



Institut für Energieverfahrenstechnik und
Chemieingenieurwesen



Institute of Energy Process Engineering and Chemical Engineering

Activities regarding IGCC-Technology

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Gasification Technologies Conference October 15-16, 2007, San Francisco



Where is the IEC?



**Head of Institute:
Professor Bernd Meyer**

**Scientists: 34
Lab/Technical: 26**

→ *Known for:*



Training Courses on Gasification & Syngas production



German Center for Gasification Technologies

International Freiberg Conference on IGCC & XtL Technologies



(Contact: Isabel.Ulbricht@iec.tu-freiberg.de)

Three Routes of IEC's Research

Biomass



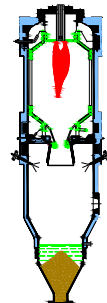
Gas/Oil



Coal

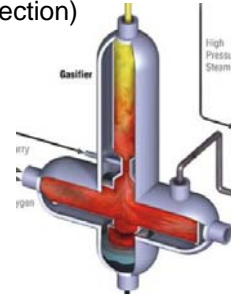


Gasification Technologies

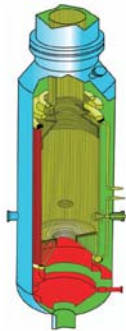


SFG

(selection)



Conoco-Phillips



SCGP



GE



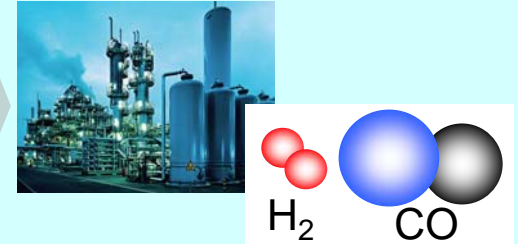
Lurgi Dry Ash

And others

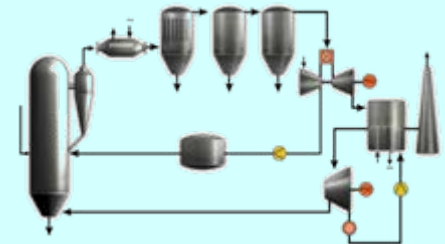
Liquid Products



Syngas production



Power Generation (IGCC)



Steady-State modelling

→ Specification data:

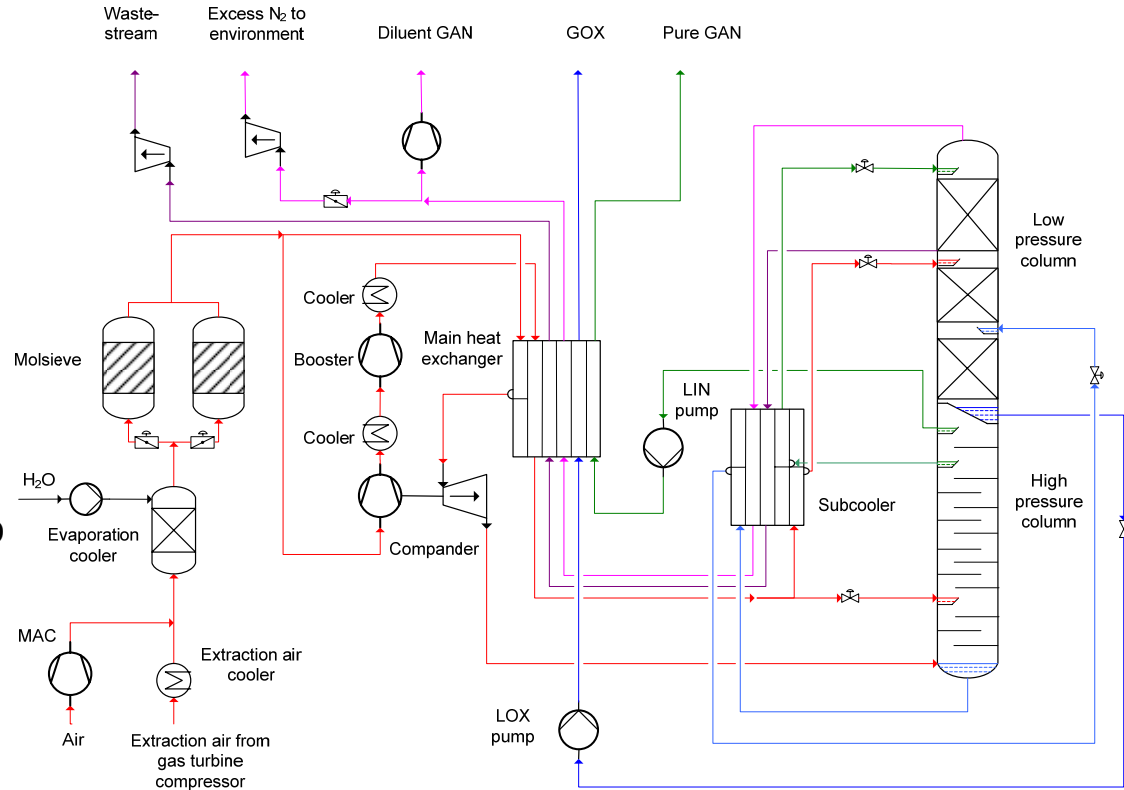
- Oxygen demand of gasifier
- Diluent nitrogen demand of GT
- Extraction air from GT compressor

