Modelling of aerosol formation

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Why aerosol formation modelling?

- Aerosols formed during combustion of woody biomass in fixed bed systems contribute to ash related problems
  - Particulate emissions
  - Deposit formation and subsequent slagging, fouling and corrosion
- Ash related problems shall be reduced by influencing aerosol formation and behaviour
- Modelling of aerosol formation clarify relevant parameters of particle formation and precipitation as a basis for influencing aerosol formation and behaviour

Model description - general model description

- **Plug flow model**
  - **1-dimensional**
- **Representation of the particle size distribution by a sectional distribution (number of size classes = 100)**
- **Determination of the gas phase composition at the beginning of each calculation step**
- **Implementation of particle formation mechanisms**
- **Implementation of particle precipitation mechanisms**
- **Modelling results**
  - **Particle size distribution**
  - **Chemical composition of aerosol particles**
  - **Amount of aerosols formed**
  - **Relevant influencing parameters on aerosol formation**

Model description - gas phase chemistry

- **The gas phase composition is determined at the beginning of each calculation step by a thermodynamic equilibrium calculation**
  - **Gaseous compounds of the following elements are implemented: Al, C, Ca, Cd, Cl, Cu, F, Fe, H, Hg, K, Mg, N, Na, O, P, Pb, S, Si, Zn**
  - **Solid and liquid compounds are excluded from the reaction products in order to achieve supersaturations of ash vapours in the gas phase**
  - **Kinetically limited reactions are considered in the case of sulphation reactions by implementation of an Arrhenius approach (*Christensen A, 1995*)**
  - **The influence of heterogeneous reactions on the gas phase composition is not considered in the stepwise calculations**

Model description - aerosol formation processes

- **Gas to particle conversion**
  - **Nucleation**
  - **Condensation of vapours on existing particles**
  - **Condensable compounds considered: K_2SO_4, KCl, $(KCl)_2$, K_2CO_3, Na_2SO_4, NaCl, $(NaCl)_2$, PbO, $PbCl_2$, ZnO, $ZnCl_2$**
- **Coagulation**
  - **Mechanisms considered**
    - **Brownian diffusion**
    - **Turbulent shear**
    - **Gravitational settling**
  - **Coagulation is considered as coalescence and particles are treated as spheres**

Model description - particle and vapour deposition

- **Particle deposition processes (fire tube boiler)**
  - Gravitational settling
  - Thermophoresis
  - Deposition by particle diffusion
  - Turbophoresis
  - Consideration of particle rebound, erosion and shedding by a re-entrainment factor
- **Vapour condensation on furnace and boiler walls**
  - Condensable compounds considered: K_2SO_4, KCl, $(KCl)_2$, K_2CO_3, Na_2SO_4, NaCl, $(NaCl)_2$, PbO, $PbCl_2$, ZnO, $ZnCl_2$

Model description - input values

Input data required for the aerosol formation model

- Time - temperature profile of the combustion plant
  - Gas volume flow
  - Furnace and boiler geometry
  - Flue gas temperature and pressure distribution in the biomass furnace and boiler sections
- Element concentrations in the gas phase considered for the thermodynamic equilibrium calculations at the starting point
- Properties of primary particles at the starting point of the calculation
  - Particle size distribution
  - Chemical composition of primary particles

Comparison of measured and calculated aerosol data

- **Particle mass load [mg/Nm³ 13 vol% O_2, dry flue gas]**
  - **before boiler inlet (waste wood)**
  - **at boiler outlet (waste wood, beech)**
- **Particle size distribution**
  - **before boiler inlet (waste wood)**
  - **at boiler outlet (waste wood, beech)**
- **Chemical composition of aerosol particles**
  - **before boiler inlet (waste wood, qualitative comparison of results from spruce and beech)**
  - **at boiler outlet (waste wood, beech)**

