MODELLING OF INDUSTRIAL THERMAL PROCESSES- THE IMPORTANCE OF INPUT DATA

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OUTLINE

- ✓ **Background**
- ✓ **Objectives**
- ✓ **Approach * 3**
- ✓ **Results**
- ✓ **Conclusions**

BACKGROUND

- ✓ **Thermal processes as combustion of waste- and biofuels lead to ash related problems:**
  1. Bed Agglomeration
  2. Fouling
  3. Corrosion
- ✓ **Pyrolysis and gasification gives tars and carbon rich solid products containing ash.**

- ✓ **Experimental methods reveal valuable information regarding ash-related problems in thermal system**

- ✓ **But, full understanding of mechanisms behind ash transformation behaviour is not attainable by experimental methods**

BACKGROUND

Modelling can be a good help to understand real processes:

- ✓ Computational Fluid Dynamics, CFD, is used to se the flow scheme, temperature gradients etc.

- ✓ Thermodynamic equilibrium modelling to model what compounds are formed at specific conditions

    -Temperature

    -Pressure

    -Composition

NOTE! Thermal equilibrium is only valid at high temperatures! $\geq$ 400°C

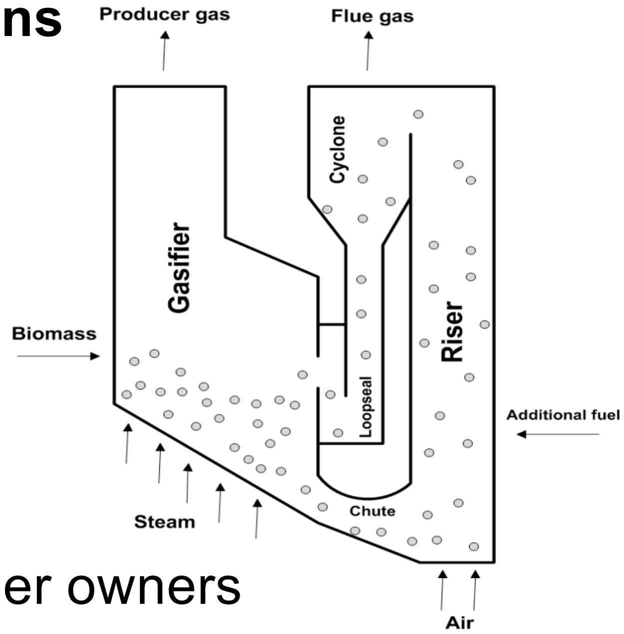
OBJECTIVE

- ✓ **Model thermal processes in Fluidized Bed applications**
  - -Bubbling fluidized Bed (BFB) Boiler
  - -Circulating fluidized bed (CFB) boiler
  - -Dual fluidized bed (DFB) gasifier

- ✓ Compare with full scale operation (or lab scale)

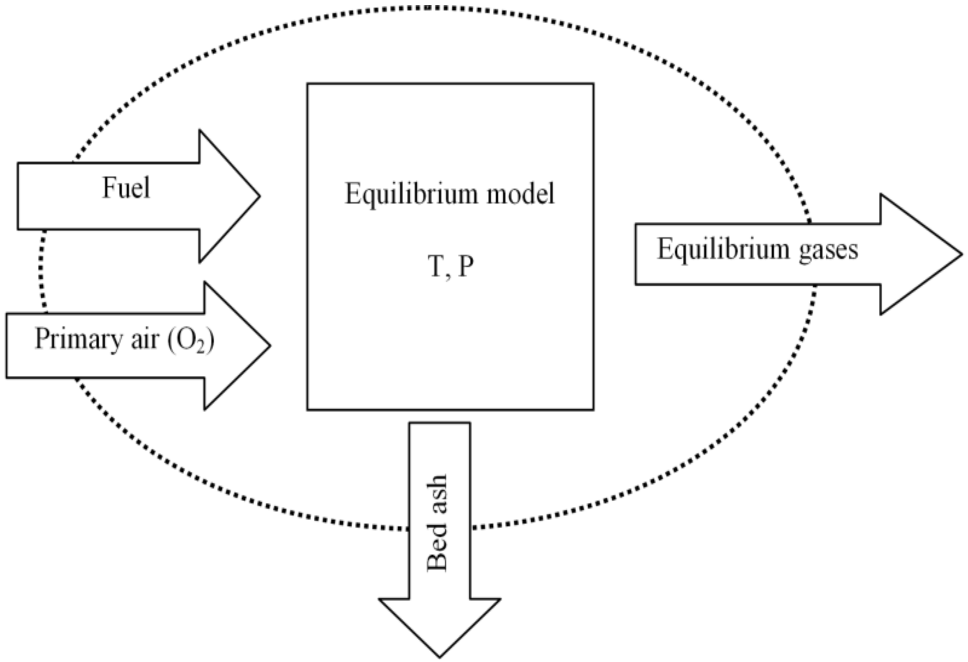
- ✓ Find suitable models that are useful for boiler and gasifier owners

DFB



APPROACH

- ✓ **Find the boundaries of the new model**
- ✓ **Find relevant data for the real process**
  - -Temperature profile
  - -Fuel flows and composition
  - -Air/fuel ratio
  - -Pressure
- ✓ **Decide and evaluate input data!!!!**



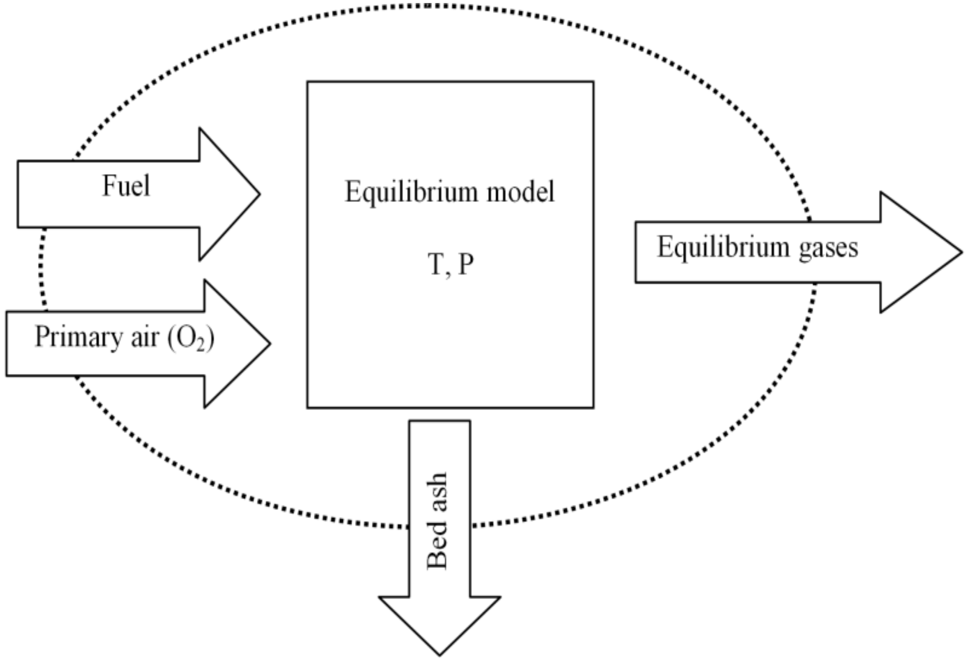
APPROACH

Input data are most important because:

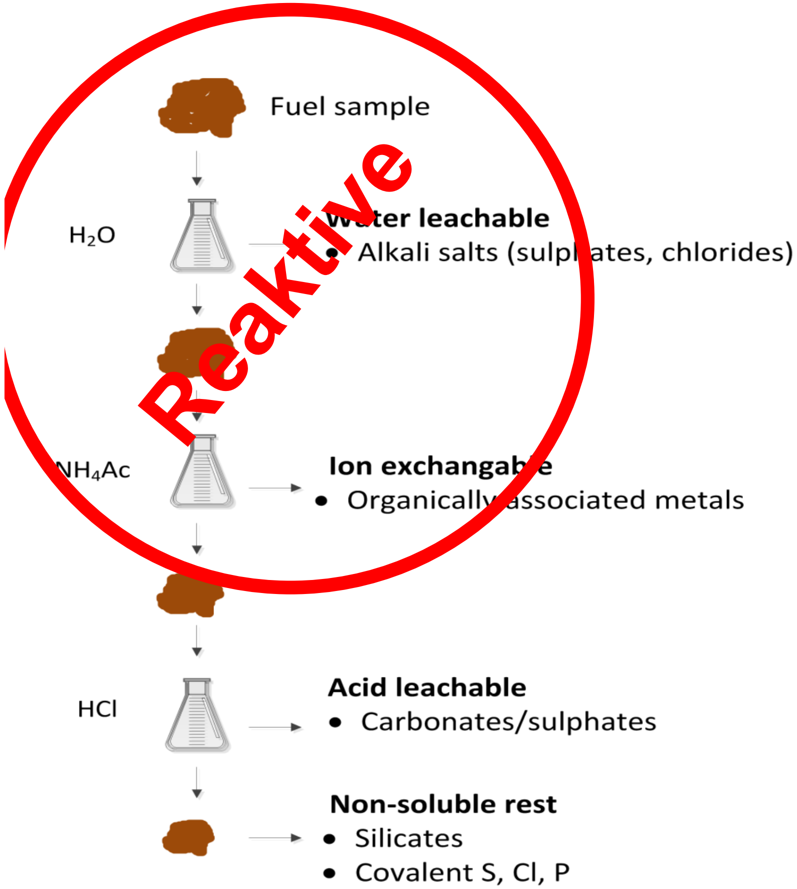
✓ They decide what elements are available
- O
- S
- Ca
- Cl