→ Calculation procedure:

- Flow sheet simulation (ASPEN)
- Concept studies regarding pressure level and pressure ratio

→ Results:

- Power consumption of nitrogen and air compression
- Concept optimisation:
 - a) Air integration of GT
 - b) Pressure level
 - c) Pressure ratio



Dynamic modelling (at the beginning)

→ Specification data:

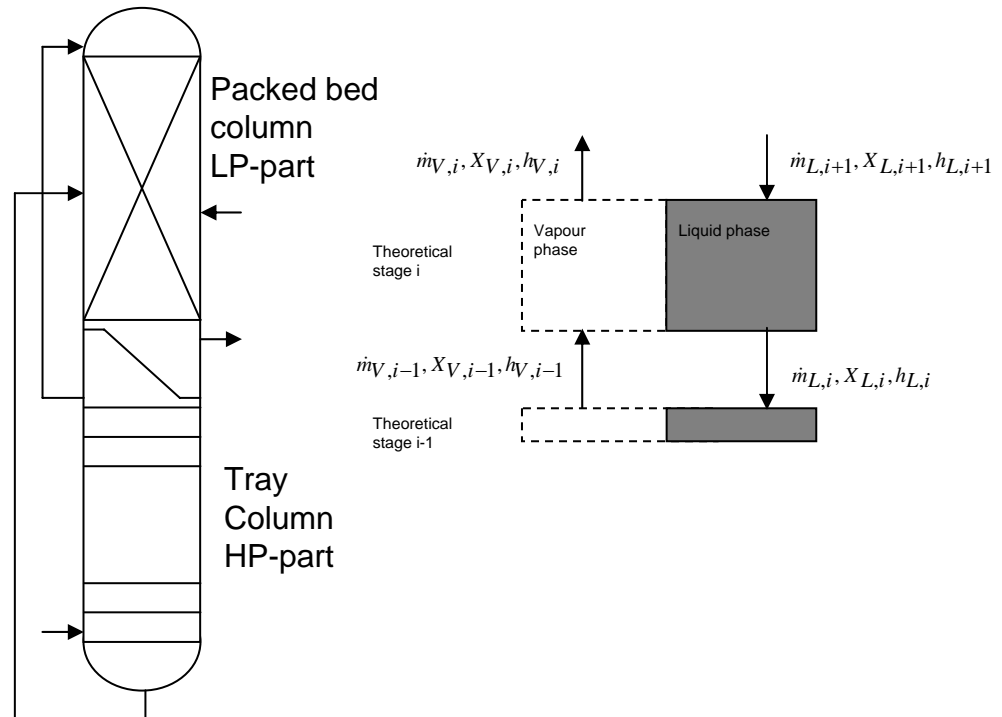
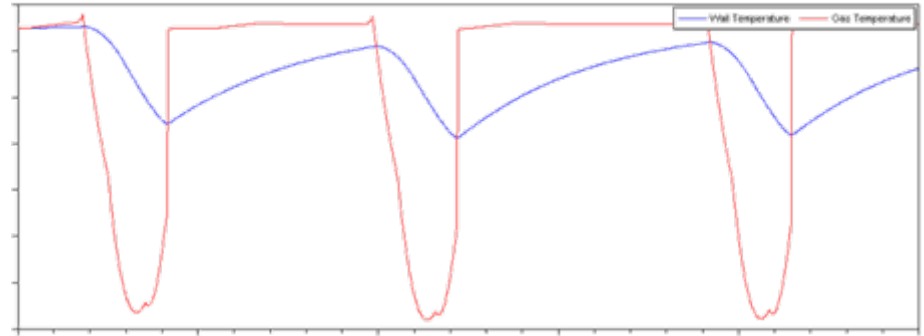
- Capacities and hold-up
- Pressure drops of equipment
- Geometry of columns and pipes
- Mass flow

→ Calculation procedure:

- Tools: Modelica/Dymola
- Non-ideal data on chemical media
- Component balances

→ Predicted results in future:

- Dynamic interaction of ASU and GT
- Load change behaviour
- Start-up and Shut-down
- Programming functions for actuators



Thermodynamic modelling

→ Specification data:

