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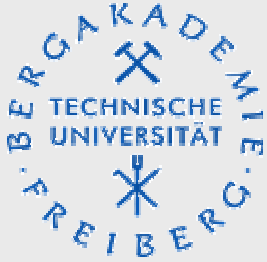

Using SimuSage for the modelling of diverse processes in energy conversion

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Content

- General steps in thermochemical modelling
- Slagging and fouling behaviour in a pulverized coal-fired boiler
- Slagging and fouling behaviour in pulverized coal-fired boiler for co firing of biomass
- Modelling of BGL-gasification processes - alkali metal cycle

General steps in thermochemical modelling

Why FactSage™ and SimuSage™ ?

FactSage™

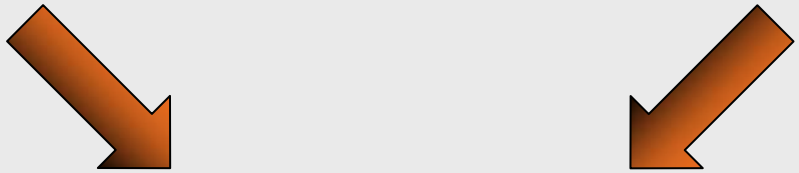
- Thermochemical databases

➢ Data file

SimuSage™

- local equilibrium stages
- material streams
- mixer, splitter, iterator

➢ interacting of single stages (recirculation, counter flow)
➢ Load/Save of interim results
➢ direct connecting to Excel™ (convenient result files, parameter calculations)

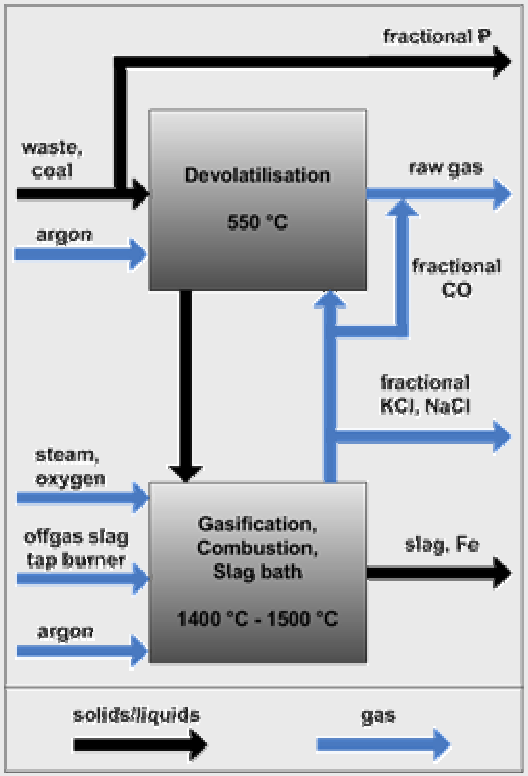


Thermochemical Model

General steps in thermochemical modelling

Real process

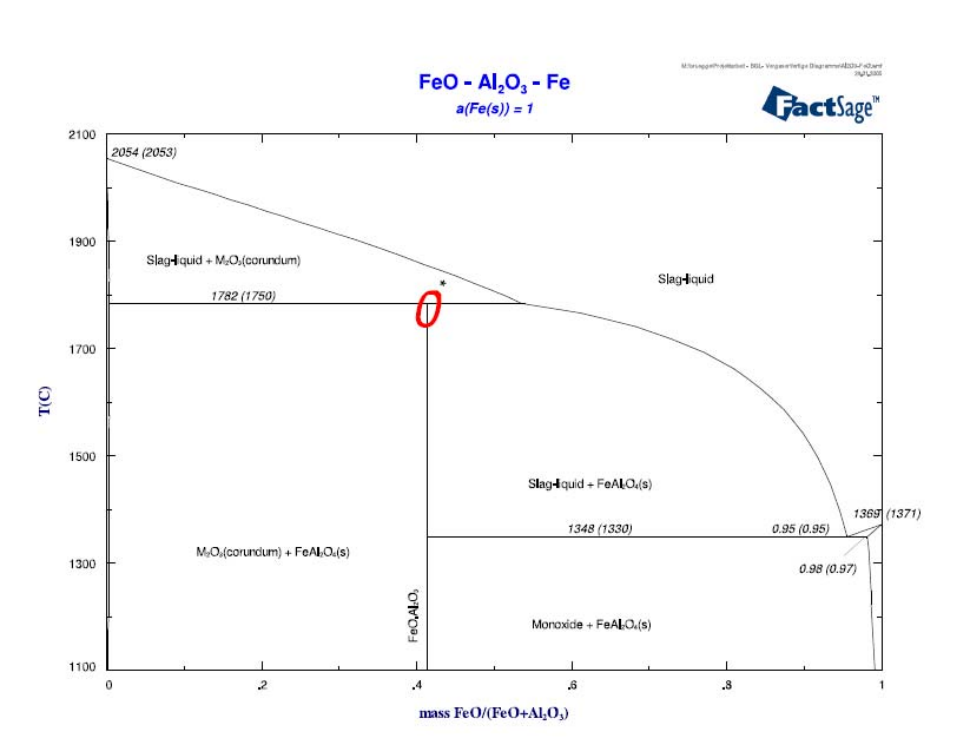
- Material balance, process parameters (as much information as possible, XRF, XRD…)
- Flow sheet for Stage Model
  - assembling of equilibrium units
  - isothermal/isenthalpic/isochoric?
  - definition of material flows
  - Equilibrium ?