✓ What compounds can be formed

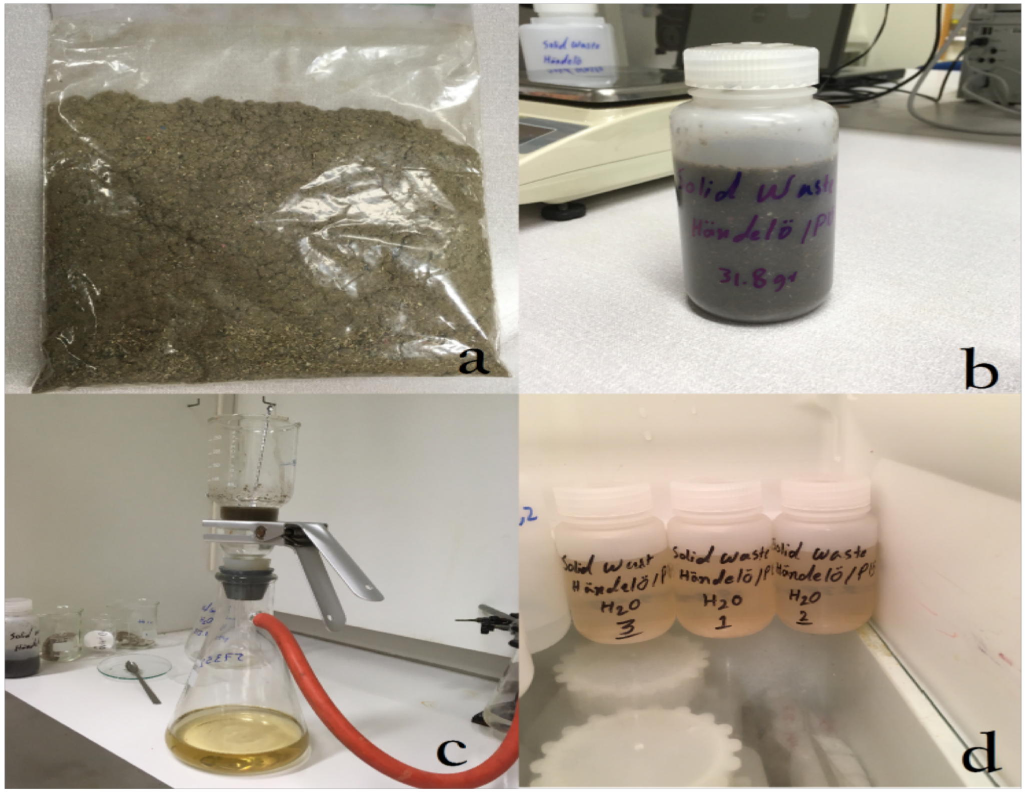
Shit in → shit out!