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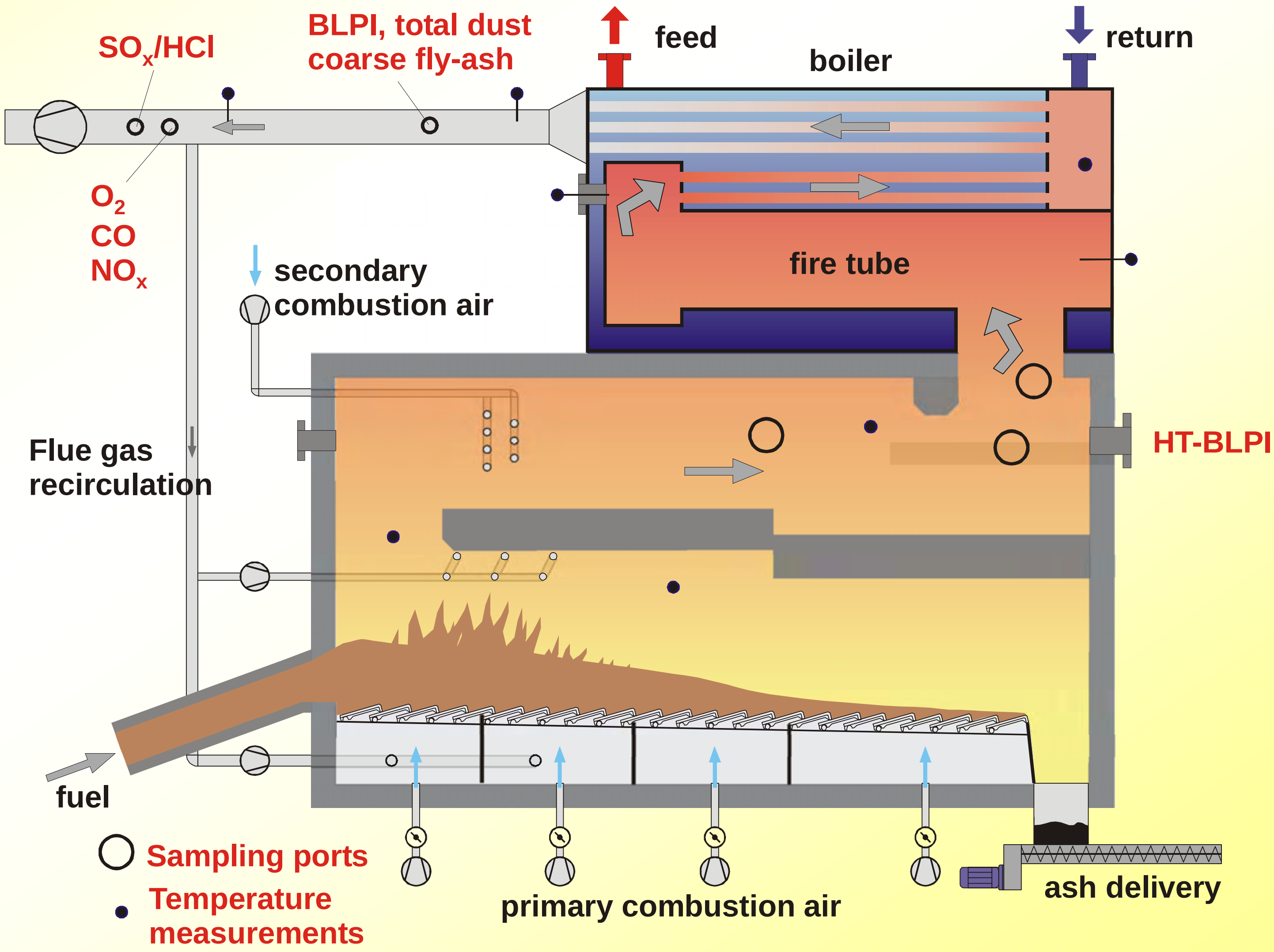
Scheme of the combustion plant and measurement ports

- Combustion plant equipped with a horizontally moving grate, staged combustion air supply and flue gas recirculation
- Nominal boiler capacity ... 440 kW
- BLPI ... Berner-type low pressure impactor
- HT-BLPI ... high temperature BLPI



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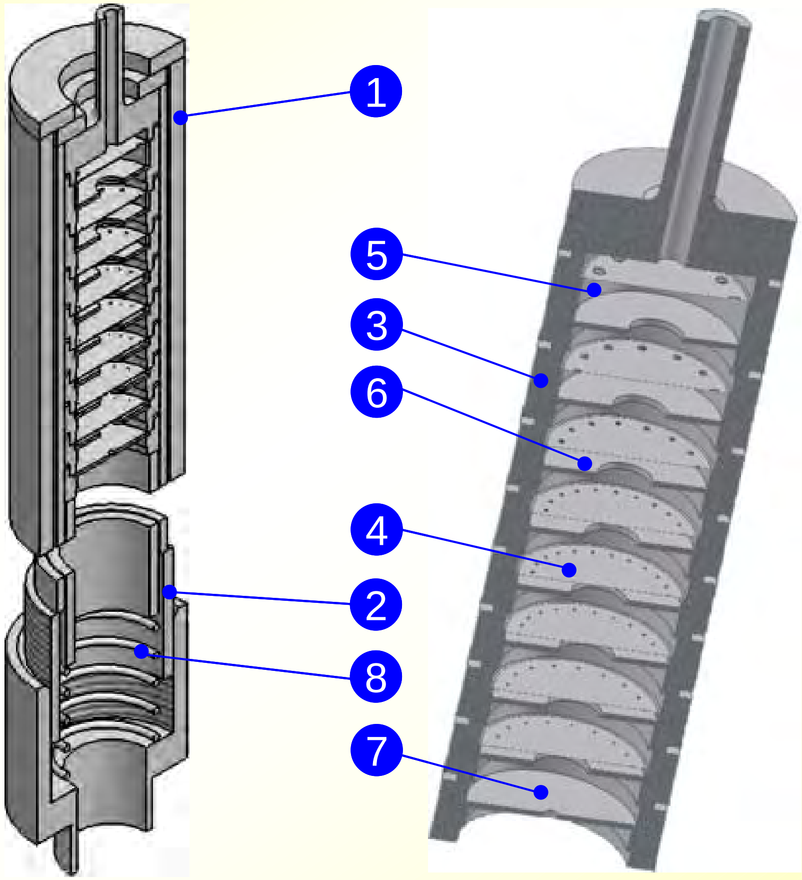
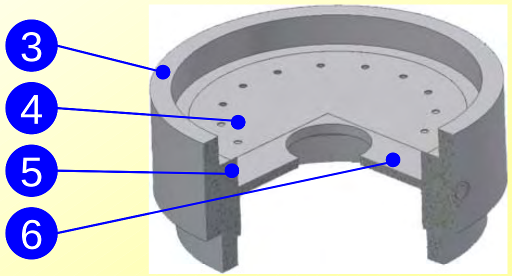
High temperature Berner-type low pressure impactor (HT-BLPI)