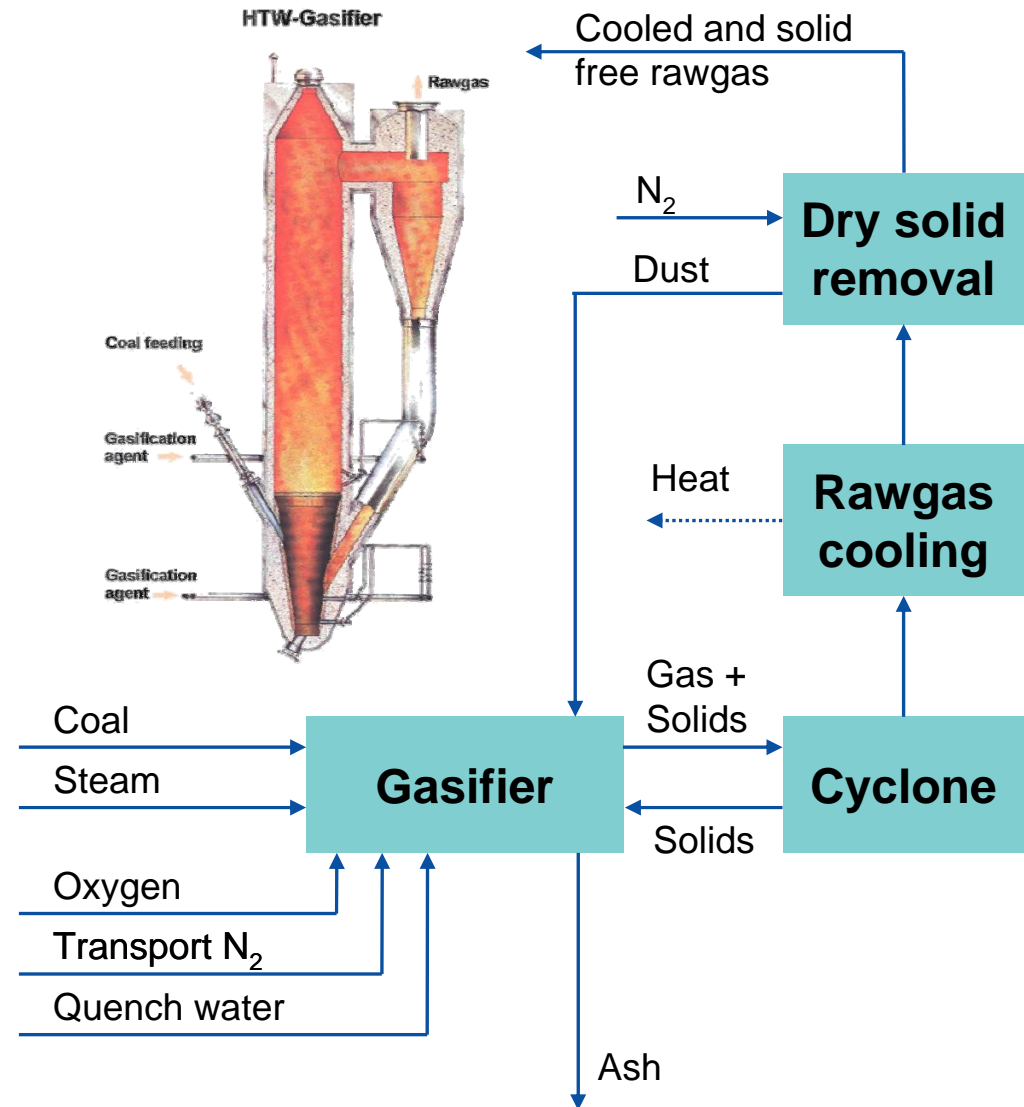
- HHV, elemental/proximate analysis of feed stream
- Type of process (HTW, SCGP, ...)
- Process conditions

→ Calculation procedure:

- Flow sheet simulation (ASPEN)
- Temperature approaches for equilibrium based modelling
- User defined functions for feed treatment

→ Results:

- Gas composition (including trace elements)
- Steam/oxygen/air consumption
- Consumption of auxiliaries (quench water, transport nitrogen, cooling water,...)



Numerical flow simulation

→ Specification data:

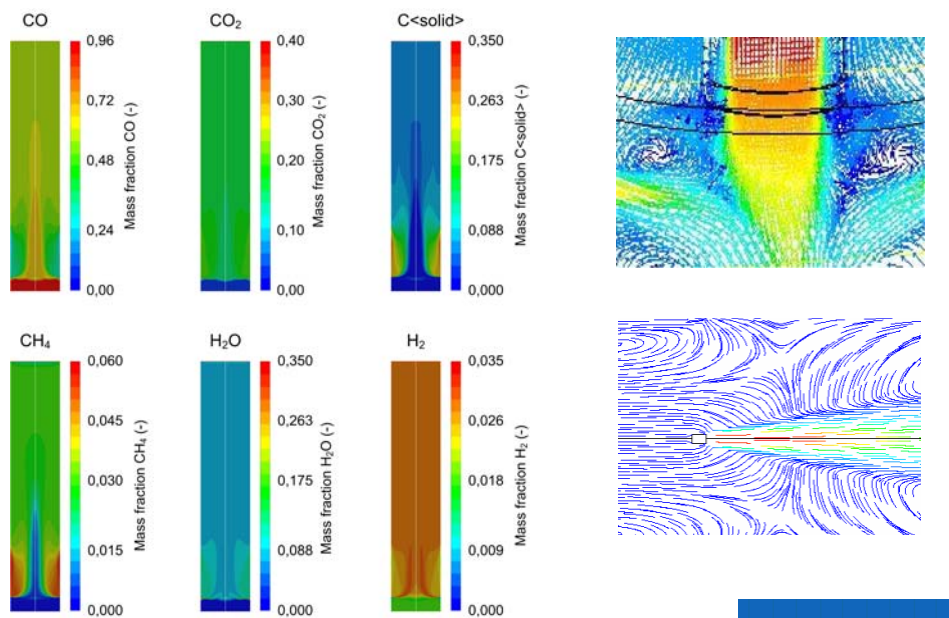
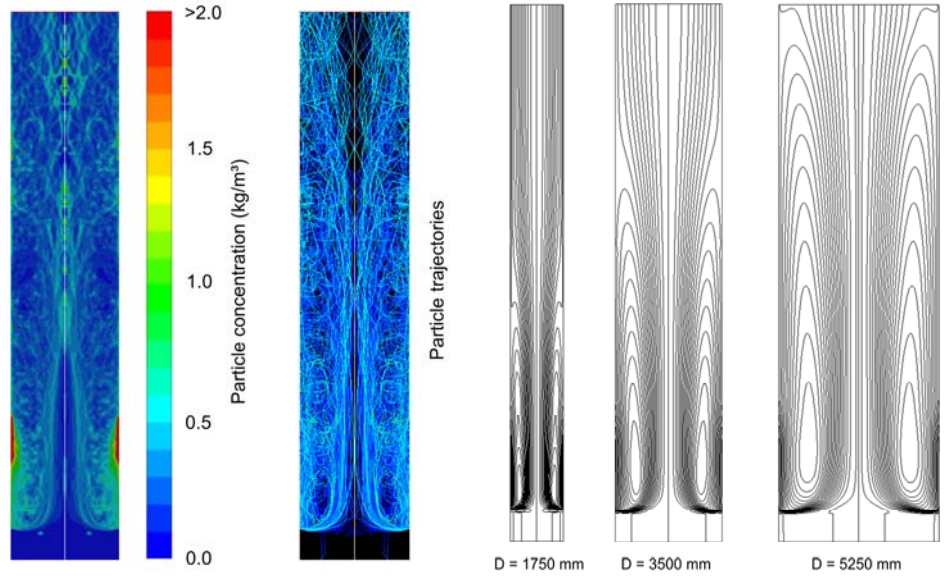
- Properties of inlet flows
- Geometry of reactor
- Process conditions
- Particle properties

→ Calculation procedure:

- Ansys Fluent (soon: OpenFOAM)
- RANS and LES modelling
- Reduced mechanisms for gas phase kinetics
- Eulerian-Lagrangian approach for particle modelling

→ Results:

- Flow pattern inside the gasifiers
- Peak temperatures
- Validation on experimental data (radio active tracer experiments)
- Optimisation of design



Modelling of ash and slag behaviour

→ Specification data:

- Elemental/proximate analysis of feed stream
- Elemental (XRF) and phase (XRD) analysis of mineral content
- Operating conditions

→ Calculation procedure:

Flow sheet simulation (SimuSage)