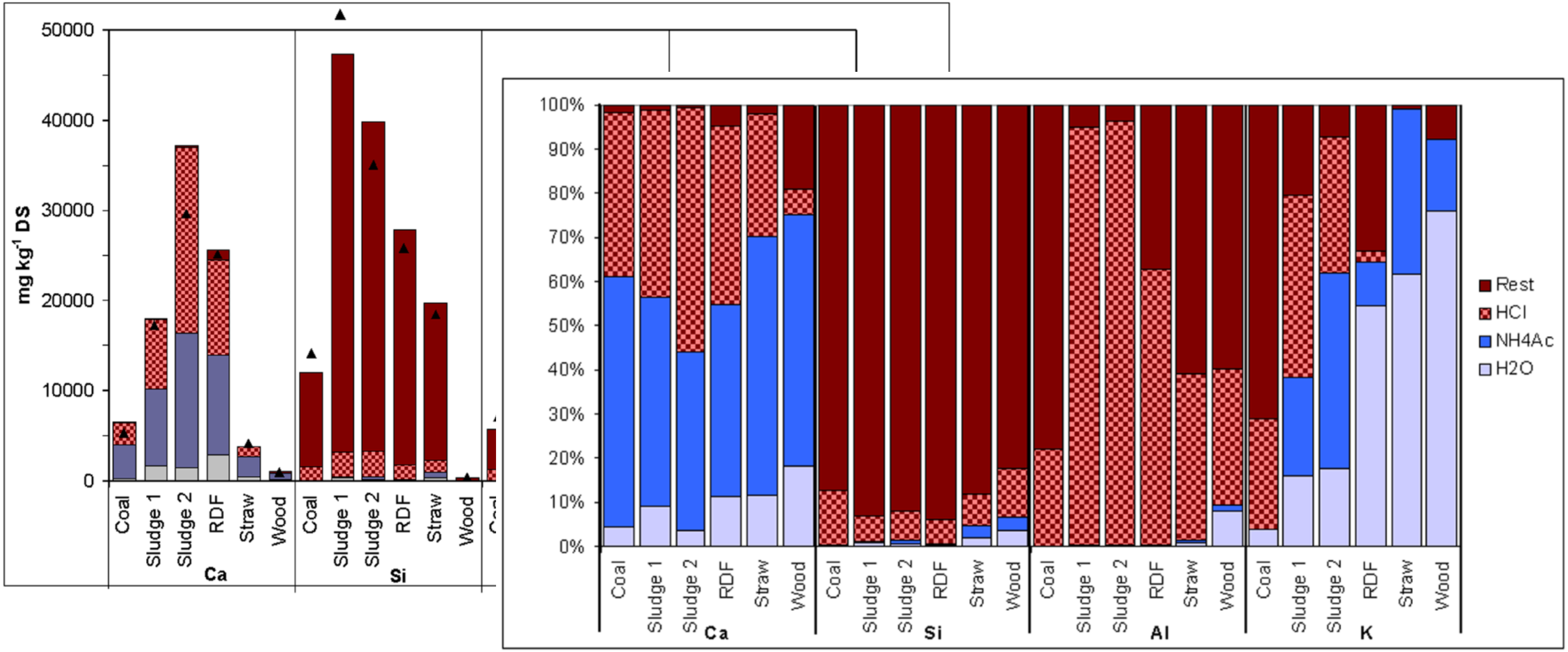
APPROACH



CHEMICAL FRACTIONATION

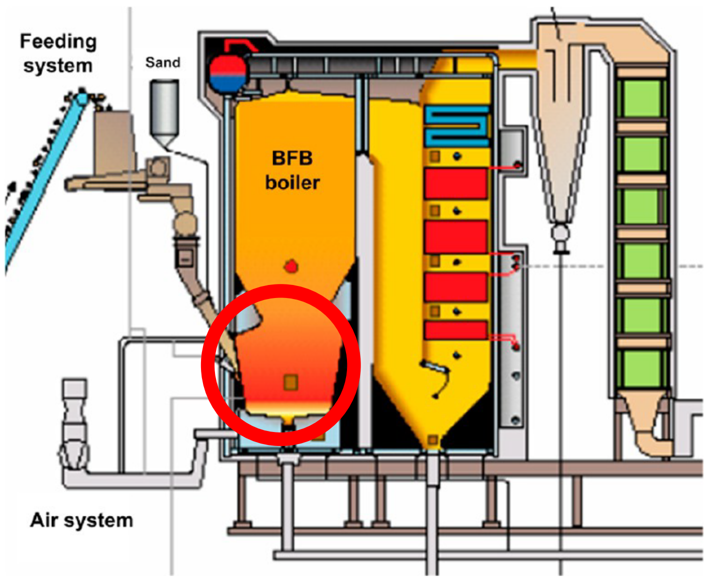


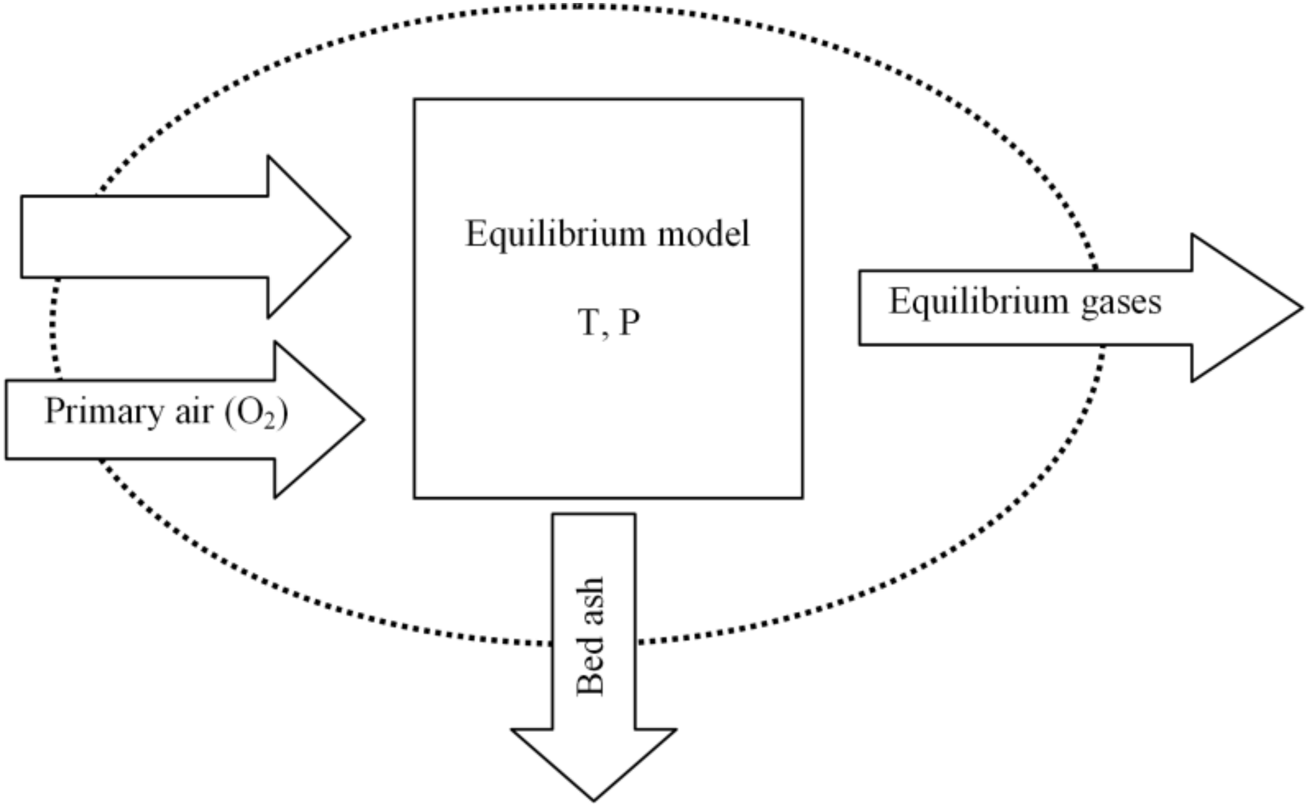
APPROACH CHEMICAL FRACTIONATION



APPROACH IMPROVED MODEL MODEL 1

Reaktive part of the fuel!





APPROACH

MODEL 2

1

40% of Fuel (RF)

2

Secondary and Tertiary Air

3

60% of Fuel (RF)

Primary air

Bed Zone (eq1)

$T=T_{bed}$
P=1 atm

Gas Phase

Freeboard (eq2)

$T=T_{Freeboard}$
P=1 atm

Gas Phase

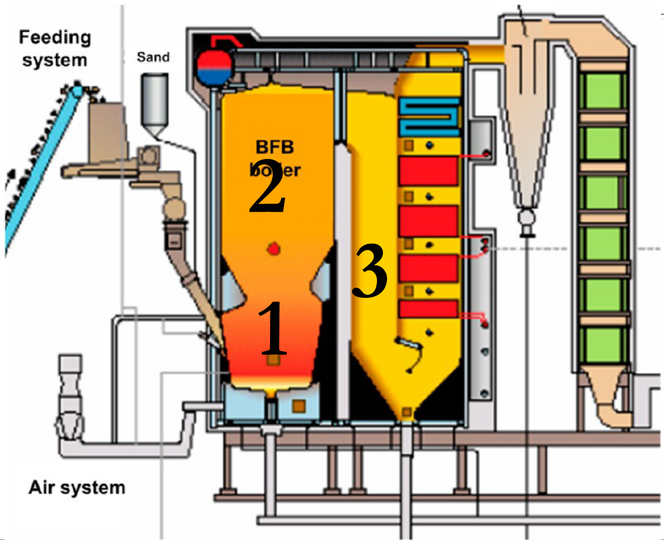
Gas Phase Cooling Down (eq3)

(1000 – 350 °C)

Fouling Prediction

Condensed Phase

Condensed Phase



Assumptions for the model!

APPROACH DATABASES

Important to choose the right databases

Often used by us:

For stoichiometric gas and the condensed phase

FactPS

FToxide

FTsalt

For solid and liquid (molten) solution phases

FToxide-SLAFGA

FT-salt-CSOB

FT-salt-SALTF

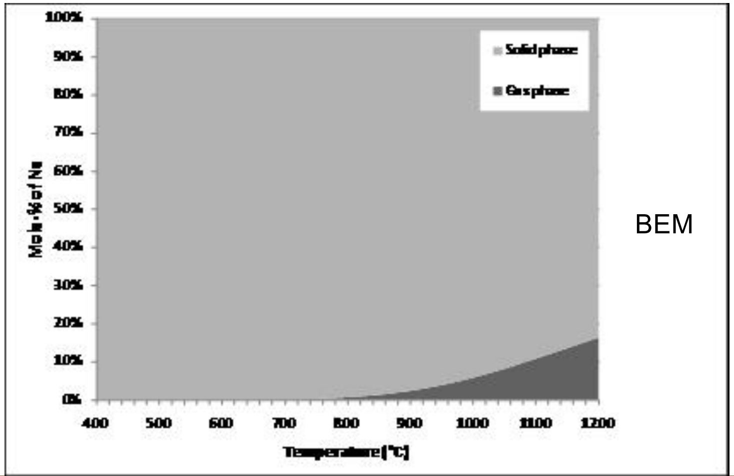
APPROACH SENSITIVITY ANALYSES

Sensitivity analyses of the input data has to be done!

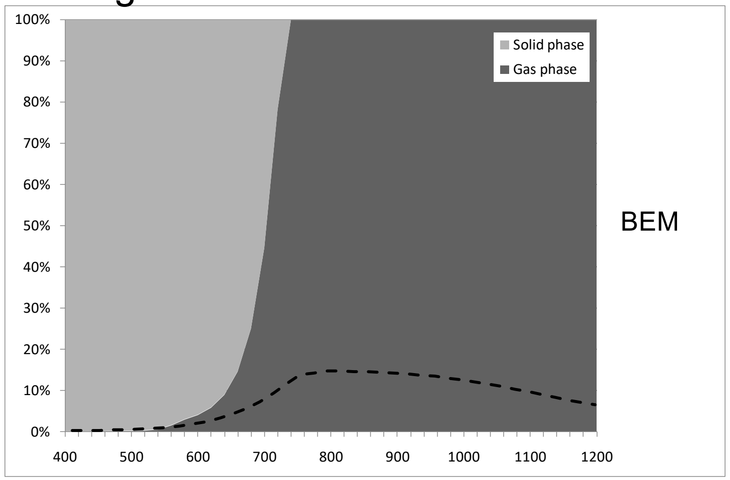
- ✓ **Small changes in one or more input data could give large differences in results**
- ✓ **These has to be found**