- Newly developed in cooperation with Prof. Axel Berner
- Temperature range: up to 1,050°C



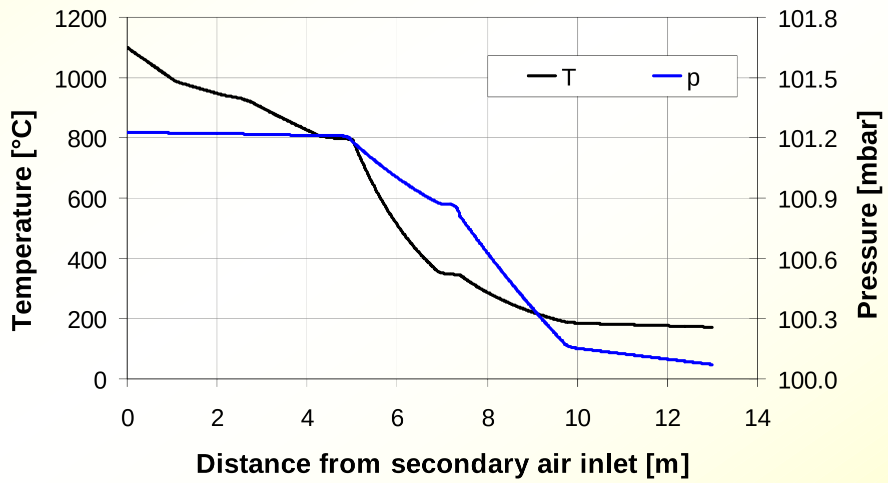
1 Outer casing
2 Inner casing
3 Impactor stage
4 Nozzle plate
5 Spacer
6 Stagnation plate
7 Critical nozzle
8 Spring

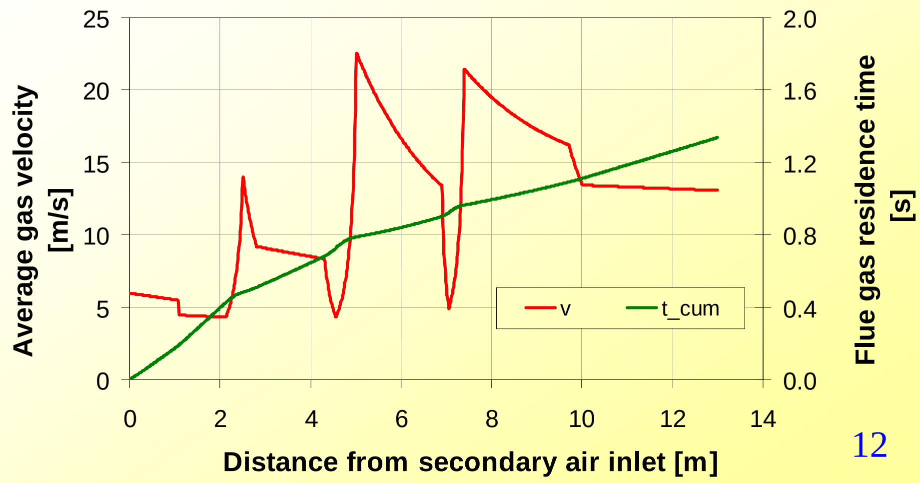


Calculation input

Input data for modelling calculations

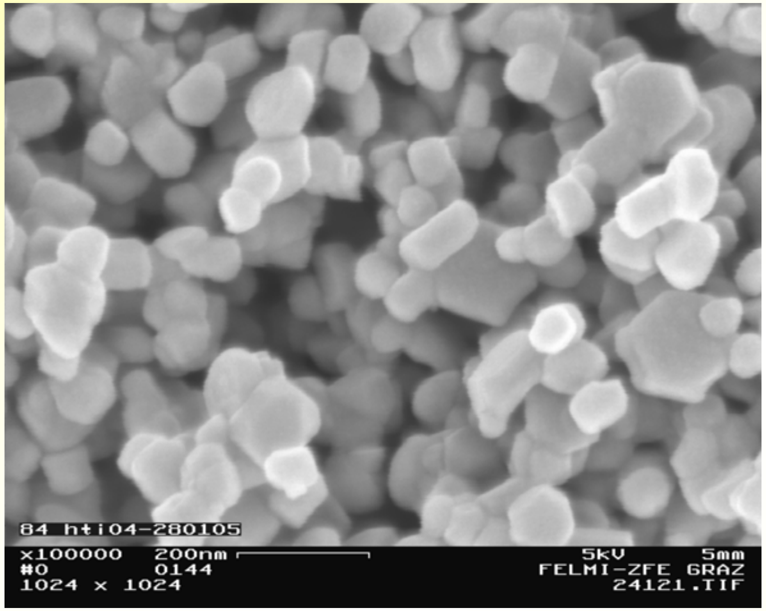
- **Element concentrations in the gas phase at the starting point of the calculation- gained from element balances over the combustion plant**
- **Primary particle composition - determined by thermodynamic equilibrium calculations**
- **Profiles of temperature, pressure, gas velocity and residence time – gained through the evaluation of plant operating data**





