A Status Report on Multiphase CFD for Gas-Particles Systems

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2005 ANNUAL MEETING
OF THE
CHEMICAL REACTION ENGINEERING LABORATORY (CREL)
Thursday, October 6, 2005
Washington University
NETL
Three Premises

- The US will need to rely on fossil fuels for electricity and transportation fuels well into 21st century

- It is prudent to rely on a diverse mix of energy resources

- Better technology can make a difference in meeting environmental needs at acceptable cost

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Outline

- Hierarchy of models
- Eulerian-Eulerian approach
- Fundamental set of equations
- Constitutive laws
- Examples
Outline

• *Hierarchy of models*

• Eulerian-Eulerian approach

• Fundamental set of equations

• Constitutive Laws

• Examples
CAD/CAE Modeling

Integrity with 3 D model
Schematic diagrams
P&IDs
Loop diagrams
Structural
Report generation
Reduce rework
Standards/Specifications
Process Simulation

Process Optimization
Economic Evaluation
Component Sizing
Sensitivity Analysis

Unit Operations Library
Physical Properties Database
Control Systems

tightly coupled systems … with disparate time scales

Normal operation
Start Up/Shut Down
Load Following
Transients Upsets
Safety
...

NETL
Mechanistic Modeling

CFD Simulations
- single/multi-phase
- heat transfer
- chemical reactions

Finite Element Structural Simulations

Event Based Simulations

Material/Property Simulations
Hierarchy of Models

- Enterprise
- System Models
- Integrated Models
- Component Models
  - empirical models
  - physics based models: CFD
Hierarchy of CFD models - 1

- **Single-phase fluid**
  - Continuum hydrodynamics (stress-law: ideal gas, …)
  - Turbulence model (steady-state, turbulent stress, etc.)
  - Heat transfer
  - Chemical kinetics (global/mechanistic, homogeneous)

- **Single-phase granular flow**
  - Discrete Element Method (DEM)
    - Soft particle (enduring collisions)
    - Hard particle (instantaneous, binary collisions)
  - Continuum hydrodynamics (stress-law: kinetic theory, …)
  - Turbulence model (not well developed!!!)
  - Heat transfer
  - Chemical kinetics
Hierarchy of CFD models - 2

- **Multiphase**
  - Eulerian-Lagrangian
    - Eulerian – non-interacting particles
    - Eulerian - DEM
  - Eulerian-Eulerian
    - Continuum hydrodynamics (stress-law: ideal gas, …)
      - Turbulence model (steady-state, turbulent stress, etc.)
    - Heat transfer
    - Chemical kinetics (global/mechanistic, homogeneous)
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Local variables
Navier-Stokes eq. for fluid
Newton’s Laws for particles

\[
\int_{V_f} g dy^3
\]

Mean variables
Navier-Stokes-like eqs.
for fluid and granular phases
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E-E Multiphase Model Equations

Continuity Equations

\[ \frac{\partial}{\partial t} (\varepsilon_m \rho_m) + \nabla \cdot (\varepsilon_m \rho_m \vec{v}_m) = \sum_{l=1}^{M} R_{ml} \]

Momentum Equations

\[ \frac{\partial}{\partial t} (\varepsilon_m \rho_m \vec{v}_m) + \nabla \cdot (\varepsilon_m \rho_m \vec{v}_m \vec{v}_m) = \nabla \cdot \vec{S}_m + \sum_{l=1}^{M} \vec{I}_{ml} \]

Chemical Rates

Stresses

Interaction Term
Cascade of Energy

- Single-phase flow
  - Large scale fluid flow >>
    >> Small scale fluid flow >>
    >> Molecular dissipation
Cascade of Energy

- Fluid-particle flow
  
  Large scale fluid flow >>
  >> Small scale fluid flow >> Molecular dissipation

  >> Large scale particle motion (bubbles/clusters) >>

  >> Relative particle motion (granular temp) >>

  >> Inelastic particle collisions >>
Energy Balance

\[
\frac{\partial}{\partial t} (\varepsilon_m \rho_m h_m) + \nabla \cdot (\varepsilon_m \rho_m h_m \mathbf{u}_m) = \varepsilon_m \left( \frac{\partial \rho_m}{\partial t} + \mathbf{u}_m \cdot \nabla \rho_m \right) + \overline{S} : \nabla \mathbf{u}_m + S_m
\]

\[
- \nabla \cdot \mathbf{q}_m + \sum_{l=1}^{M} \left( \gamma_{ml} (T_l - T_m) + R_{ml} h_{ml} \right)
\]
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• Hierarchy of CFD models

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• Constitute Laws:
  closure – dependence on mean variables

• Examples
Constitutive Laws: Phase Interaction

- Bouyancy
- Drag
- Lift
- ...

\[ \vec{I}_{ml} = -\delta_{gm} \varepsilon_l \nabla P_g - F_{ml} (\vec{v}_l - \vec{v}_m) + R_{ml} \left[ \xi_{ml} \vec{v}_l + \xi_{ml} \vec{v}_m \right] \]