General steps in thermochemical modelling

- selection of elements and possible products (solution phases!)
- rough calculation (reducing product list, equilibrium?)
- check thermodynamic data (calculation of binary and ternary systems, comparison to literature)

➢ **data file**

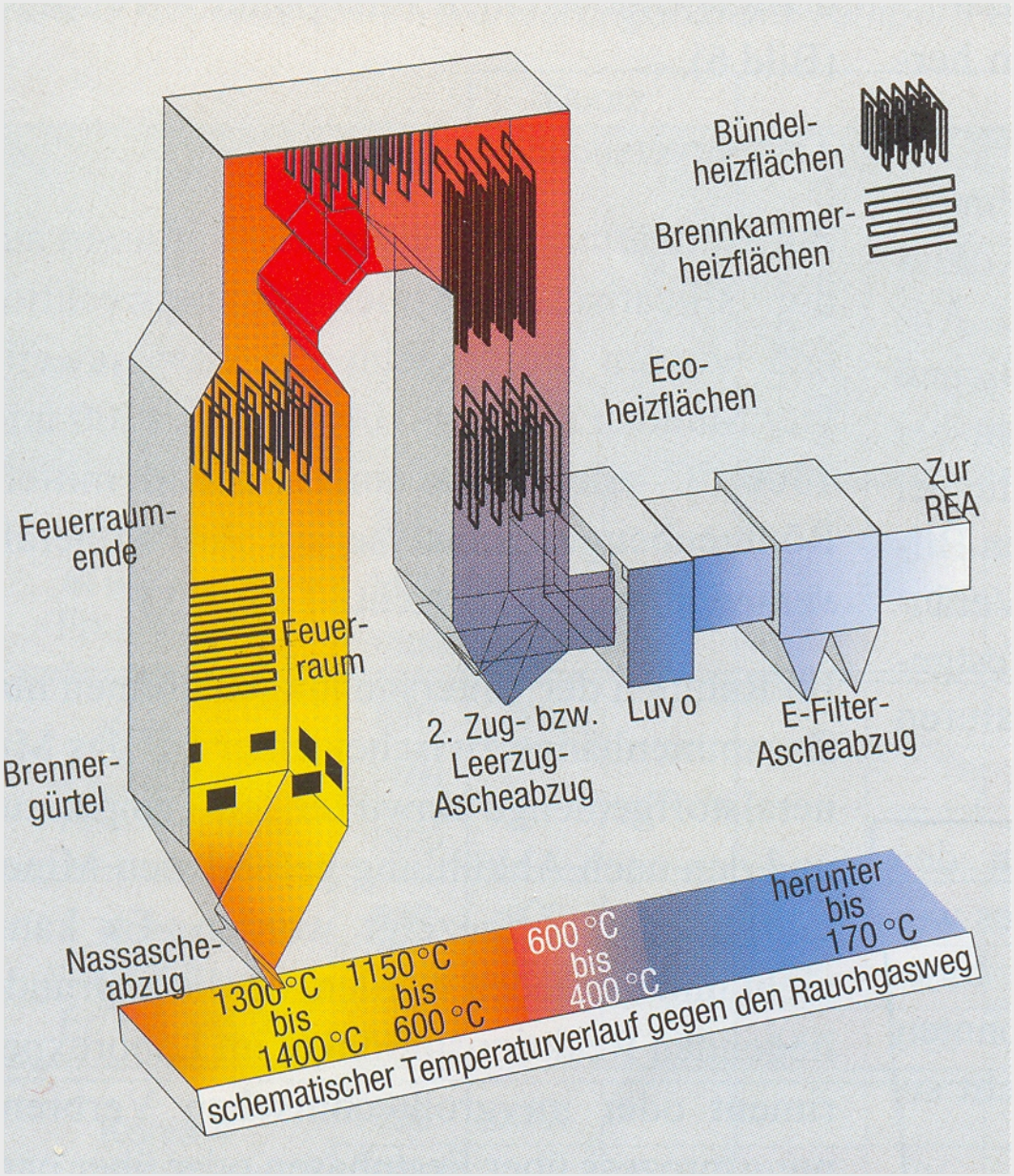


General steps in thermochemical modelling

SimuSage™

- definition of equilibrium stages