Measurement and calculation results - waste wood (I)

SEM/EDX analysis of particles sampled in the furnace during the combustion of waste wood (950°C)



Element	wt%
Al	0.4
Ca	0.3
Fe	1.1
K	0.8
Mg	0.0
P	0.1
S	0.5
Si	1.6
Zn	95.2

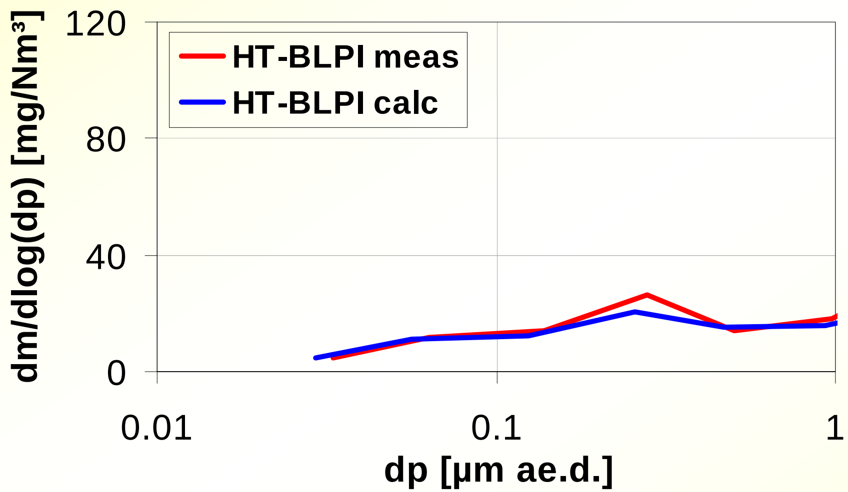
Sampling equipment … HT-BLPI; impactor stage cut diameter … 0.208µm (aerodynamic diameter); measurement point HT-BLPI … secondary combustion chamber (950°C); material of sampling foil … Pt; sample preparation … sample sputtered with Au; analysis results excluding C, Cr, Mn, O, Pt and Ti; analysis method … EDX measurement performed as area scan on particle peaks of a single impactor measurement

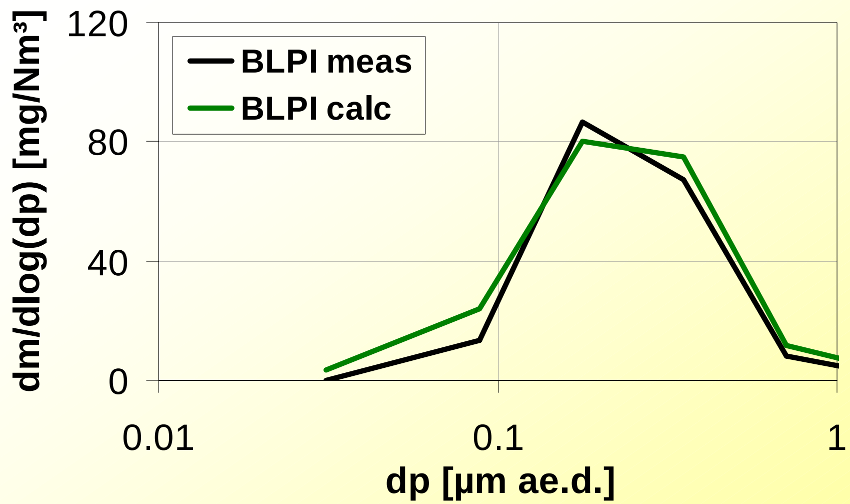
Measurement and calculation results - waste wood (II)