Ex: Only the available oxygen is changed

Na-distribution solid/gas



BEM



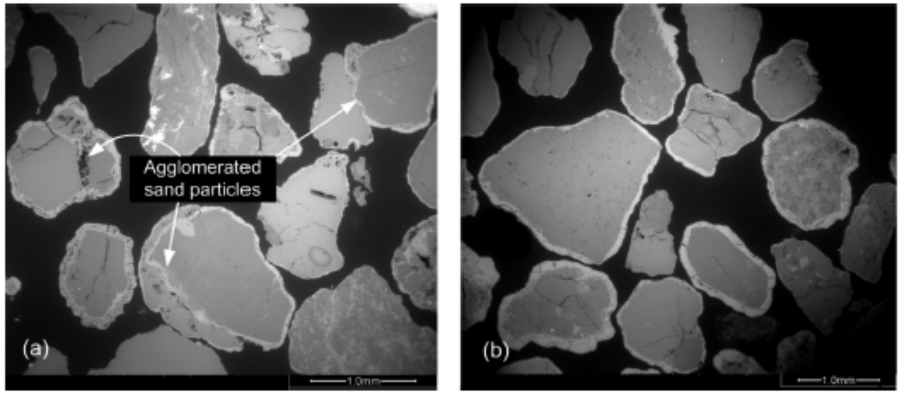
BEM

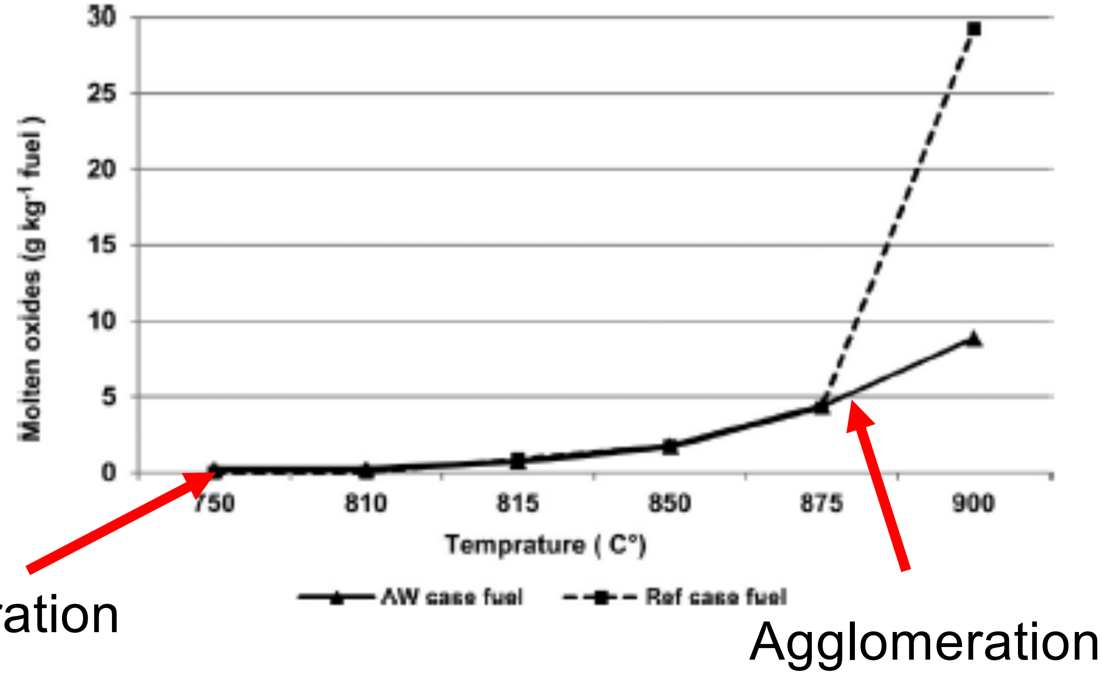
Source: Frida Claesson, VOKAB

RESULTS MODEL 1

AGGLOMERAION OR NOT

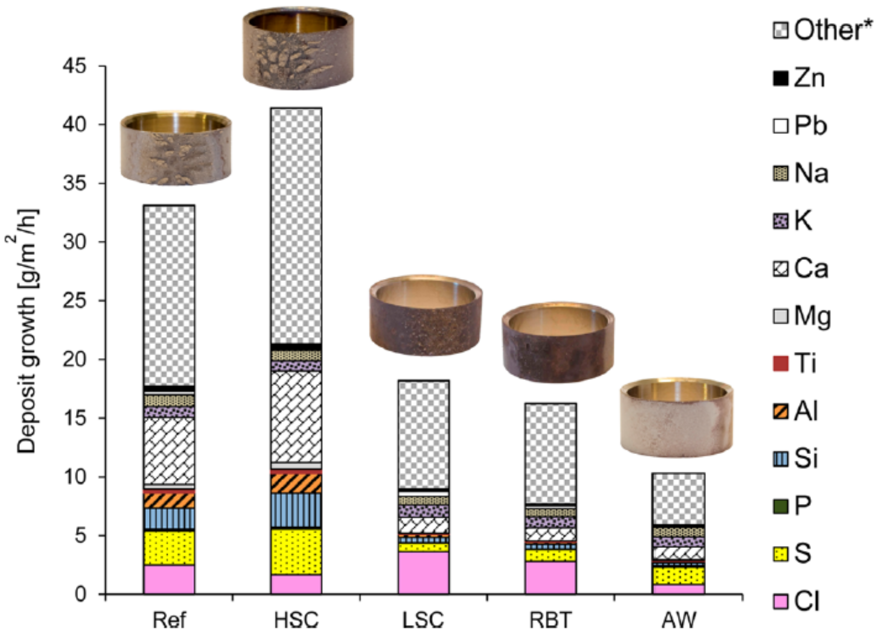
Ref 870°C **AW 750°C**

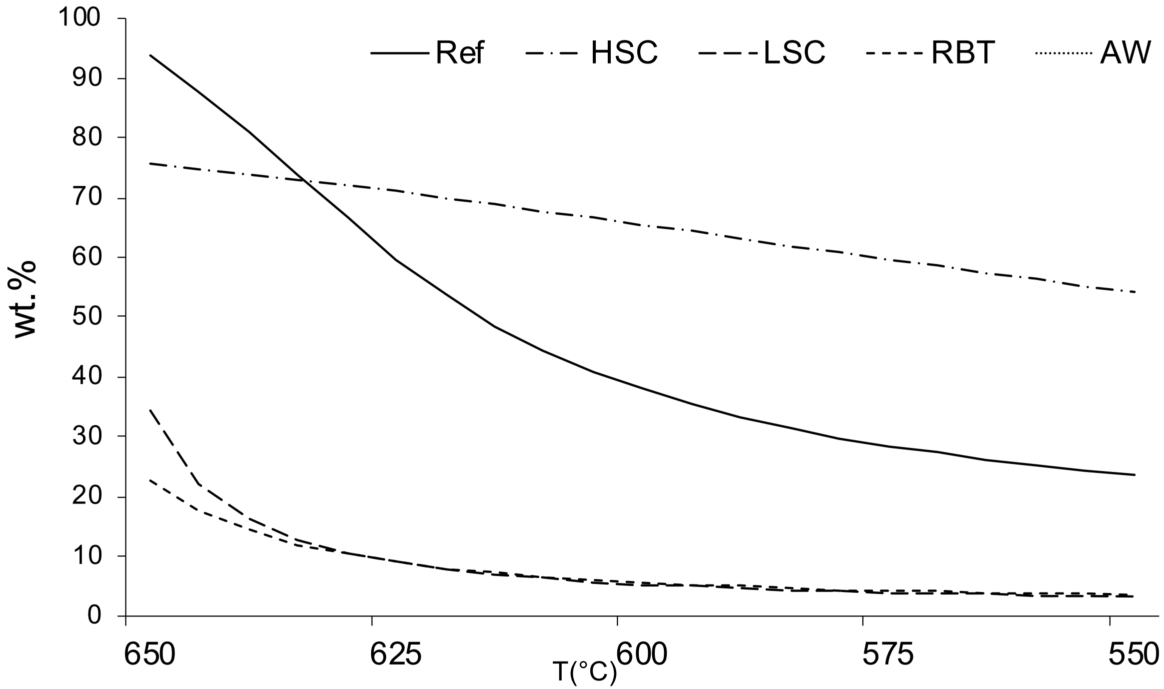




RESULTS MODEL 2

AMOUNT OF MELT IN THE CONDENSED PHASE CAUSING DEPOSIT FORMATION

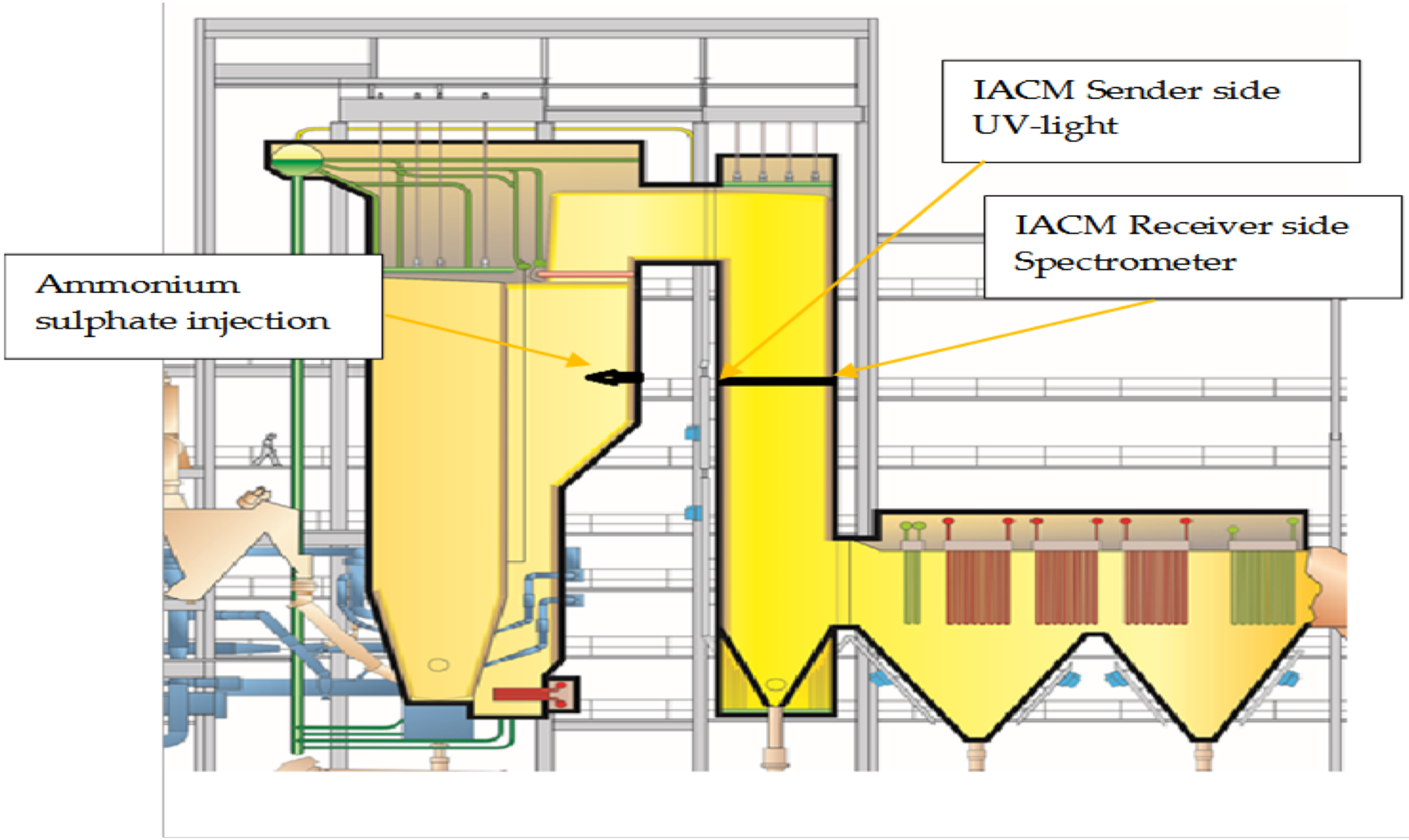




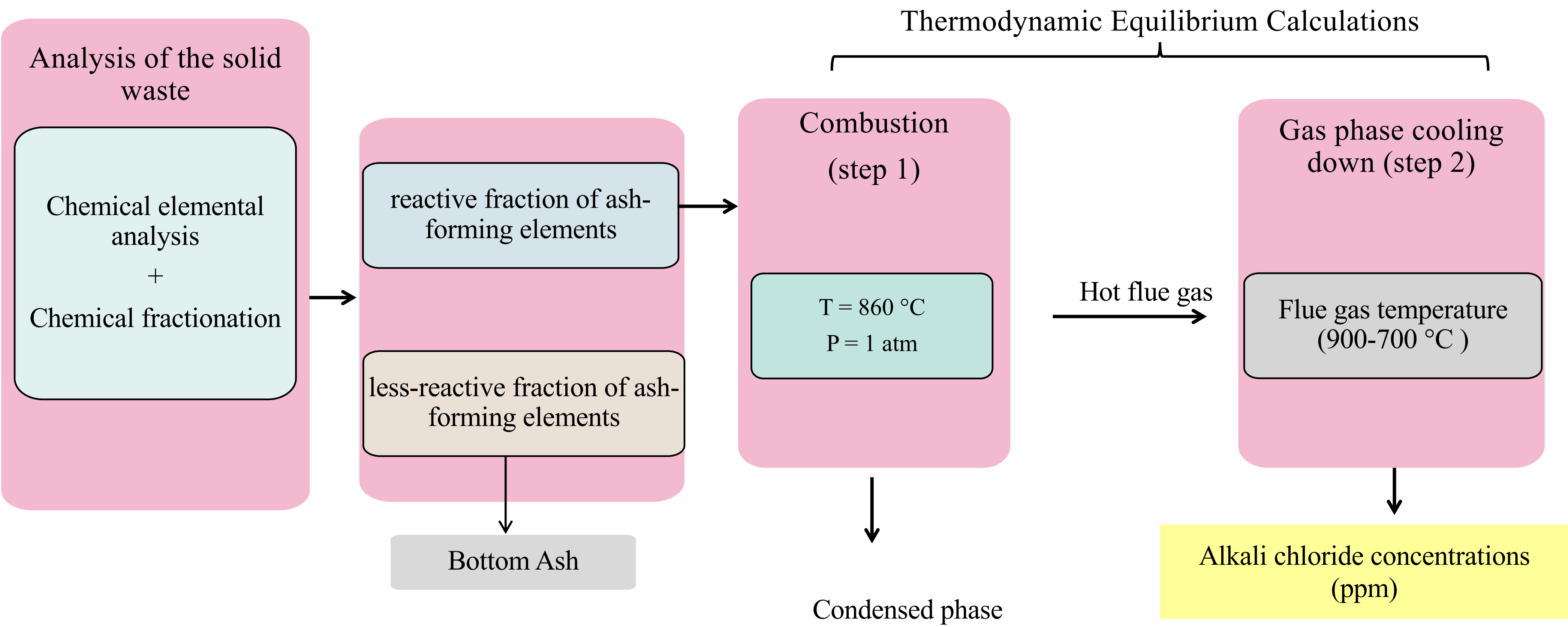
(a) quantity of melt in the condensed phase and (b) percentage of melt in the condensed phase, with a flue gas temperature of 650 to 550 °C, calculated by thermodynamic equilibrium modeling ***(Paper IV Farzad Modarian PhD-thesis)***

APPROACH