- definition of input and material flows
- adjusting equilibrium stages to non-equilibrium conditions (bypass, eliminated phases)
- evaluation with process data/samples (HT-XRD)
- application of the validated model

Slagging and fouling behaviour in a pulverized coal-fired boiler

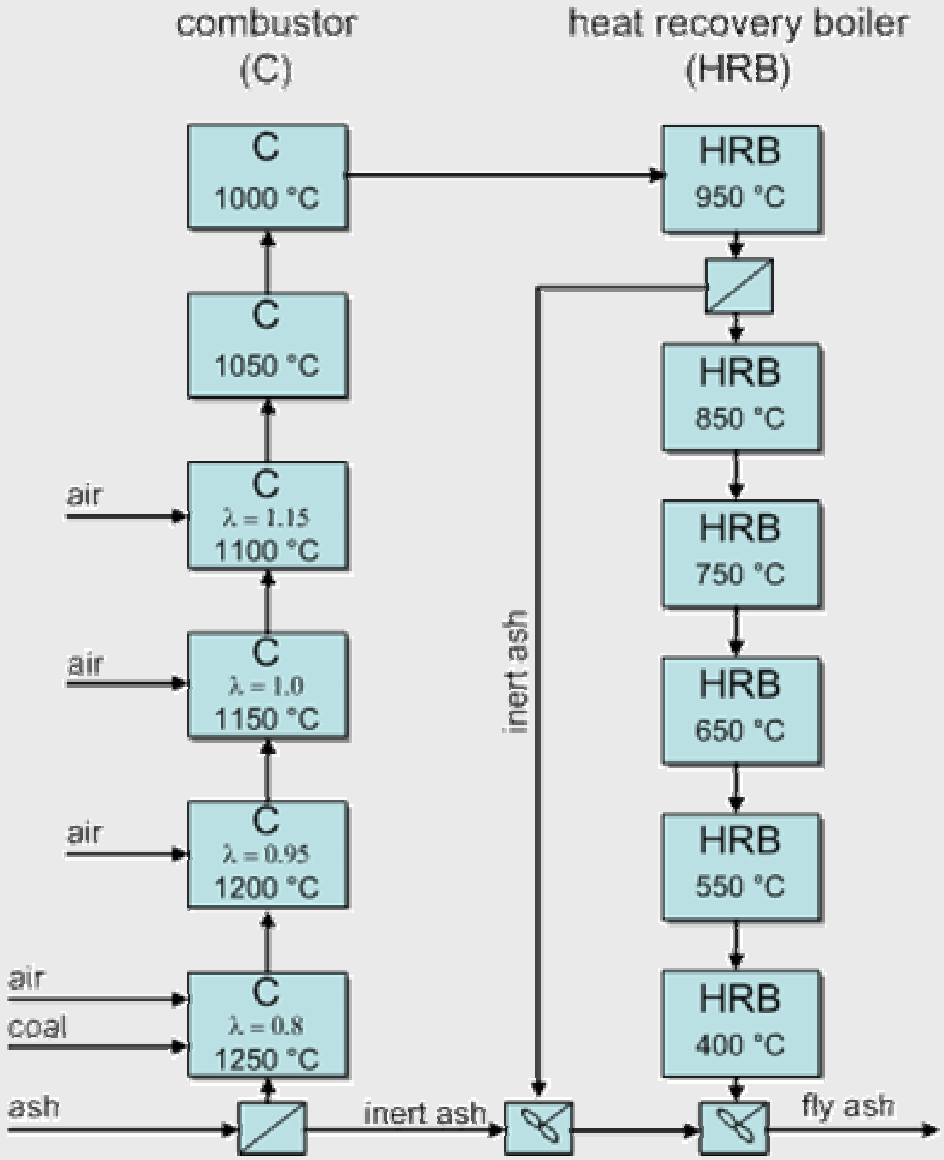


Model of pulverized coal-fired boiler (Dr. Muhammadieh)

- estimation of slagging and fouling for different coal mixtures
- kinetic inhibition for ash components is considered
- evaluated with HT-XRD of coal ashes and process samples
- development of classification numbers for the estimation of the slagging and fouling behaviour of new coal mixtures

Reference: M. Muhammadieh; 2007, "Beitrag zur Ermittlung des Ansatzbildungspotenzials von Braunkohlen in Dampferzeugern"; Dissertation TU-Freiberg [1]

Slagging and fouling behaviour in a pulverized coal-fired boiler

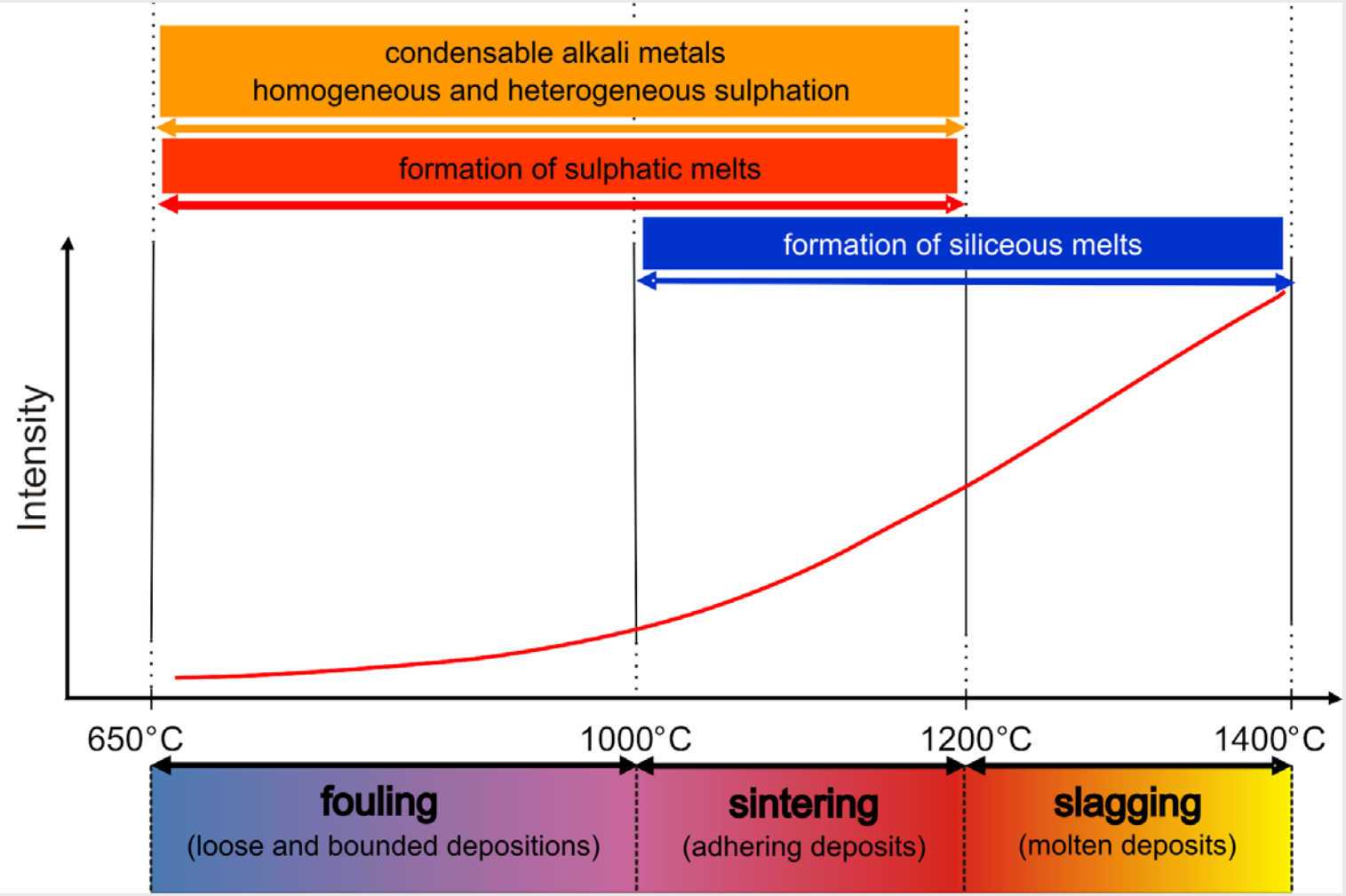


Reference: [1]