Measured and calculated mass of aerosols (dp < 1 µm) and particle size distributions of aerosols before boiler inlet and at boiler outlet

	measured	calculated
HT-BLPI	13.6	16.6

	measured	calculated
BLPI	68.5	62.7

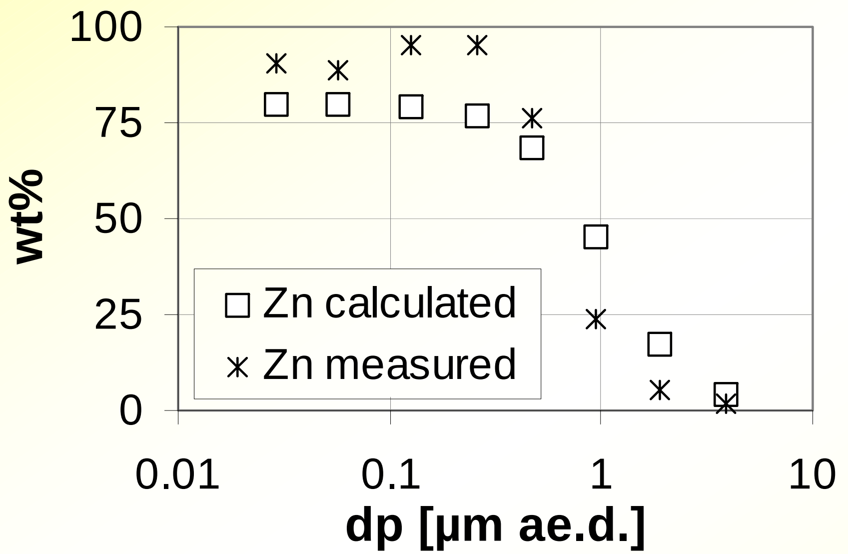


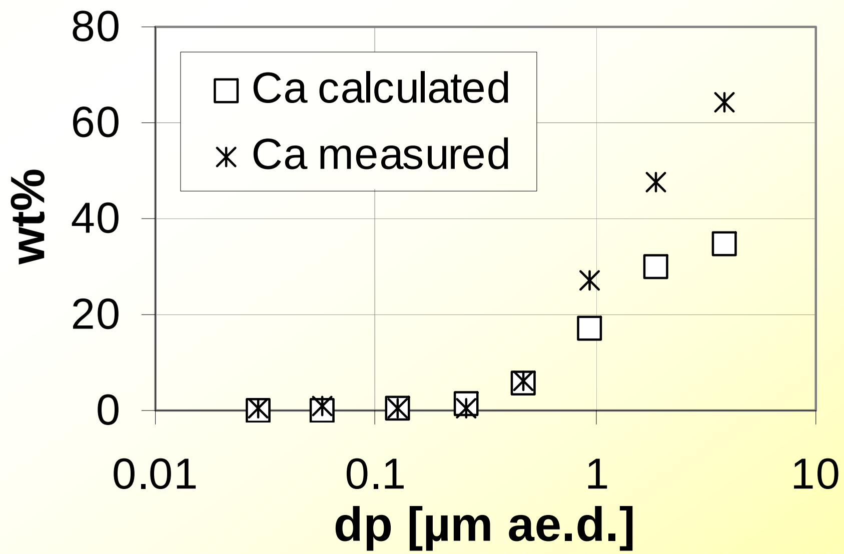


Values in mg /Nm³ 13 vol% O_2, dry flue gas; BLPI … Berner-type low pressure impactor; HT-BLPI … high temperature BLPI; ae.d. … aero-dynamic diameter

Measurement and calculation results - waste wood (III)

Comparison of measured and calculated concentration trends of Zn and Ca in aerosol particles before boiler inlet





wt% … weight %; ae.d. … aerodynamic diameter

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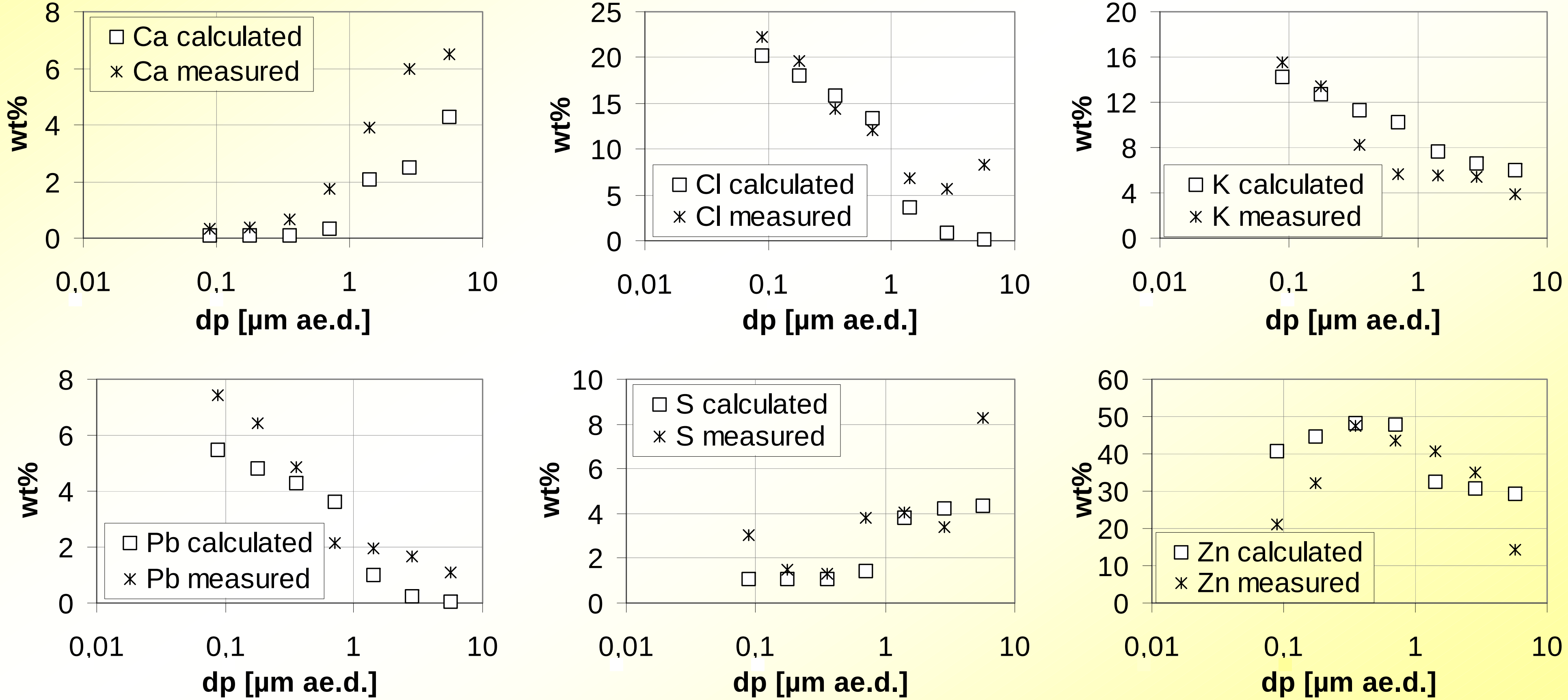
Measurement and calculation results - waste wood (IV)