\( F_{ml} \) is:

1) empirical
2) function of: velocity, voidage,
Constitutive Laws: Granular Stresses

Plastic flow
- slowly shearing
- enduring contacts
- frictional transfer of momentum

Viscous flow
- rapidly shearing
- transient contacts
- translational or collisional transfer of momentum

Slowly and Rapidly Shearing Granular Flows
Multiphase Model - Granular Stress

\[
S_{sm} = \begin{cases} 
- P_{sm}^p I + \tau_{sm} & \text{if } \varepsilon_g \leq \varepsilon_g^* \\
- P_{sm}^v I + \tau_{sm} & \text{if } \varepsilon_g > \varepsilon_g^* 
\end{cases}
\]

Plastic Regime
(Schaeffer – 1987)

Viscous Regime
(Lun et al. – 1984)
**Multiphase Model - Granular Stress Viscous Regime**

**Granular Pressure**

\[ P_{sm}^v = K_{1m} \varepsilon_{sm}^2 \Theta_m \]

\[ K_{1m} = 2 \left(1 + e_{mm}\right) \rho_{sm} g_{0mm} \]

**Granular Temperature**

**Shear Stress**

\[ \tau_{sm} = 2 \mu_{sm}^v D_{sm} + \lambda_{sm}^v \text{tr} \left( D_{sm} \right) I \]

\[ \lambda_{sm}^v = K_{2m} \varepsilon_{sm} \sqrt{\Theta_m} \]

\[ K_{2m} = \frac{4 d_{pm} \rho_{sm} \left(1 + e_{mm}\right) \varepsilon_{sm} g_{0mm}}{3 \sqrt{\pi}} - \frac{2}{3} K_{3m} \]
Multiphase Model - Granular Stress
Plastic Regime

\[ P_{sm}^p = \varepsilon_{sm} P^* \]

\[ P^* = A(\varepsilon_{g}^* - \varepsilon_{g})^n \]

\[ \tau_{s1} = 2 \mu_{s1}^p \overline{D}_{s1} \]

\[ \mu_{s1}^p = \frac{P^* \sin \phi}{2 \sqrt{I_{2D}}} \]

\[ I_{2D} = \frac{1}{6} \left[ (D_{s11} - D_{s22})^2 + (D_{s22} - D_{s33})^2 + (D_{s33} - D_{s11})^2 \right] \]

\[ + D_{s12}^2 + D_{s23}^2 + D_{s31}^2 \]

Second Invariant of the Deviator of the Strain Rate Tensor
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Modeling of Gas-Solid Transport in the Chemical Industry

The Goal is Fully Coupled Simulations

- Dense Phase Gas/Fluid Hydrodynamics
- Heat and Mass Transfer
- Chemical Kinetics
- 3-D
- Transient

Applications: coal gasification, O₃, SiH₄, SiHCl₃, CH₄, TiCl₄, -CH₂-
MFDRC - NETL MFIX Code

- MFIX - Multiphase Granular Flow Code

MFIX Application - Ozone Decomposition

- Fryer and Potter (1976)
- 117 mm, 2650 kg/m³ catalyst particles
- 0.229 m diameter x 2 m height
- bed height = 0.115 m
- $U_{mf} = 1.7$ cm/s
- Gas flow: 2, 4, 6, 8, 10, 12, 14 cm/s
- axisymmetric cylindrical coordinates
- Grid resolution: 36 x 56, 72 x 112, 144 x 224
- First order kinetics
  \[ \text{O}_3 \rightarrow 1.5 \text{O}_2 \]
- Catalyzed by sand impregnated with iron oxide
MFIX Code - Ozone Decomposition

Ozone Conversion

Cout/Cin vs Gas Velocity, cm/s

Fryer and Potter (1976)

MFIX-72x112
MFIX Code - Ozone Decomposition

Void fraction 0.8
(yellow isosurface)

Ozone mass fraction 0.05
(green isosurface)
U = 8 cm/s; Hmf = 11.5 cm
SiH$_4$ Pyrolysis

“Silicon Deposition from Silane and Disilane in a Fluidized Bed
- Part I: Experimental Study”
B. Caussat, M. Hemati, and J. P. Couderc
- Part II: Theoretical Analysis and Modeling”
Hydrogenation of SiCl₄

“Investigation of the Hydrochlorination of SiCl₄”
J. Y. P. Mui, Solarelectronics, Inc.

Process for the hydrochlorination of SiCl₄ with H₂ to form SiHCl₃ in a fluidized bed of Si (m.g.)