- Principle of local equilibrium stages

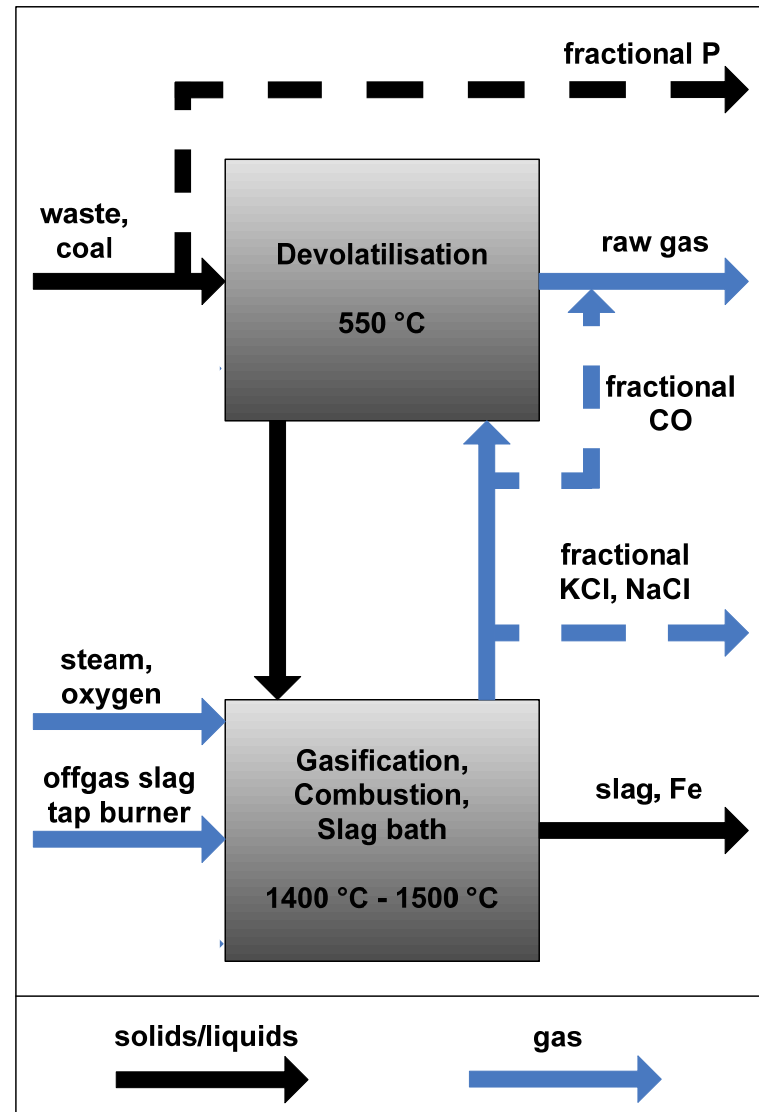
Thermodynamic simulation (FactSage)

- Data base for pure condensed substances and solution phases (non-ideal interaction)

→ Results:

- Behaviour of volatile ash compounds (alkalies, Cl, S, trace elements)
- Ash melting behaviour
- Fouling prediction in HRSG
- Phase separation (slag vs. metals)

BGL model



Multi-concept modelling of gas treatment

→ *Freely combinable modules for each process type and each process step*

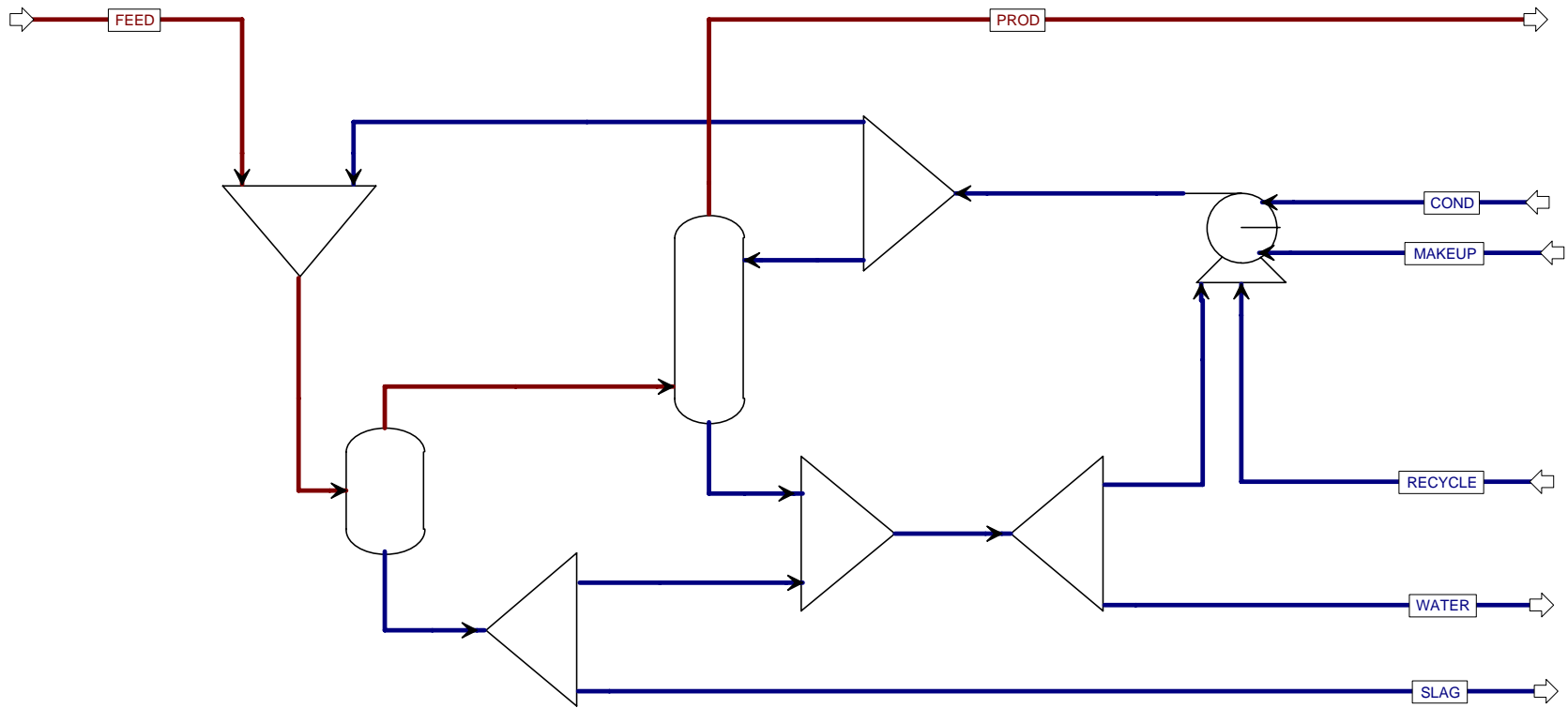
Dry Dust Removal	Raw Gas CO Shift	Acid Gas Removal chemical	Sweet Gas CO Shift
Water Treatment	Hydrolysis	Acid Gas Removal physical	CO ₂ -Treatment
Water Wash	Dry Desulphurisation	Sulfur Recovery	Fuel Gas Conditioning

→ *Configuration of desired process chain*



Example for Module 1: Water wash

- **Specification data:** Gas composition, temperature, pressure and flow rates
- **Calculation procedure:** Electrolyte reactions, experimental data user subroutines
- **Results:** Water/energy demand, chloride removal rate, gas composition



Example for module 2: Raw gas CO-conversion**→ Specification data:**

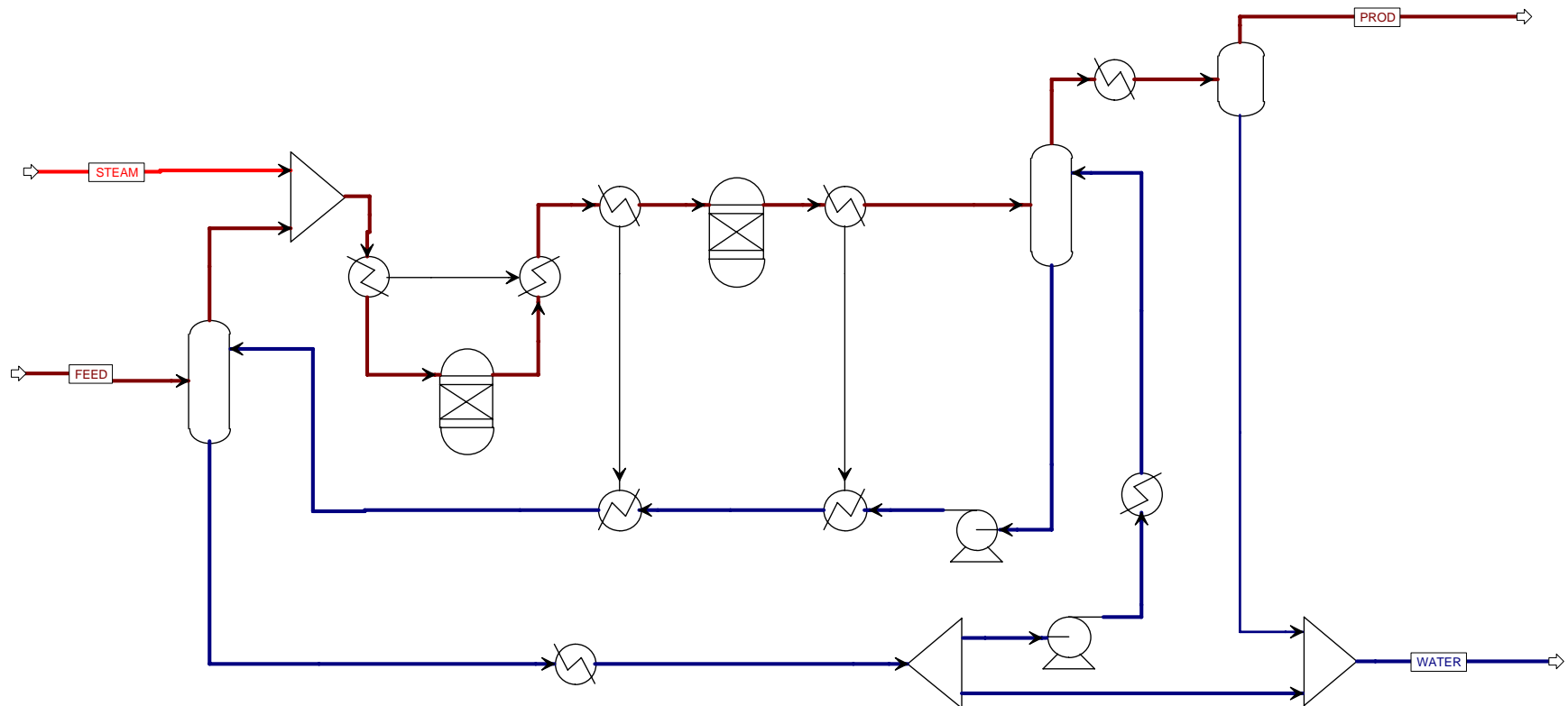
Gas composition, temperature, pressure and flow rate,
type of reactor and intercooler

→ Calculation procedure:

Cycle calculation with electrolyte reactions and non ideal gas
properties

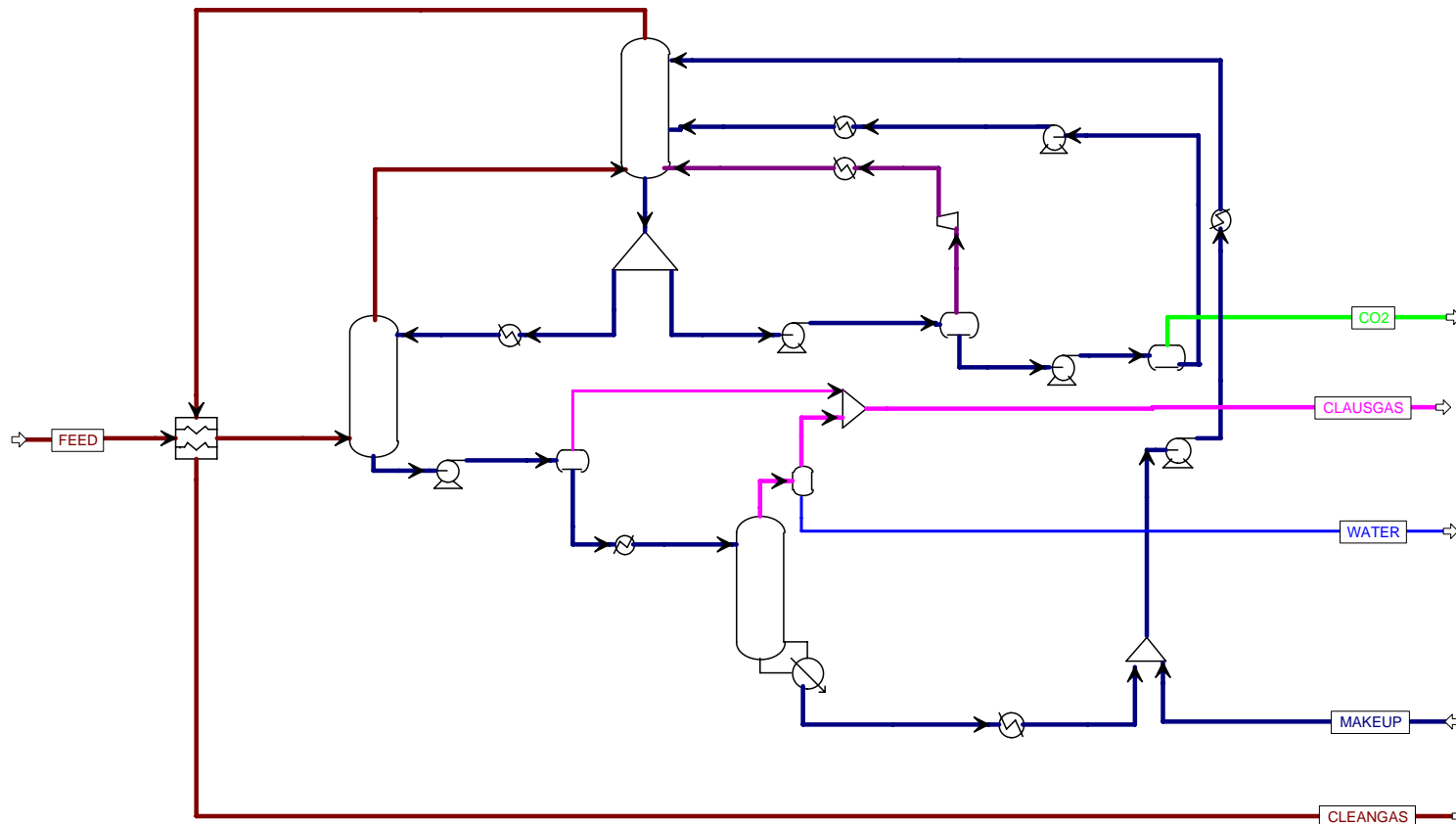
→ Results:

Steam demand, conversion rate, efficiency losses



Example for module 3: Acid gas removal (physical absorption)