Comparison of measured and calculated concentration trends of Ca, Cl, K, Pb, S and Zn in aerosol particles at boiler outlet



wt% … weight %; ae.d. … aerodynamic diameter

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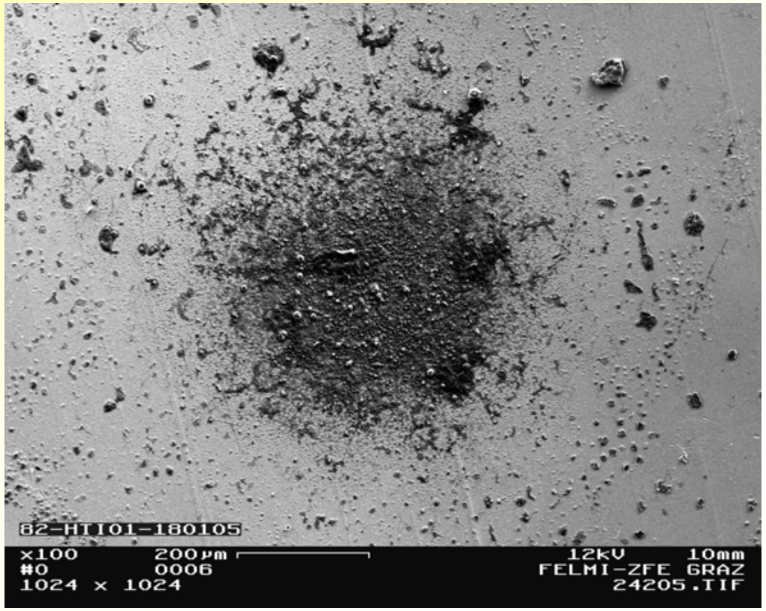
Measurement and calculation results - wood chips (I)

SEM/EDX analysis of particles sampled in the furnace during combustion of chemically untreated wood chips (spruce, 1,020°C)



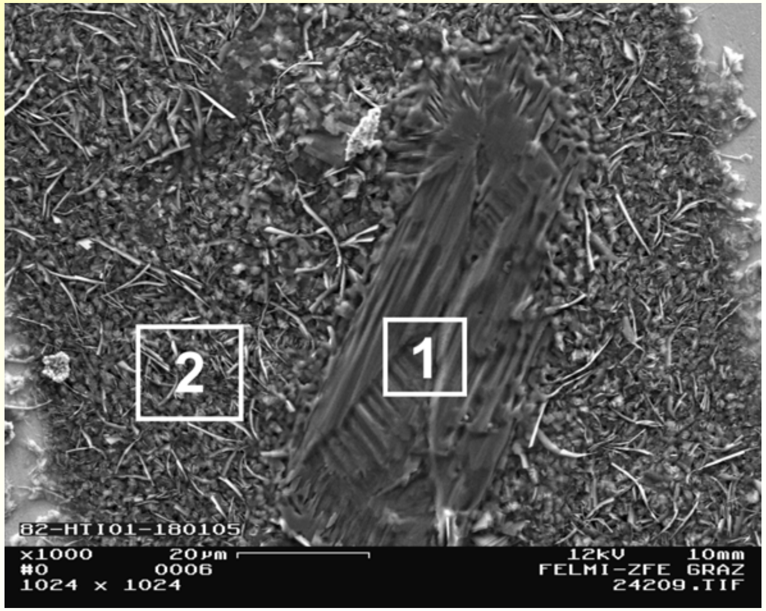
Element	wt%
Al	0.9
Ca	12.4
Fe	1.1
K	45.6
Mg	4.5