KME711: CORROSION EXPOSURES IN THE WASTE FIRED CFB P15 AT HÄNDELÖ



MODELLING APPROACH



THERMODYNAMIC EQUILIBRIUM CALCULATIONS

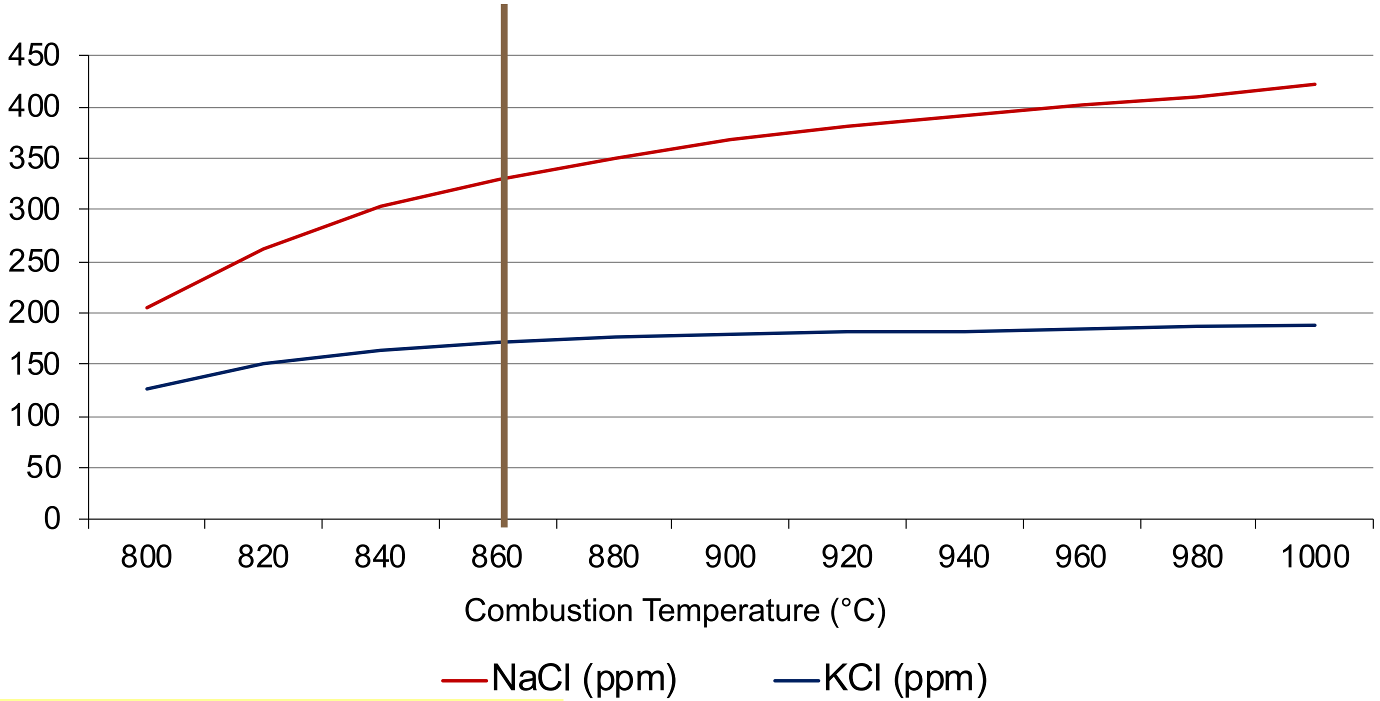
➢ **Tool : FactSage 7** (the thermochemical software and databases)

✓ Thermodynamic databases used: FactPS, FToxid and FTsalt

➢ **Input data and assumptions:**

- ✓ Input elements (reactive fraction): C, H , N , O , Cl , S , K , Na , Ca, Mg, Si, P, Zn and Pb
- ✓ Other elements excluded, owing to their less-reactive nature or very low concentrations
- ✓ Air/fuel ratio: 6 vol % excess O_2 in the flue gas
- ✓ One step combustion due to the uniform temperature profile in the furnace of the CFB bolier

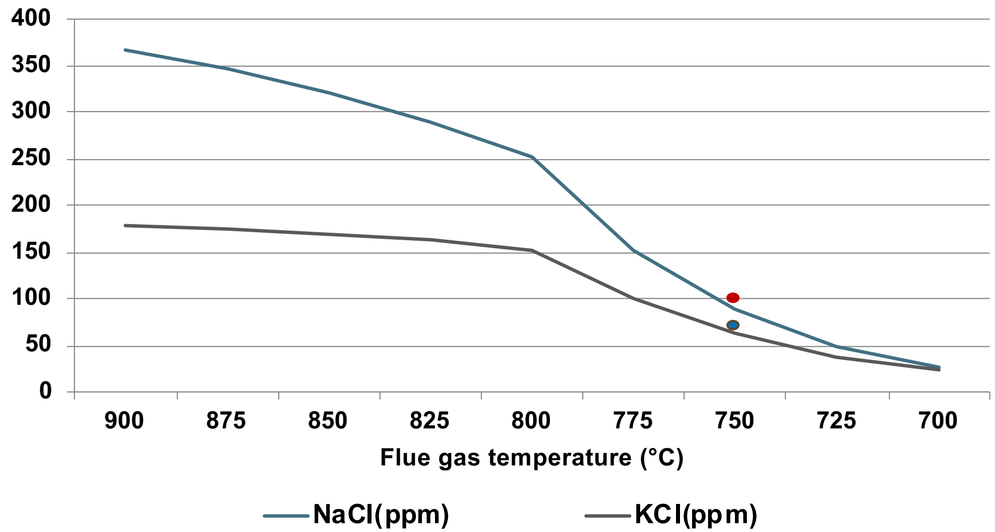
ALKALI CHLORIDE CONCENTRATIONS IN THE HOT FLUE GAS (REF CASE)