- **Specification data:** Gas composition, temperature, pressure and flow rate, requirements to gas quality
- **Calculation procedure:** Activity coefficient model for different solvents: glymes (DEPG), methanol, water
- **Results:** Clean gas composition, energy demand



Generic modelling of IGCC-gas turbine

→ Specification data:

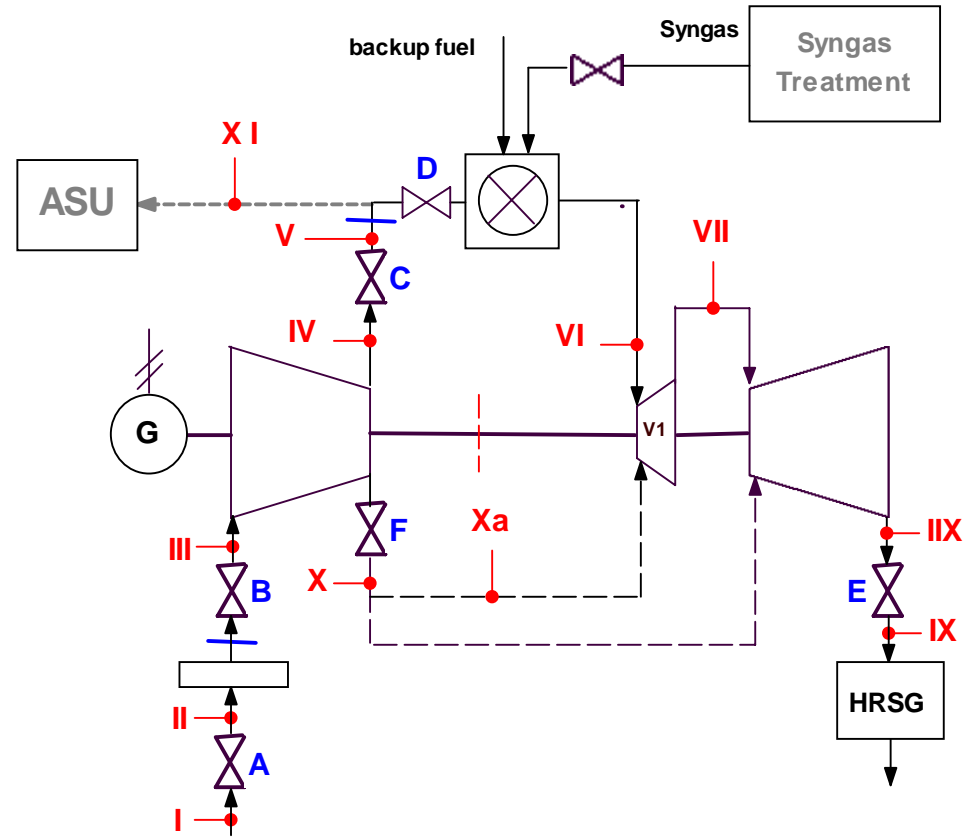
- Fuel gas (syngas) composition
- Preheat temperature
- Air extraction for ASU, inlet mass flow

→ Calculation procedure:

- Generic equation modelling (EES)
- Polytropic change vs. compressor map
- Turbine cooling mass flow
- Material constraints
- Balances and losses

→ Results:

- Power output
- Surge margin
- Blade temperature
- Rotor torque
- Exhaust temperature
- ISO mixing temperature (TIT)
- Definition of operation windows



Future challenges are identified as ...**→ Deep modelling of gasification:**

- Integration of complex kinetics in reactive flows
- Mathematical implementation of particle-interactions (agglomeration)
- Virtualisation of processes (www.virtuhcon.de)

→ Modelling of ash and slag reactions:

- Prediction of T-250 by mineral composition
- Modelling of eutectics and flux properties
- Paths of trace elements

→ Dynamic modelling:

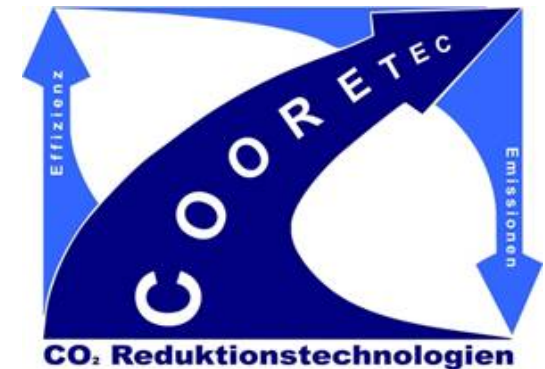
- Description of all components of an IGCC and integration into one concept

→ Conceptual Optimisation:

- Expansion from IGCC to polygeneration concepts
- Concept studies on capture-ready IGCC technology
- Integration of low temperature shift conversion

→ Experimental investigations up to pilot scale:

- Validation of models
- Improvement of design



→ All activities are part of Germany's R&D Lighthouse Project COORETEC