Element	wt%
Na	3.9
P	0.0
S	30.6
Si	1.1
Zn	0.0

sampling equipment … HT-BLPI; impactor stage cut diameter … 0.669µm (aerodynamic diameter); measurement point HT-BLPI … secondary combustion chamber (1020°C); material of sampling foil … Pt; sample preparation … sample vaporised with C; analysis results excluding C, Cr, Mn, O, Pt and Ti; analysis method … EDX measurement performed as area scan on particle peaks of a single impactor measurement

Measurement and calculation results - wood chips (II)

Precipitation of liquid K_2SO_4 and liquid Na_2SO_4 could be confirmed by thermodynamic equilibrium calculations which showed a stable liquid sulphate phase between 950 and 1,100°C



Element	1	2
Al	0.0	0.2
Ca	0.8	21.0
Fe	0.0	0.3
K	65.9	41.0
Mg	0.1	0.0
Na	0.6	0.3
P	0.0	0.0
S	32.7	37.3

sampling equipment … HT-BLPI; impactor stage cut diameter … 0.669µm (aero-dynamic diameter); measurement point HT-BLPI … secondary com-bustion chamber (1020°C); material of sampling foil … Pt; sample preparation … sample vaporised with C; analysis results excluding C, Cr, Mn, O, Pt and Ti; analysis method … EDX measurement performed as area scans; values in wt%

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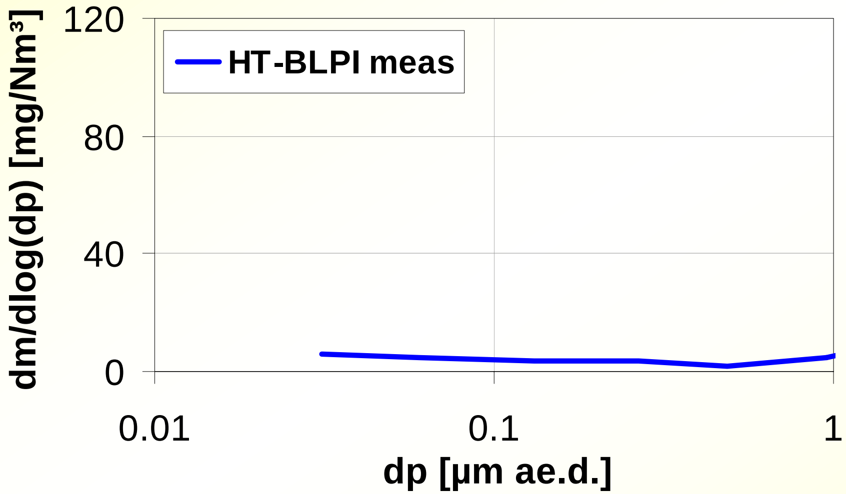
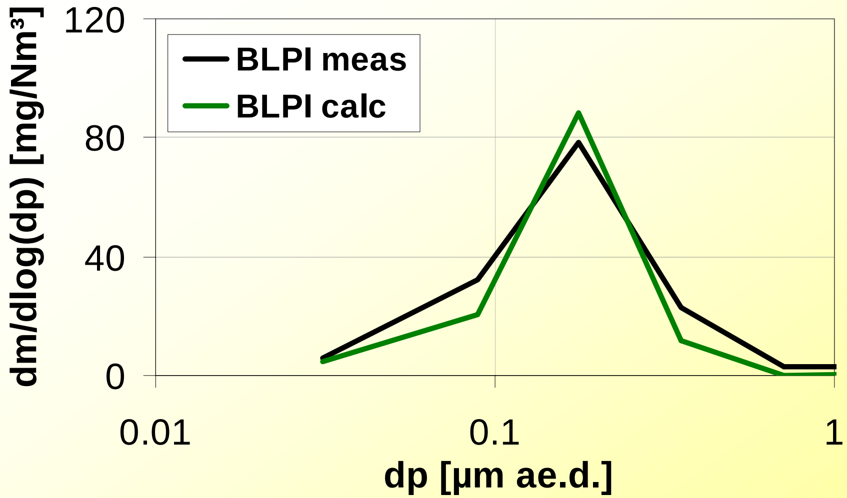
Measurement and calculation results - wood chips (III)

Measured and calculated mass of aerosols (dp < 1 µm) and particle size distributions of aerosols before boiler inlet and at boiler outlet

	measured	calculated
HT-BLPI	4.9	-

	measured	calculated
BLPI	46.6	42.0





Values in mg /Nm³ 13 vol% O_2, dry flue gas; BLPI … Berner-type low pressure impactor; HT-BLPI … high temperature BLPI; ae.d. … aero-dynamic diameter