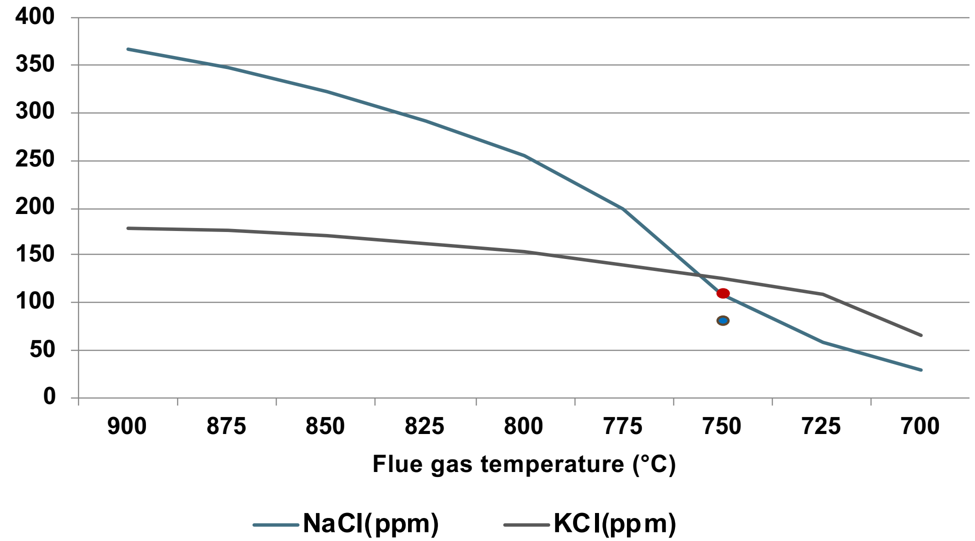
Combustion temperature (860 °C):
$NaCl$ = 329 (ppm)
KCl = 170 (ppm)

ALKALI CHLORIDE CONCENTRATIONS DURING GAS PHASE COOLING DOWN (REF CASE)

Condensation as solution phase (A)

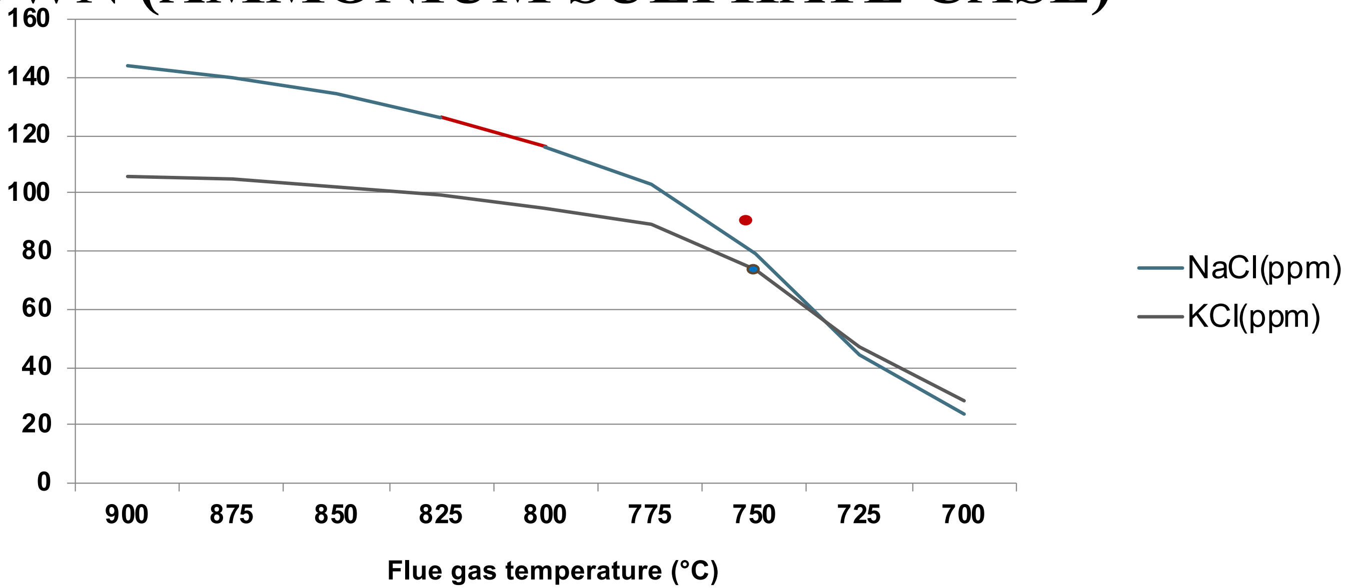


Condensation as pure solid (B)



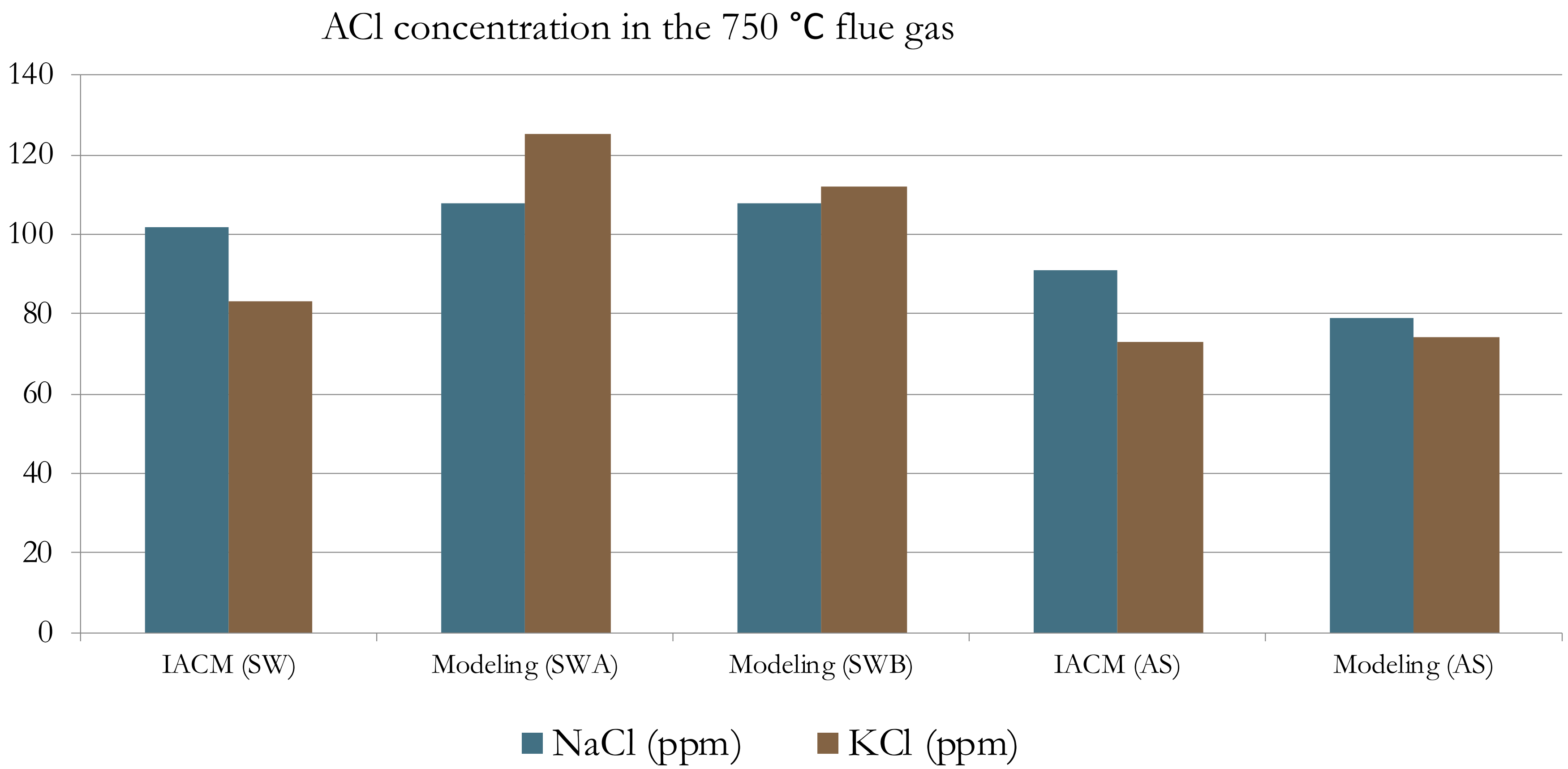
IACM vs Modeling	KCl (ppm)	NaCl (ppm)
IACM at 750 °C (average)	83	102
Modeling 750 °C (A)	62	88
Modeling 750 °C (B)	125	108

