Institute of Energy Process Engineering and Chemical Engineering

Research project HotVeGas and coupling of ChemApp with OpenFOAM

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Outline

1st part of presentation:

- Project HotVeGas
  - Aims
  - Partners
  - Tasks of IEC
- Preliminary results
  - Thermodynamic modelling (FactSage/ SimuSage)
  - Overview General concept

2nd part of presentation:

- Coupling of ChemApp and OpenFOAM

Aim of the project HOTVE

In general:

Fundamental investigations for the development of future high-temperature gasification and gas cleaning processes for IGCC power plants and for production of synthetic energy sources

In detail:

Research into the behaviour:

- of coals and other heterogeneous energy sources
- at highest temperatures and pressures
- considering their mineral content and trace elements
- at reducing conditions/ atmosphere

Project partners and time period

Cooperation partners:

- **3 research institutions**
  - Department of Energy Process Engineering and Chemical Engineering (IEC) TU Bergakademie Freiberg
  - Chair of Energy Systems - TU Munich
  - Department of Energy Research - Forschungszentrum Jülich

- **6 industry partners**
  - GTT-Technologies
  - Siemens (Future Energie) - Freiberg
  - E.ON
  - RWE
  - EnBW
  - Vattenfall

Project period: 01.09.2007 – 31.08.2011

Tasks of the IEC

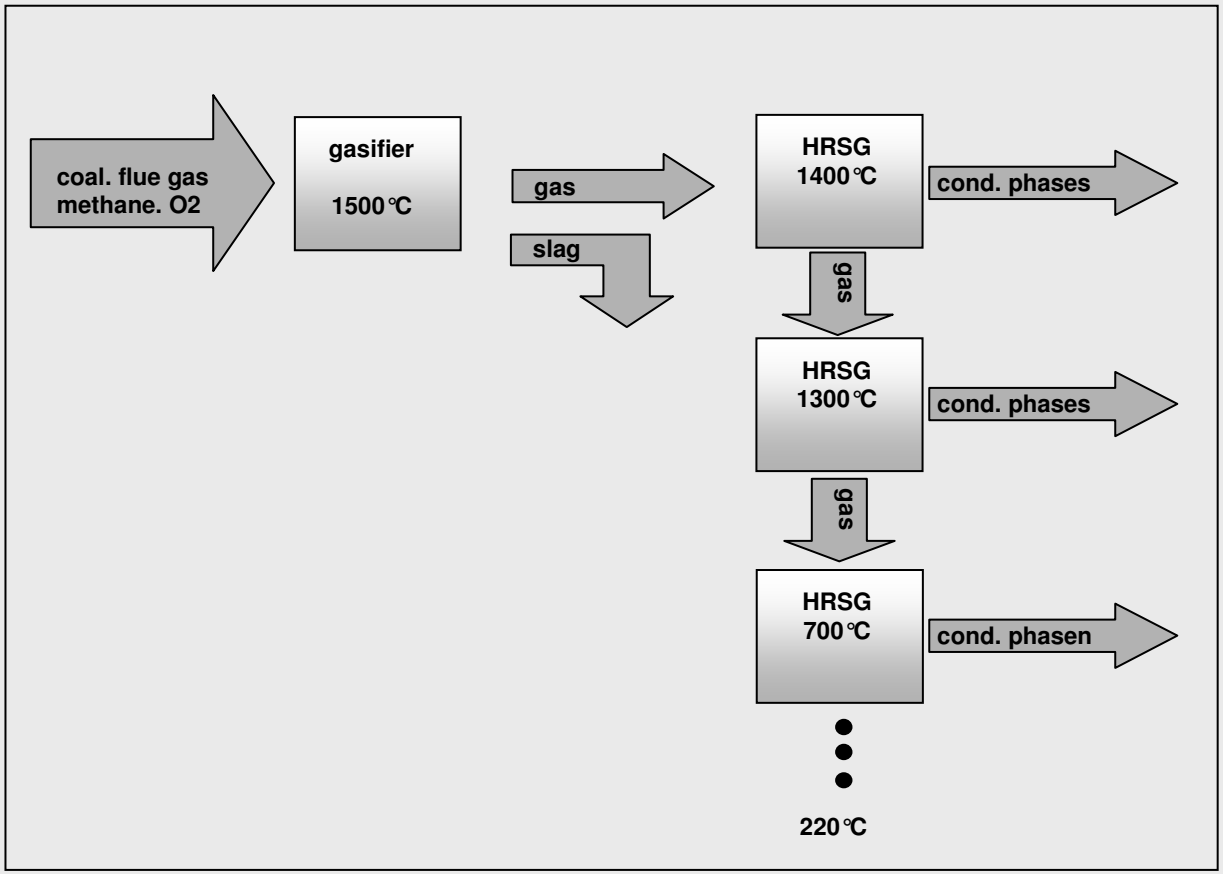
- Investigations of the influence of pressure on pyrolysis of heterogeneous energy sources
- Characterisation of real ashes and slags of different gasification processes
- Thermo-chemical calculations of sub-systems with SimuSage®
- CFD-modelling of the gasification, including calculations of ash/slag behaviour and raw gas cleaning, using OpenFoam including ChemApp