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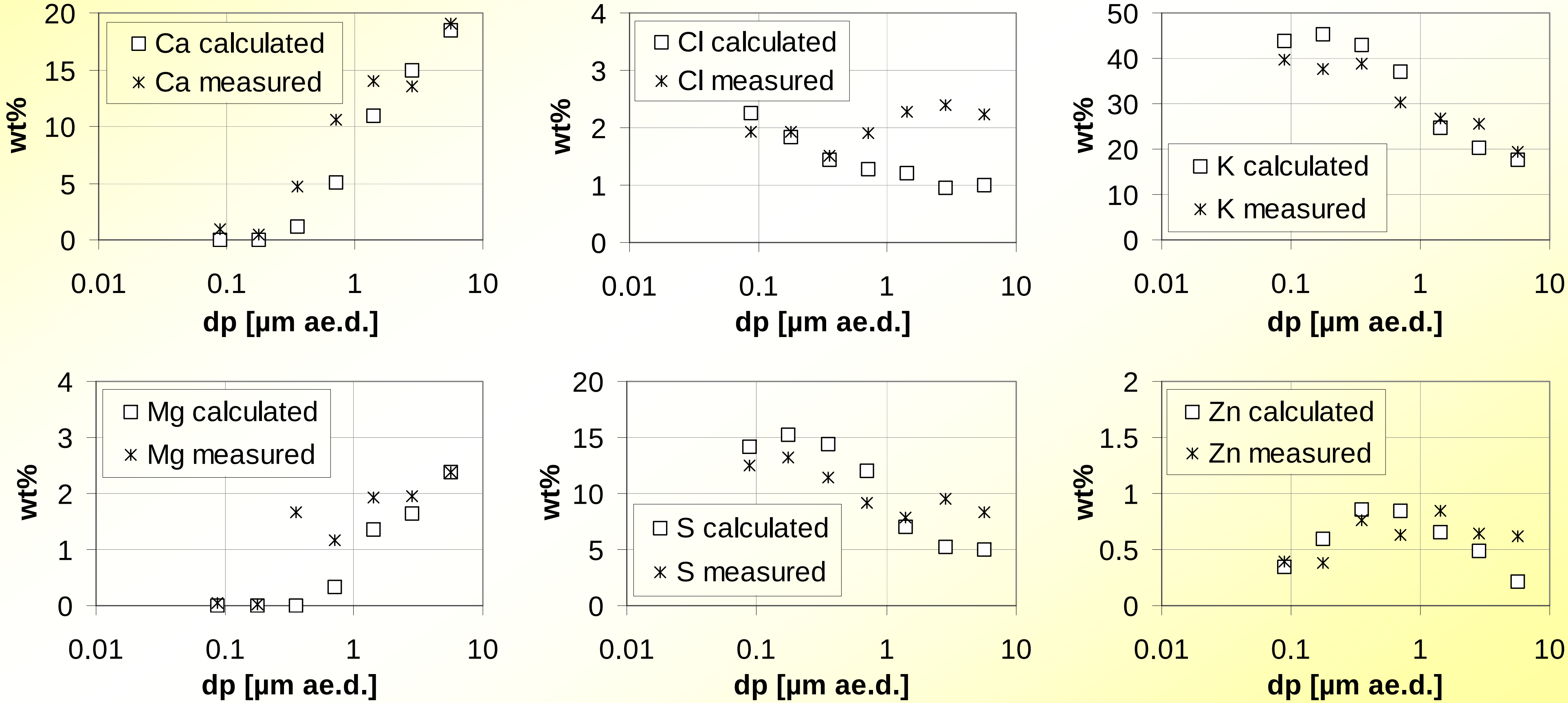
Measurement and calculation results - wood chips (IV)

Comparison of measured and calculated concentration trends of Ca, Cl, K, Mg, S and Zn in aerosol particles at boiler outlet (beech)



fuel … beech; wt% … weight %; ae.d. … aerodynamic diameter

Summary and conclusions (I)

- An aerosol formation model was developed in order to evaluate relevant influencing parameters on aerosol formation and behaviour during combustion of woody biomass in fixed bed combustion systems
- The model covers the determination of the gas phase composition, gas to particle conversion processes (nucleation, condensation), coagulation, particle deposition mechanisms and vapour condensation on furnace and boiler walls
- Input values for the model are element concentrations in the gas phase, size distribution and composition of primary particles, and data concerning the flue gas (mass flow, temperature and pressure) as well as furnace and boiler geometry

Summary and conclusions (II)

- Modelling results are mass, particle size distribution and chemical composition of aerosols at a defined point of the combustion plant
- A new HT-BLPI was developed and successfully used for high temperature aerosol measurements
- A validation of the aerosol formation model was performed by a comparison of calculated aerosol data (mass load, particle size distribution, chemical composition) with measured values gained from test runs for two biomass fuels (waste wood, wood chips)
- The model validation showed a good mach of the data compared before boiler inlet and at boiler outlet

Summary and conclusions (III)

- **The identification of different aerosol formation pathways was possible and could be confirmed by the impactor measurements performed**
- **The model shall be further developed and a coupling between aerosol formation modelling and CFD simulations shall be performed**