Definition of inert ash:

- fractionation of raw ash
- analysis of ash fraction (XRF, HT-XRD, AFT)
- definition of particle-size-effects
  - coarse ash fraction (quartz, layered silicates, siderite) as inert ash
  - fine-grained fraction (silt, clay) as reactive ash

Slagging and fouling behaviour in a pulverized coal-fired boiler



Reference: [1]

Classification numbers:

Slagging potential (T) = Fraction of siliceous melts * Ash fraction in coal

Fouling potential (T) = Fraction of sulfatic melts * Ash fraction in coal

Model of pulverized coal-fired boiler and estimation of the co-combustion of biomass on the slagging and fouling behaviour (Dr. Schreiner)

actual state: pulverized coal-fired boiler (hard coal – mixtures)

additional biomass feeding:

- external pyrolysis of wheat straw
- gaseous pyrolysis products to combustor
  - ➢ low alkali metal input

Model development:

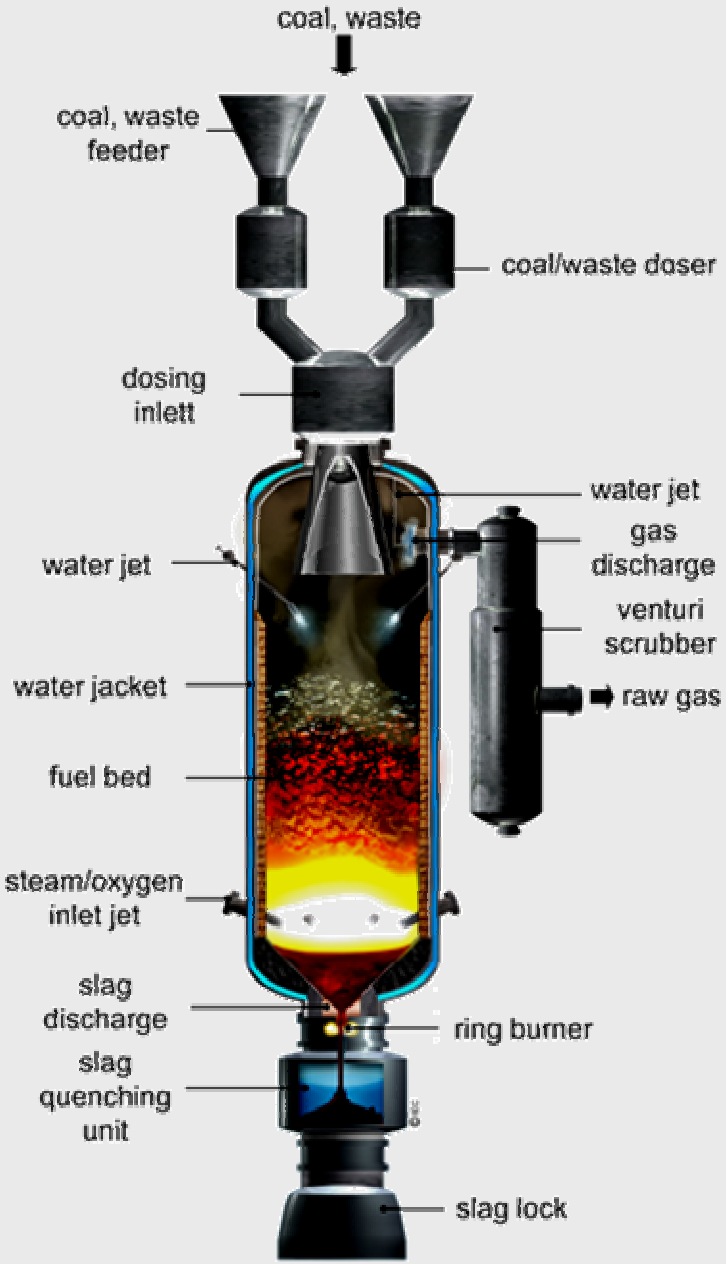
- modelling of the hard-coal combustion, based on the previous shown model
- validating of the model
- implementing the gaseous pyrolysis products into the model
  - amount and composition (K, Na, Cl, S) from laboratory tests and test facility
- estimation of the slagging and fouling behaviour for the biomass feeding

Modelling of BGL-gasification processes - alkali metal cycle

- Motivation: deposit in the British Gas-Lurgi gasifier of the Sustec-Schwarze Pumpe-GmbH linked to alkali metal condensation
  - ➢ description of alkali metal volatilisation and condensation