Pseudo-first order JPL data being analyzed by Dow Corning personnel

\[ 3 \text{SiCl}_4 + 2 \text{H}_2 + \text{Si} \iff 4 \text{SiHCl}_3 \]
Hydrogenation of SiCl4

"3 SiCl₄ + 2 H₂ + Si ⇌ 4 SiHCl₃"

SiCl₄ $\xrightarrow{\text{Cu-Si}}$ SiCl₂

$\begin{bmatrix}
\text{SiCl}_2 \\
\text{SiH}_2\text{Cl}_2
\end{bmatrix}$ $\xrightarrow{\text{HCl}}$ SiHCl₃

- Si - Cu - Cl - $\xrightarrow{\text{H}_2}$ - Si - Cu - + HCl
Coal Gasification: Carbonizer Chemistry

$$\text{CO}_2 + \text{H}_2\text{O} + \text{CO} + \text{CH}_4 + \text{H}_2$$

$$\text{O}_2$$

$$\text{CO}_2 + \text{H}_2\text{O}$$

$$\text{O}_2$$

$$\text{CO}_2 + \text{H}_2\text{O} + \text{CO} + \text{CH}_4 + \text{H}_2 + \text{Fixed Carbon}$$

$$\text{H}_2\text{O}$$

$$\text{CO} + \text{H}_2\text{O} \oplus \text{CO}_2 + \text{H}_2$$

Coal

Moisture

Ash

CaO

CaCO_3

CaMg(CO_3)_2

MgO

Volatile Matter

Fixed Carbon

sorbent

CO_2

H_2

CO

CH_4

H_2O

H_2 + CO
Power Systems Development Facility
Kellogg, Brown & Root Transport Reactor

- Transient, 3-D cylindrical coordinated
  >250K computational cells

- 8 gas species: $\text{O}_2$, $\text{CO}$, $\text{CO}_2$, $\text{CH}_4$, $\text{H}_2$, $\text{H}_2\text{O}$, $\text{N}_2$, Tar

  4 solid species: Ash, Volatile Matter, Moisture, Fixed Carbon

- Parallel runs at Pittsburgh Super Computing Center (PSC)
  < week CPU time ~ 10 seconds of simulation
CH4  H2  H2O
Kellogg Brown and Root, Inc. Transport Gasifier

Mass Fractions of Gas and Solids

- **Oxygen (20%)**
- **Oxygen (2%)**
- **Coal (1-2%)**
- **Solid Pathlines**

Coal Feed

Recycled Solids
Kellogg Brown and Root, Inc.
Transport Gasifier

Isosurface Void Fraction

Gas Temperature (F)
- 1675
- 1241
- 808

Axial Temperature (F)

Recycled Solids
Coal Feed
Simulations using PC Coal Lab to determine yields and composition of volatile matter

Powder River Basin Coal
- air and oxygen blown
- with/without lower mixing zone

- Hiawatha Coal
  - air and oxygen blown
  - with lower mixing zone

#Niksa Energy Associates
Kellogg Brown and Root, Inc.
Transport Gasifier

Mass Fractions of Gas and Solids

- **Oxygen** (20%)
- **Oxygen** (2%)
- **Fixed Carbon** (2%)
- **Solid Pathlines**

Coal Feed

Recycled Solids
TC09 Hiawatha Air Blown

Molar Fraction

- MFIX/PC Coal 1763/68/.3
- MFIX 1756/69/.46
- Exp. 1779/89/.4

CO, CO2, CH4, H2, H2O
TC06-52 PRB Air Blown

Molar Fraction

- **CO**
- **CO2**
- **CH4**
- **H2**
- **H2O**

Lines:
- MFIX/PC Coal 1749/98/.3
- MFIX (old rates) 1755/80/.75
- Exp 1757/98/1.5

**NETL**
MFIX Code: General Description

(Multiphase Flow with Interphase eXchanges)

- general-purpose computer code
- developed at the National Energy Technology Laboratory (NETL)
- describes the hydrodynamics, heat transfer and chemical reactions in fluid-solids systems
- used for describing bubbling and circulating fluidized beds and spouted beds
- calculations give transient data on the three-dimensional distribution of pressure, velocity, temperature, and species mass fractions
- used as a "test-stand" for testing and developing multiphase flow constitutive equations.
MFIX Features

- Mass, momentum, energy and species balance equations for gas and multiple solids phases
- Granular stress equations based on kinetic theory and frictional flow theory
- Three-dimensional Cartesian or cylindrical coordinate systems with nonuniform mesh size
- Impermeable and semi-permeable internal surfaces
MFIX Features (cont.)

- Set up the simulation with an input data file
- Define chemical reactions and kinetics with the input data file or with a user-defined subroutine
- Error checking of user input
- Multiple, single-precision, binary, direct-access output files that reduces disk space and increases data retrieval speed
- Post-processing codes for the animation and retrieval of output data
- Fortran 90 code base with allocatable arrays
- Generate serial, shared-memory parallel (SMP) or distributed-memory parallel (DMP) executables from the same code base
Acknowledgements

- Dr. Madhava Syamlal (NETL-DOE)
- Dr. Chris Guenther (NETL-DOE)
- Philip Nicoletti (NETL-Parsons)
- Dr. Sreekanth Pannala (DOE-ORNL)
- Dr. Sofiane Benyahia (NETL-Fluent, Inc.)
- Dr. