MATHEMATICAL MODEL OF THE PARTIAL OXIDATION OF COAL PARTICLES
FOR THE MODELLING OF SYNGAS PRODUCTION: VIRTUCON

P.A. Nikrityuk, B. Meyer
Institute of Energy Process- and Chemical Engineering

Centre for Innovation Competence
Virtual High Temperature Conversion Processes

4th Int. Conference on Clean Coal Technologies, CCT2009
3rd Int. Freiberger Conference on IGCC & XtL Technologies, Dresden, Germany 18-21 May 2009
Centre for Innovation Competence (CIC) Virtuhcon

Objective:
- Establishment of a leading international research centre for fundamental and applied research in the field of high temperature conversion processes for Chemical, Energy and Metallurgical applications

Integration:
- Initiated by 8 institutes of TU Bergakademie Freiberg (combining engineering, natural sciences, mathematics and computer sciences)

Structure:
- 3 research groups with 21 young scientists
- Start: 05/2009 at Reiche Zeche, Institute of Energy Process- and Chemical Engineering, Freiberg University of Technology - Mountain Academy

Funding:
- First funding phase from 2009-2014: approx. 10 Mio. EUR excluding additional investments in laboratory equipment and construction costs (appr. two thirds from the Federal Ministry of Education and Research of Germany and the rest from federal state of Saxony)
Strategic objectives

- focussing on stable supply of materials and energy

Material and energy conversion process chains

- ... obtaining resource-intensive high temperature conversion processes based on *partial oxidation*

Products of our daily life

- Syngas production in sectors, like:
  - Production of hydrogen-rich energy sources
  - Production of chemical products
  - "CO₂-free" power generation

- Metallurgical processes in sectors, like:
  - Production of pig iron
  - Production of *steel and ferro* alloys
  - Nonferrous metallurgy

Market analysis

- high demand and broad potential customer and market base for Virtuhcon

Virtuhcon relevant business volume

- USA
  - 185 Mrd. EUR
  - 108 Mrd. EUR

- Germany
  - 46 Mrd. EUR
  - 29 Mrd. EUR

Joint criteria

- High investment costs
- Long development cycles (< 5 - 10 years)
- High potential of optimisation

Reduction of 1% costs gives ~10⁷ EUR profit
Development of new technologies through numerical simulations

Strategic objectives

Aim

... virtual prototype processes

... basis of the virtual process engineering

Innovative new Technologies for:

- Power Plant Technology
- Fuel Synthesis
- Production of H₂-rich fuels
- Production of Chemicals
- Nonferrous Metallurgy
- Iron and Steel Technology

Potential for development of fundamentally new technologies:

- at a shorter development time
- with lower effort
- at minimum risk
New process development via multidiscipline and innovative research

- **Mathematics & computer science**
  - Institute for Numerical Mathematics and Optimisation
  - Institute for Computer Sciences

- **Fluid dynamics & materials science & thermodynamics**
  - Institute of Heat Engineering and Thermodynamics
  - Institute for Mechanics and Fluid Dynamics
  - Institute for Materials Science

- **Institute for Iron and Steel Technology**
  - Institute for Nonferrous Metallurgy and Purest Substances
  - Institute for Energy Process Engineering and Chemical Engineering

- **Energy source conversion**
- **Metallurgy**

... realistic simulation and virtualisation of HT conversion processes
Complete theoretical description of high temperature conversion processes by three system components:

Three research groups

- Multi-phase systems
- Inter-phase phenomena
- Reactive flow systems

Example: syngas production

Example: Production of steel and iron

Strategic objectives

Virtualisation

... accelerated development of sustainable HT conversion processes
Multi-Level Modeling Scheme for Fluidized Beds Reactors

The whole Reactor
$\Delta x \sim 0.1 \text{ m}$

$(10^5)$ Chemical Reacting Particles
$\Delta x \sim 10^{-4} \text{ m}$

$N (1-100)$ Chemical Reacting Particles
$\Delta x \sim 10^{-6} \text{ m}$

Semi-Empirical Drag Closure for Bubbles

Discrete Bubble Model
(E.g. Screen Saver)

Lagrangian (Gas Phase)-Eulerian (Solid Phase)

Semi-Empirical Drag Closure for Gas-Solid

Two-Fluid Model

Euler (Gas Phase)-Euler (Solid Phase)

Semi-Empirical or Direct Modeled Drag Closure
for Solid + Effective Model for Particle-Particle Interactions

Unresolved and Resolved
Discrete Particle Model
(UDPM, RDPM)

Euler (Gas Phase)-Lagrangian (Solid Phase)

DNS (Lattice Boltzmann Model (LBM), Immersed Boundary Model (IBM), Elastic Collisions)

No Closure Required, Direct Modeling of Particle-Fluid and Particle-Particle Interactions

After Deen et al. 2007, Van der Hoef et al. 2008
Objectives:

- Modeling of a chemical-reacting interface in multi-phase systems including phase changes: solid-gas, solid-liquid and liquid-gas
- Modeling of the fluid-particle, particle-wall interactions including heterogeneous chemical reactions

Tasks

- Modelling of boundary layers and drag forces
- Modelling of kinetics of heterogeneous reactions and homogeneous reactions near the interface
- Modeling of the evolution of the coal-particle shape during the gasification including particle tracking by use of DNS approach

\[2\left(\frac{\alpha+1}{\alpha+2}\right)C + O_2 \rightarrow \frac{2\alpha}{\alpha+2}CO + \frac{2}{\alpha+2}CO_2\]

\[C + H_2O \rightarrow CO + H_2\]

\[CO + \frac{1}{2}O_2 \leftrightarrow CO_2\]

\[H_2 + \frac{1}{2}O_2 \rightarrow H_2O\]

\[CO + H_2O \rightarrow H_2 + CO_2\]
Fixed Grid Concept. Full Coupled Euler-Lagrange Model

\[ \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{u}) = 0 \]

\[ \rho \frac{\partial \vec{u}}{\partial t} + \rho (\vec{u} \cdot \nabla) \vec{u} = -\nabla \cdot \sigma + \vec{F} \]

\[ \rho \frac{\partial (c_p T)}{\partial t} + \rho (\vec{u} \cdot \nabla) (c_p T) = \nabla \cdot (\lambda_m \nabla T) + \Delta H_c \rho \frac{\partial \varepsilon_s}{\partial t} + \varepsilon_f \sum \Delta H_i \mathcal{R}_i + k_e \sigma_B T^4 \]

\[ \rho \frac{\partial C_i}{\partial t} + \rho (\vec{u} \cdot \nabla) C_i = \nabla \cdot (D_i \nabla C_i) + \rho \sum \omega_i \mathcal{R}_i \]

\[ M_j \frac{d \vec{U}_j}{dt} = \Delta M_j \vec{g} + \vec{F}_{j,\text{colis}} + \vec{F}_{j,\text{hydro}} \]

\[ \bar{I}_j \frac{d \omega_j}{dt} + \omega_j \times (\bar{I}_j \omega_j) = T_j \]
Code and Model Validation

Re=100
Illustration of the heat and mass transfer simulation

Sc=1, Pr=1

Re=10

Re=40

Re=80

Temperature, K
Example of the Interface Tracking
Mass Concentration of Cu by Dendritic Growth of Al 4wt% Cu

- Modified CA
  (Beltran-Sanches & Stefanescu, MMTB, 2003, 2004)
- Stefan Conditions on the Interface
- Full Coupling: momentum, heat and mass transfer
- SIMPLE algorithm
- SIP solver

\[
\frac{\partial T}{\partial t} = \frac{30}{s} \frac{K}{\Delta T = 3.3K}
\]
Full Coupled Euler-Lagrange: Particle Sedimentation
Tasks To Study

• Update of the drag force between the gas phase and the coal particles, especially the impact of the volume fraction of particles has to be studied more precisely

• Update the heat and the mass transfer coefficients for the coal particles

• Prediction of the shrinking time of a particle in dependence on the temperature of a surrounding gas

• The impact of the particle porosity on the dynamics of particle gasification

• The impact of turbulence on the particle gasification
Technology leadership in the sustainable supply of materials and energy through multi-disciplinary innovative research!

Thank you for your attention!

Funded by the BMBF (Federal Ministry of Education and Research) Germany and the government of Saxony within the initiative "Centers for Innovation Competence: Create Excellence – Foster talents"