- related problems in processes with reducing atmosphere:
  - deposit at raw gas heat exchangers (Shell/Texaco)
    - ➢ reduced efficiency
    - ➢ pressure trop
  - accumulation of alkali metals in blast furnaces
    - ➢ coke-stability
    - ➢ deposit reduce fix bed diameter
    - ➢ evaporation/condensation affects energy distribution

Modelling of BGL-gasification processes - alkali metal cycle



- **operating pressure: 24 bar**
- **raw gas temperature**
  - **at discharge: 550 °C**
  - **after scrubber: 200 °C**

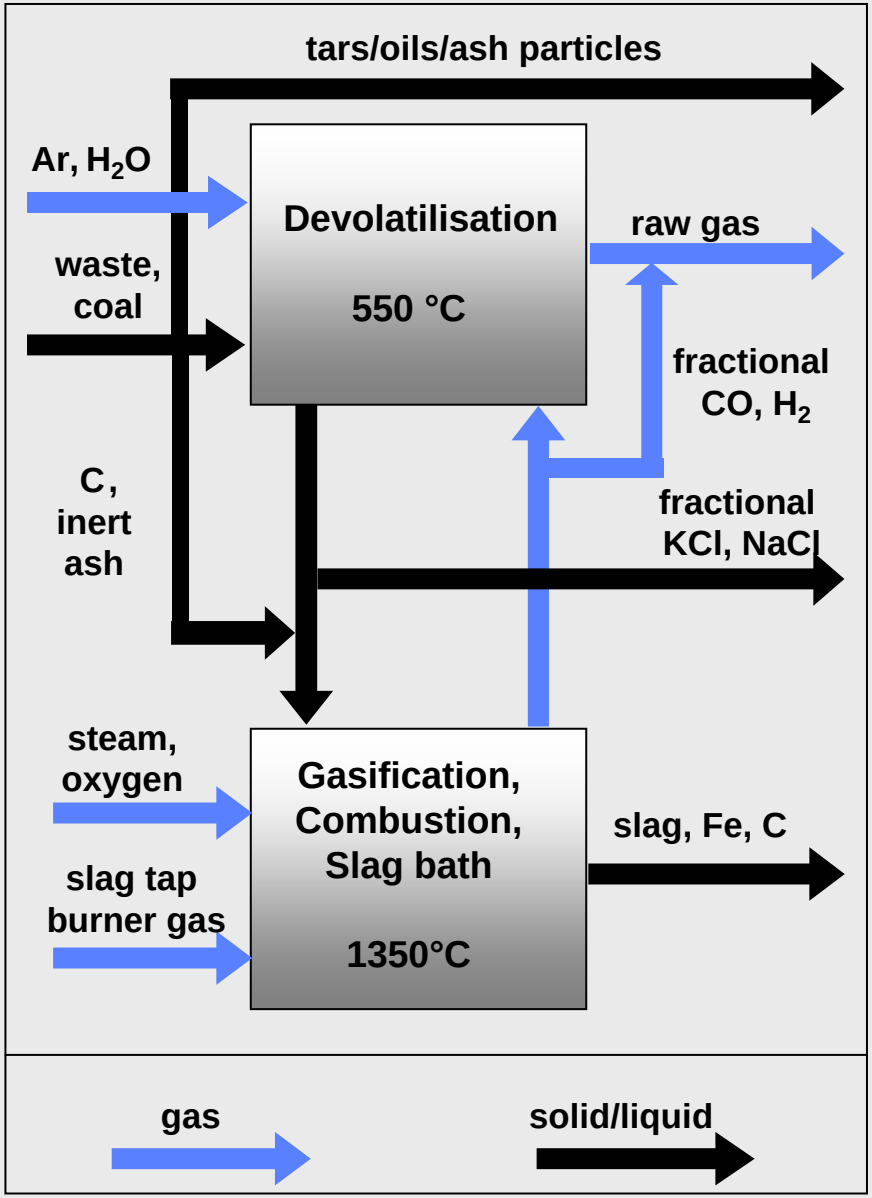
In:

- **MSW + coal: 24 - 30 t/h**
- **oxygen: 4000 - 6000 m³/h STP**
- **steam: 3.2 - 4.8 t/h**
- **steam-oxygen ratio: 0.8 – 1.2 kg/m³ STP**

Out:

- **raw gas: 35000 - 44000 m³/h STP, wf.**
- **slag: 3 – 5 t/h**

Modelling of BGL-gasification processes - alkali metal cycle

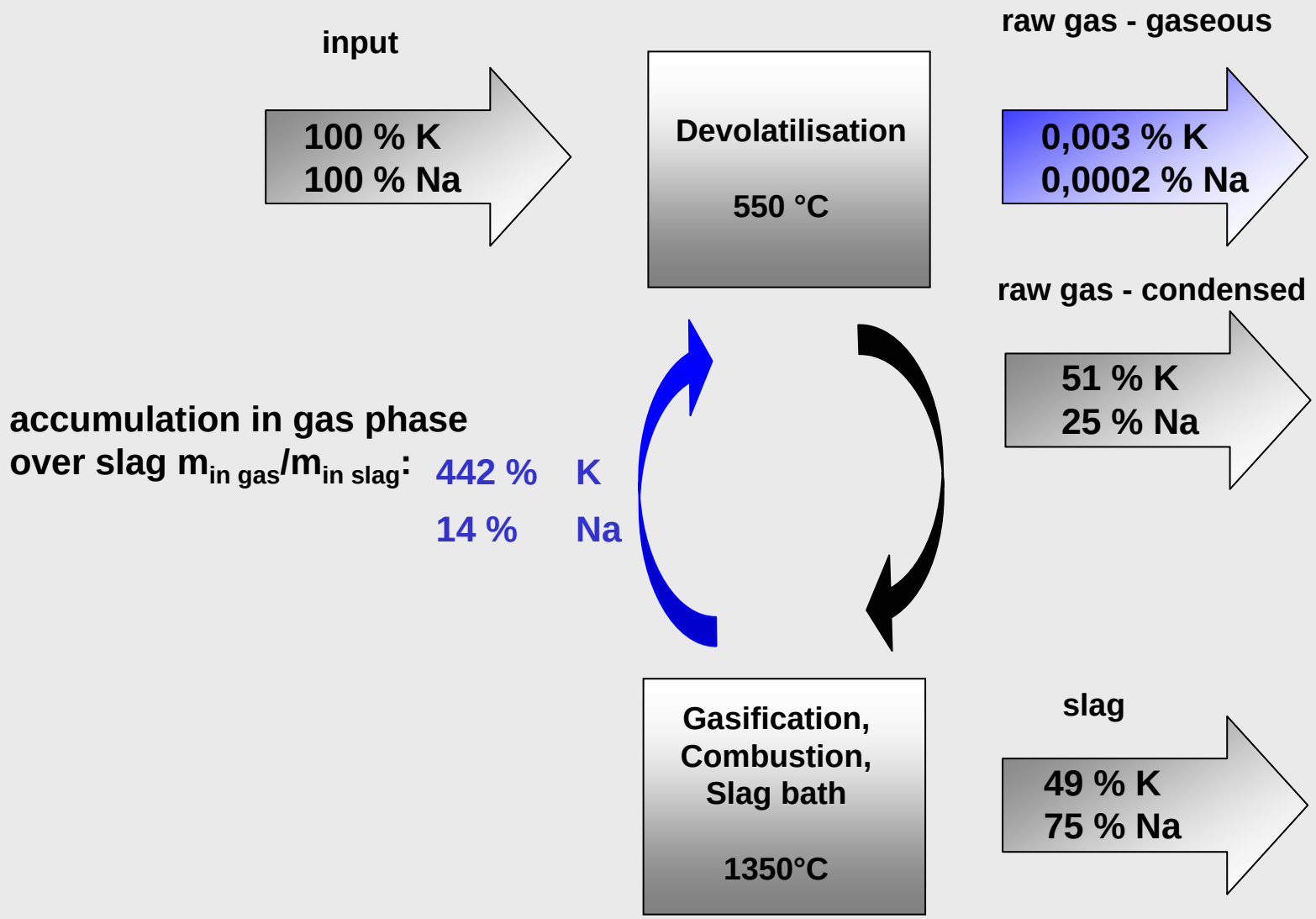


- kinetic inhibitions for permanent gases in cold stage: bypass for CO, H_2 and elimination of graphite, compensation with argon for constant partial pressures
- direct C-Input for hot stage
- bypass for tars and oils, ash of non-volatiles (material balance of process samples)
- condensed volatile ash components

  $$m_{\text{i kond. inTÖF}} = m_{\text{i,IN}} - m_{\text{i in slag}} - m_{\text{i in gas}}$$
- kinetic inhibitions for non-volatile ash components

