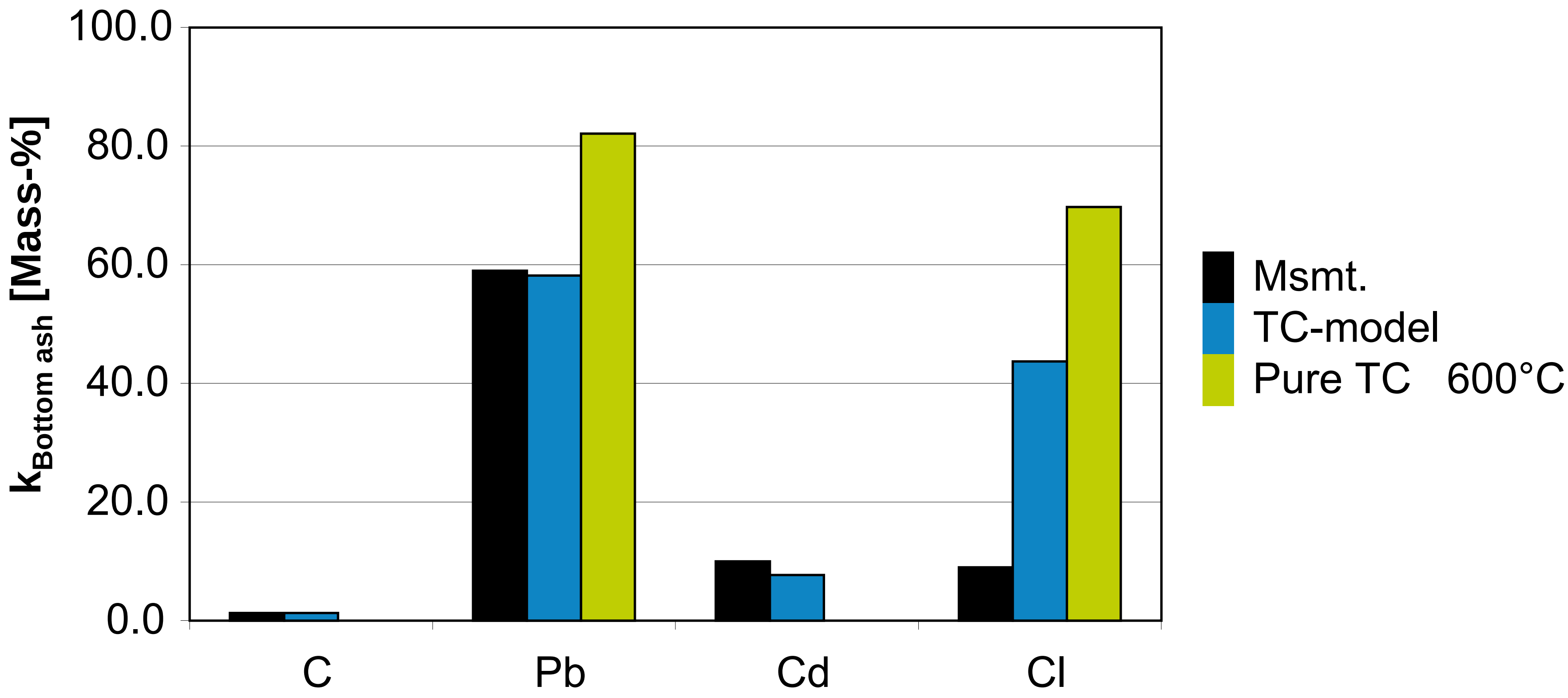
Grate Combustion – Pure TC



Grate Combustion – Qualitative Analysis

- Processes on the grate
  - Several distinct zones on the grate with separate air supply
    - ⇨ Varying temperature and oxidation conditions
  - Particles are entrained into the gas phase
    - ⇨ Fly Dust
  - Incomplete carbon burnout on the grate
    - ⇨ Residual C in bottom ash
- Modeling
  - Four equilibrium zones on the grate, different temperatures and air flow rates
  - Partial transfer of solids into the gas phase
    - ⇨ Correctly determine fly dust flow rate
  - Solid bypass around grate equilibrium zones
    - ⇨ Correctly determine residual carbon in bottom ash

Results - Grate Combustion



Mean Errors			
Pure TC	30.9 Mass-%	T Degassing Zone	620°C
TC-Model	22.2 Mass-%	T Burnout Zone	580°C

Conclusion and Outlook

- Computational thermochemistry is a strong tool to simulate the ideal behaviour of complex chemical systems
- Process analysis allows for incorporation of non-idealities by means of a properly chosen model structure and few simple and plausible assumptions

⇨ Significant improvement of modeling results

- Further improvement is possible but requires disproportion-ately more information
  - e.g. in grate combustion Cl is much easier released from PVC than from NaCl or KCl

AACHENER VERFAHRENSTECHNIK

Thank you
for your attention!