Thermodynamic modelling

- Thermodynamic modelling using FactSage® and SimuSage®
- Software enables calculation of thermodynamic equilibrium between all reactants in the system
- Kinetic aspects are not taken under consideration
- Results: compositions of solids (e.g. mineral phases), liquids (e.g. slags), condensed phases and gases
- Considerations about corrosion risks from volatile ash components and slags (compositions, presence)

Flowsheet simulation (SimuSage®)

- Gasification chamber and single temperature steps in the HRSG are represented as isobar-isothermal equilibrium stages
- Slag treated as amorphous and therefore split off before cooling down
- Separation of condensed phases and gas phases after each cooling step
- Gaseous components are in thermodynamic equilibrium at cooling down
- Condensed phases are considered to be deposit formers



Sample K1-1

K1-1			
Ultimate analysis:	wt.-% wf	**Ash analysis (XRF):**	wt.-%
Ash	11.44	SiO2	52.70
C	61.00	Al2O3	2.15
H	4.30	Fe2O3	7.05
N	0.72	CaO	19.64
SC	0.31	MgO	5.58
O	22.20	P2O5[1)]	0.00
Cl	0.03	Na2O	0.24
Sum:	100	K2O	0.49
		SO3	11.85
	wt.-% raw	TiO2	0.31
Moisture	12.96	Sum:	100

[1)] With the used database it is not possible to calculate phosphorus embedding into the slag. Therefore. P2O5 was set 0 for coal ash K1-1

Results slag embedding, condensed and gas phases

- Distribution of volatile ash elements over single process stages

element	**Slag 1500°C** [wt.-%]	HRSG 1400°C [wt.-%]	HRSG 1275°C [wt.-%]	HRSG 1150°C [wt.-%]	HRSG 1025°C [wt.-%]	HRSG 900°C [wt.-%]	HRSG 700°C [wt.-%]	Quench 220°C [wt.-%]	Σ
Cl	**0.1**	0.0	0.0	0.0	0.0	0.0	8.7	91.1	99.9
Fe	**99.8**	0.0	0.0	0.0	0.1	0.1	0.0	0.0	100
K	**89.7**	0.0	0.0	0.0	0.0	0.0	6.2	4.1	100
Na	**99.4**	0.0	0.0	0.0	0.0	0.0	0.4	0.2	100
S	**0.1**	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.1

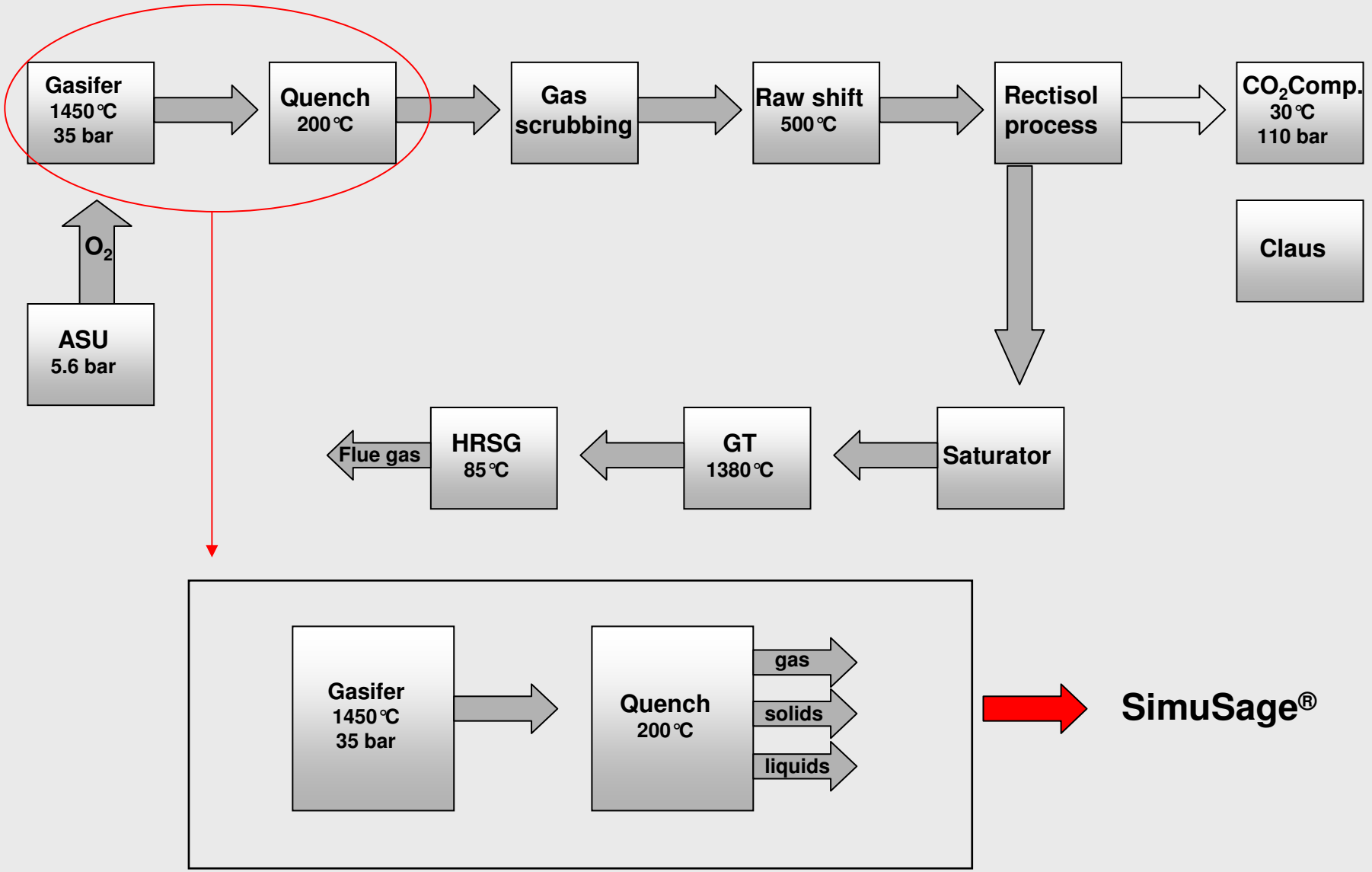
- Condensed phases:
  - Formation of monoxide phase and pyrrhotite at about 1000 °C
  - Condensation of salts (alkali chlorides) at 700 °C
  - Other chlorides at quench stage 220 °C

- Gaseous phases:
  - Considerable amount of KCl and $(KCl)_2$ found in gas phase below 700 °C
  - Traces of NaCl and $(NaCl)_2$

Summary of results

- Embedding of volatile ash elements into slag is very high
- Decreasing at higher gasification temperatures
- High content of Cl and CaO in coal (high basicity) leads to more likely deposition formation
- All elements, excluding Cl and S, condense completely at 200°C
- Alkalis condense as chlorides (KCL, NaCl) at the exit of the HRSG

General concept HotVeGas



End of 1st part of the presentation

Results condensed phases

Condensed phases in the specific process stages in g/h

Phases	Slag gasifier 1500°C	HRSG 1400°C	HRSG 1275°C	HRSG 1150°C	HRSG 1025°C	HRSG 900°C	HRSG 700°C	Quench 200°C
AMonoxide solid MP of FeO, Fe2O3, CaO, MgO	0	0	0	0.11	0.24	0.0003	0.0001	0
ASlag-liq	39159	0.12	0	0	0.003	0	0	0
BAlkCl-ss_rocksalt solid MP of KCl, NaCl	0	0	0	0	0	0	22.6	0.42
CaCO3_calcite(s2)	0	0	0	0	0	0	0	0.0005
CaMg(CO3)2	0	0	0	0	0	0	0	0.0003
FeCO3_siderite(s)	0	0	0	0	0	0	0	0.007
NH4Cl(s2)	0	0	0	0	0	0	0	122.3
NH4Cl-[KCl](ss) solid MP of NH4Cl, KCl	0	0	0	0	0	0	0	54.0
Olivine solid MP of (Mg,Mn,Fe)2[SiO4]	0	0	0.029	0.0001	0	0	0	0
Pyrrhotite solid MP of FeS, S	0	0	0	0	4.0	1.9	0.23	0
SiO2_tridymite	0	0.004	0	0	0	0	0	0
Sum:	39159	0.13	0.029	0.11	4.22	1.88	22.9	176.7