ALKALI CHLORIDE CONCENTRATIONS DURING GAS PHASE COOLING DOWN (AMMONIUM SULPHATE CASE)



IACM vs Modeling	KCl (ppm)	NaCl (ppm)
IACM at 750 °C (average)	73	91
Modeling 750 °C	74	79

ALKALI CHLORIDE CONCENTRATIONS DURING GAS PHASE COOLING DOWN MEASURED AND MODELLED

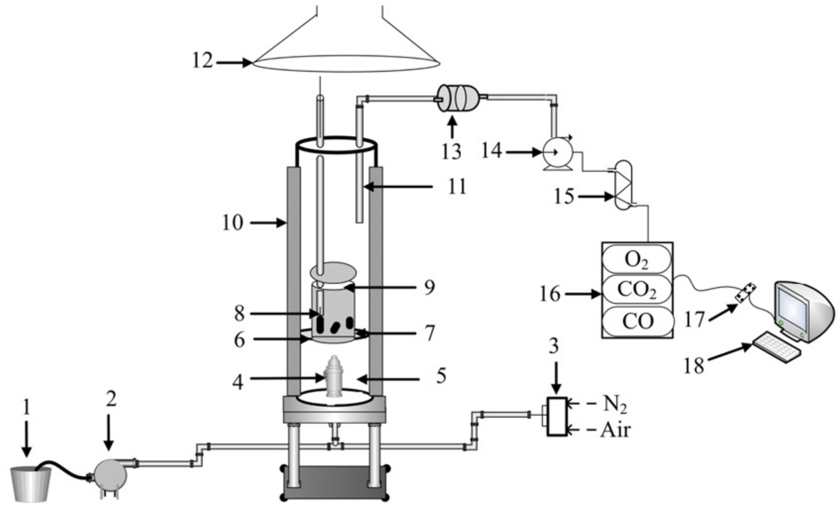


CONCLUSIONS

- ✓ Thermodynamic modelling is a useful tool for analyses of thermal processes
- ✓ Input data and data bases should be chosen carefully
- ✓ Sensitivity analyses are very important
- ✓ Not valid for low temperatures
- ✓ Could be used and developed for more complicated systems


Thank you!

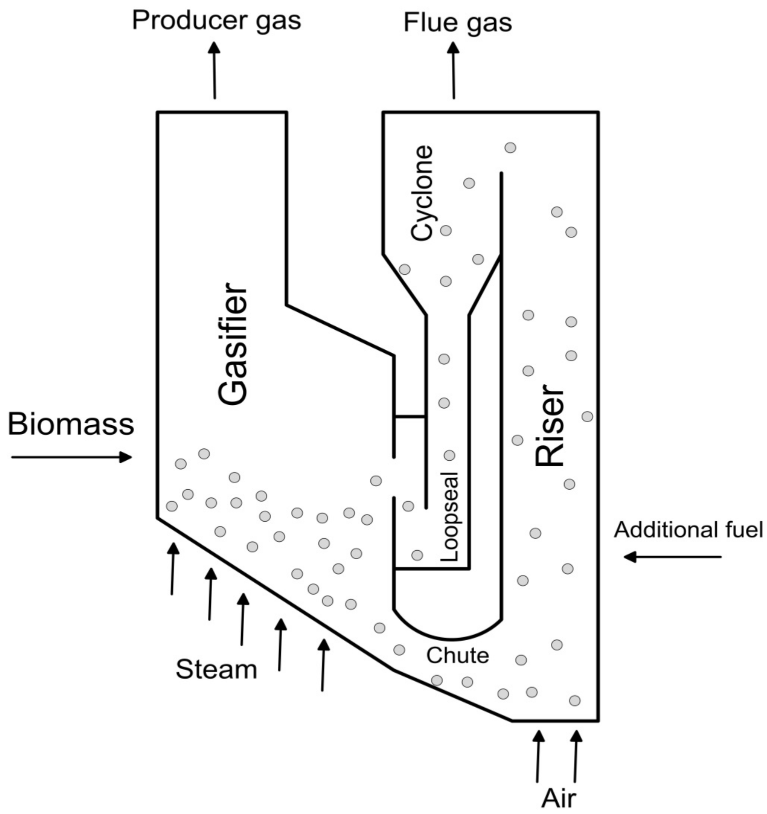
APPROACH



1-water tank, 2-water pump, 3-mass flow regulator 4-inbuilt steam generator, 5-gas preheater, 6-perforated ceramic plate, 7- sand bed, 8- thermocouple inserted into a pellet, 9-wire mesh basket, 10- heating elements, 11-gas probe, 12-exhaust hood, 13-particle filter, 14- gas pump, 15- condenser, 16-gas analyzers, 17- pc logger , 18- computer.

Labb scale BFB reactor

DFB GASIFIER



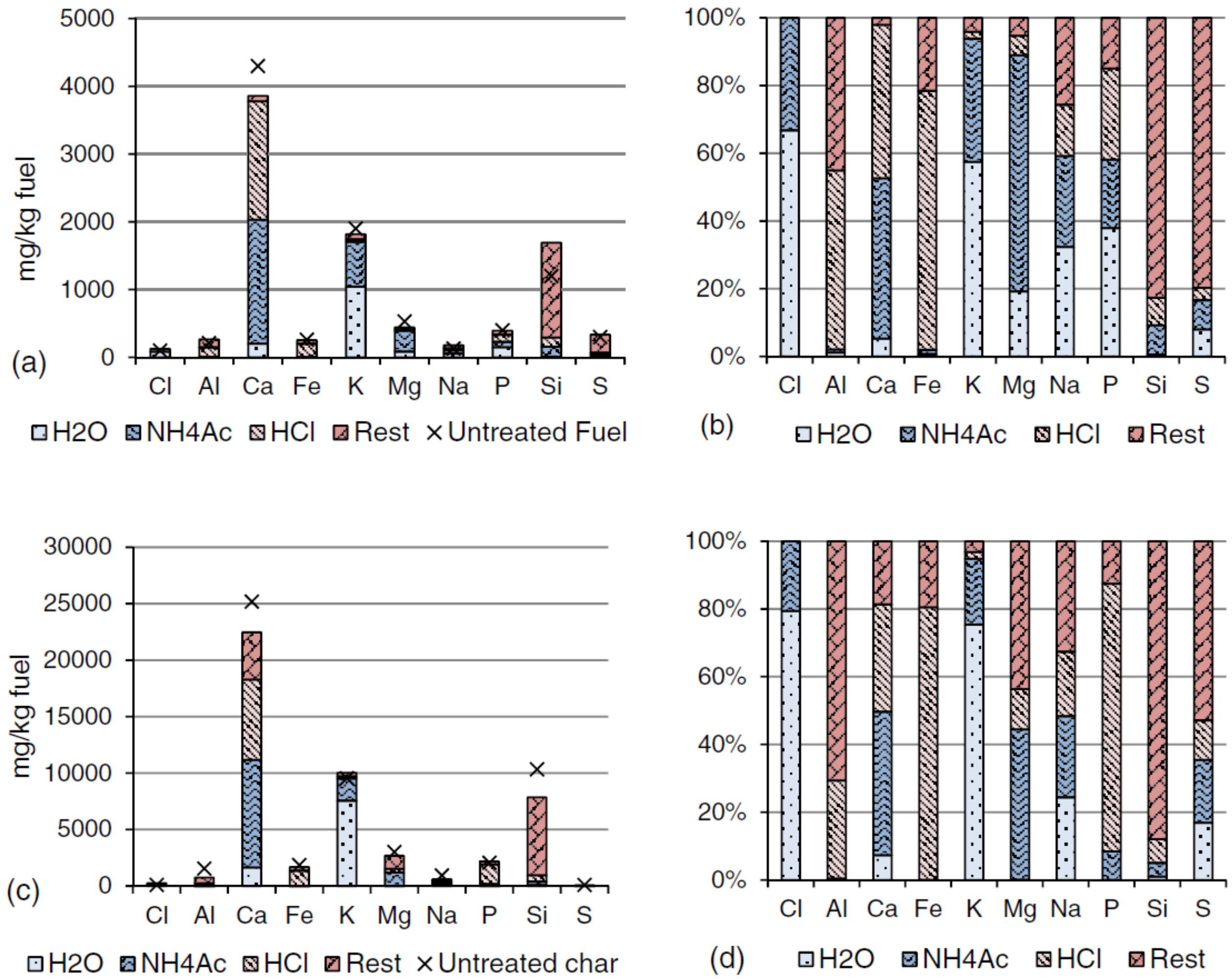
Dual fluidized-ded steam gasifier, DFB

APPROACH

FUEL AND CHAR CHARACTERISATION

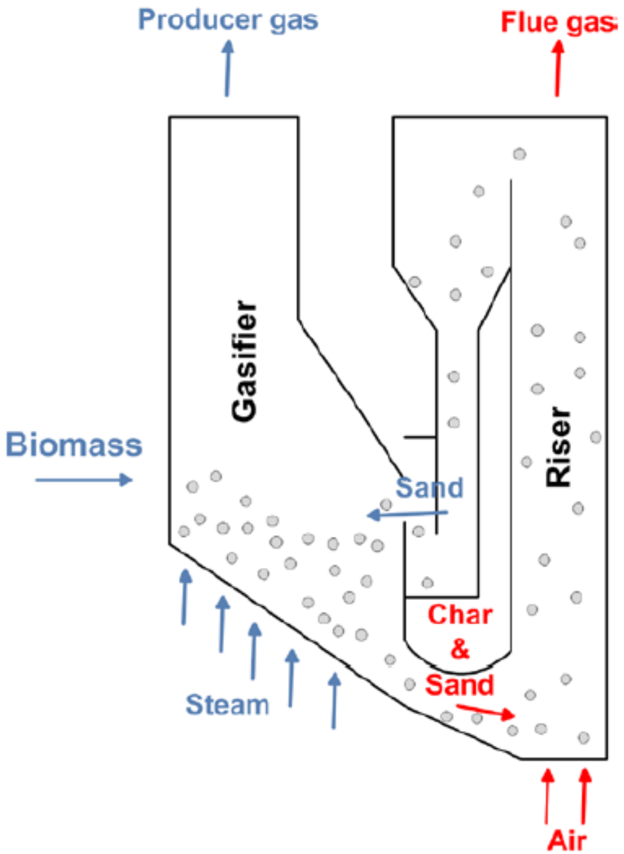
FUEL

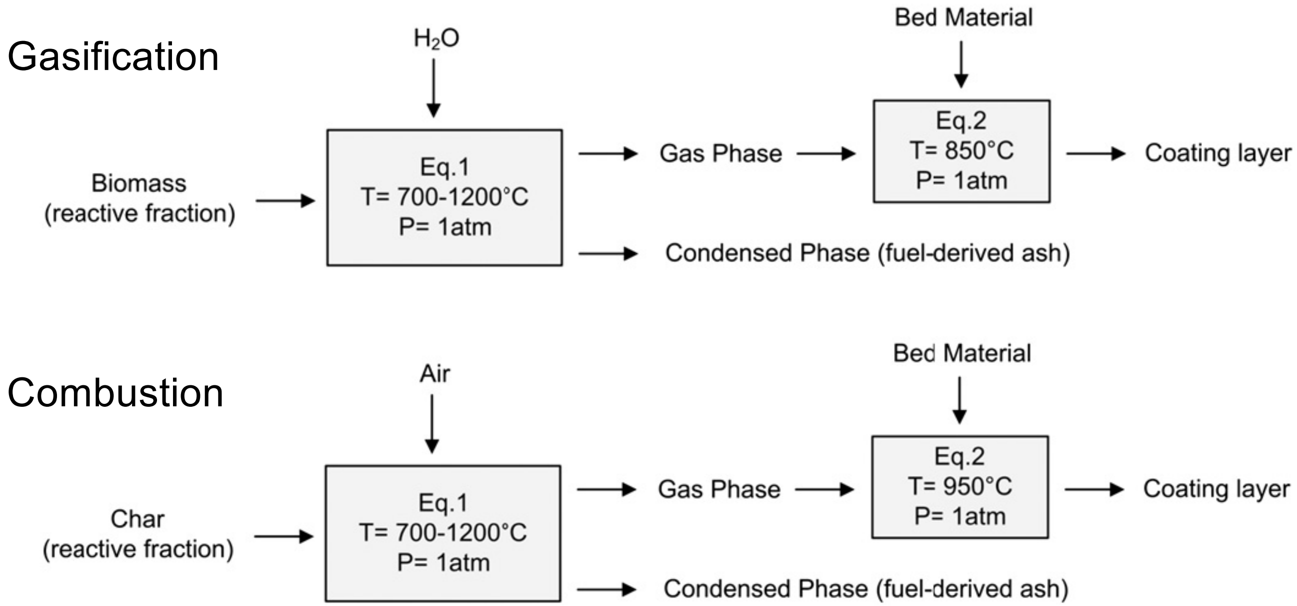
CHAR



APPROACH

DFB GASIFIER



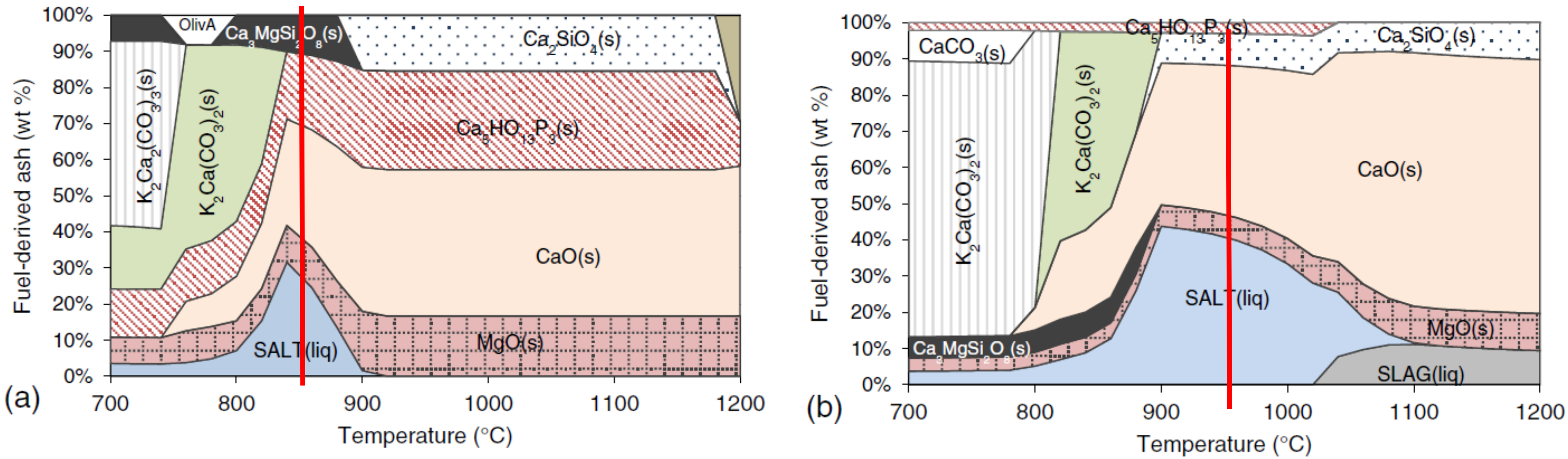


APPROACH DATABASES

Database	Solution phase
FToxid	SLAGA (molten oxide of K_2O, Na_2O, SiO_2, CaO, MgO, P_2O_5 + dilute sulphides)
FToxid	OlivA (solid solution: Mg, Ca//SiO_4)
FTsalt	SALTF (molten salt: Na^+,K^+//Cl^-, SO_4^{2-},CO_3^{2-},NO_3^-,OH^-)
FTpulp	MELTA (molten salt: Na^+,K^+//Cl^-, SO_4^{2-},CO_3^{2-},OH^-,S^{2-})

RESULTS

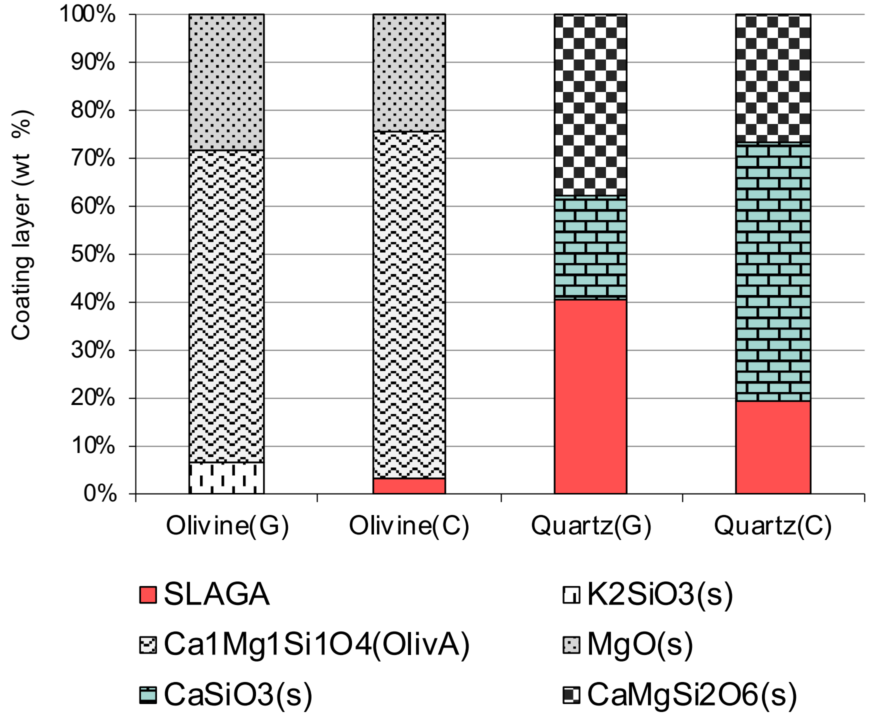
COMPOSITION AND MELTING BEHAVIOR IN DFB GASIFIER



The calculated equilibrium composition and melting behaviour of the fuel-derived ash at different temperatures in the (a) gasification and (b) combustion reactors of the DFB gasifier

RESULTS

COMPOSITION AND MELTING BEHAVIOR IN DFB GASIFIER



The calculated equilibrium composition of the bed particles coating layer in the gasification (850 °C) and combustion (950 °C) reactors of the DFB gasifier

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