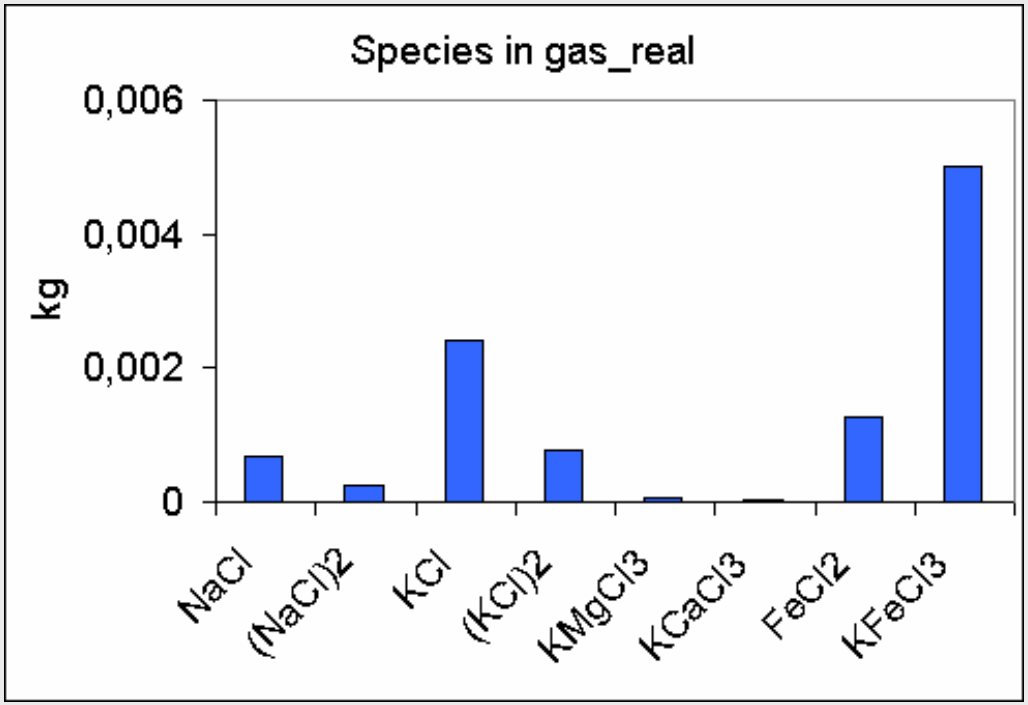
Modelling of BGL-gasification processes - alkali metal cycle

- Distribution of K and Na on outlet streams and accumulation in alkali cycle:



Modelling of BGL-gasification processes - alkali metal cycle

- Gaseous and condensed volatiles in raw gas:



	mg/m³ STP
K-Species gaseous	0.22
Na-Species gaseous	0.023
KCl condensed	4003
NaCl condensed	3774

Modelling of BGL-gasification processes - alkali metal cycle

- Composition of the slag stream (amount in kg):

ASlag-liq	**5187**
MgO	151
FeO	26
(Na2O):2.000	152
SiO2	2251
TiO2	72
CaO	1585
(Al2O3):2.000	789
(K2O):2.000	54
MgS	3
CaS	32
FeS	1
(Na2S):2.000	3
(K2S):2.000	1
NaCl	5
KCl	1
CaCl2	50
MgCl2	6
FeCl2	1

Fe-liq	**271**
Fe	226
C	9
Cu	19
Al	5,E-06
N	1,E-02
P	11
S	1,E-02
Si	1,E-03
Ti	7,E-05
O	1,E-03
SiO	3,E-06
FeS	6
C_graphite(s)	**216**

Modelling of BGL-gasification processes - alkali metal cycle

- Composition of the gas phase in the hot stage:

Spezies K	kg
KCl	330
(KCl)2	55
KCaCl3	13
KMgCl3	3.E-01
KFeCl3	2.E-01
KCN	2.E-01
K	1.E-01
KOH	2.E-02
KH	8.E-04
KAlCl4	2.E-04
(KCN)2	3.E-06

Spezies Na	kg
NaCl	39
(NaCl)2	1
NaCN	1.E-01
Na	5.E-02
NaMgCl3	8.E-03
NaOH	2.E-03
NaH	7.E-04
Na2MgCl4	2.E-04
NaAlCl4	2.E-05
NaFeCl4	1.E-05
(NaCN)2	3.E-06

- partial pressure K-species: 0.127 bar
- partial pressure Na-species: 0.018 bar

➢ concentration of alkali metal species as information for corrosion mechanisms of refractory lining

Thank you for your attention!

Questions?

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