*mass flow 450 kg/h and 2 MW

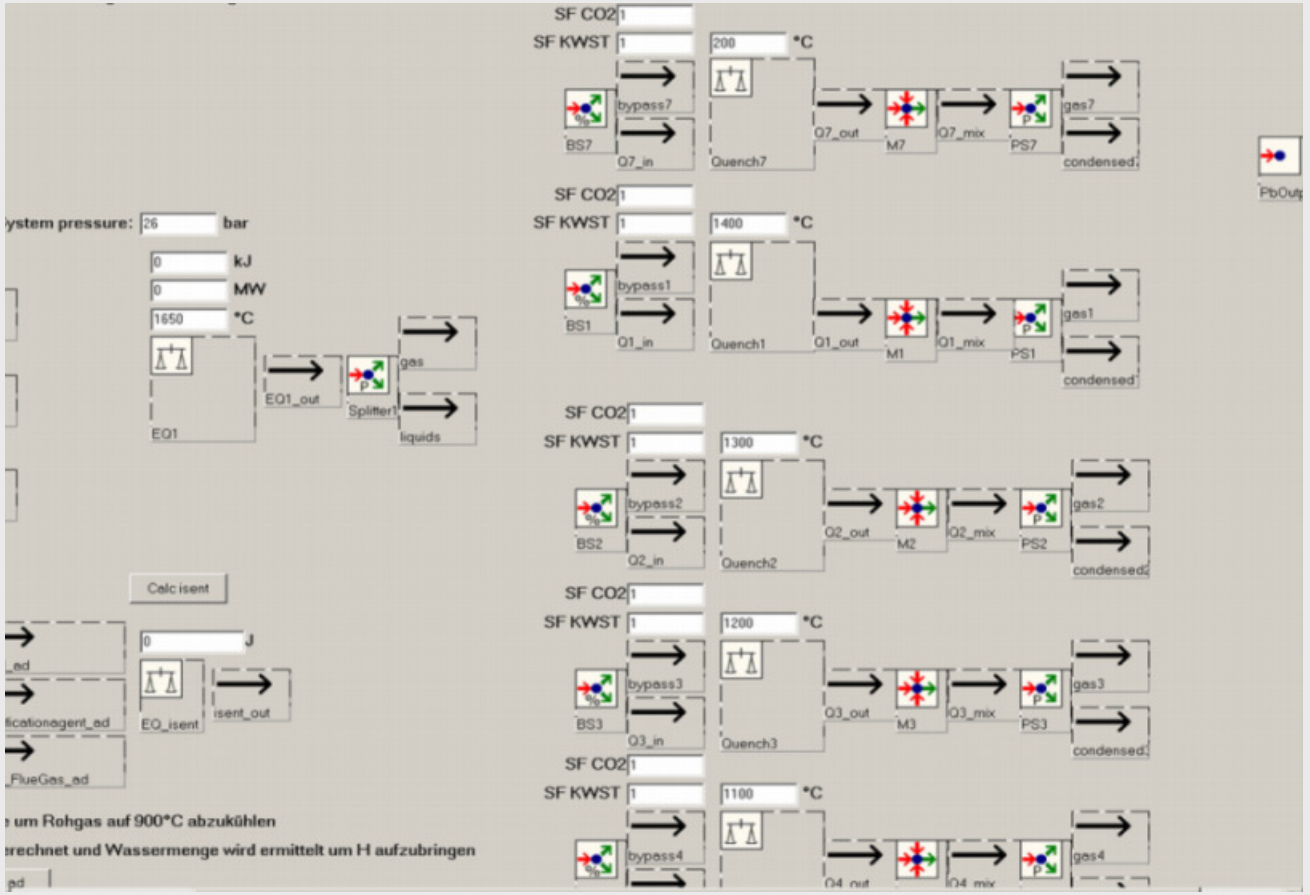
results gaseous compounds

Concentrations of gaseous compounds at the exit of the HRSG in mg/m³ raw gas STP

Gaseous compounds	700°C
Na	0.0E+00
NaCN	3.9E-05
NaOH	5.6E-05
NaCl	3.8E-01
$(NaCl)_2$	3.6E-02
K	0.0E+00
KCN	9.5E-05
KOH	1.4E-03
KCl	8.2E+00
$(KCl)_2$	6.1E+00
$Fe(OH)_2$	2.1E-03
$FeCl_2$	1.7E-03
$KFeCl_3$	5.4E-03
$KMgCl_3$	2.4E-04
$KCaCl_3$	1.1E-03

SimuSage®

- Development of a complex model which simulates a whole process in one calculation
- Results of one step are the input data for the next step of the process



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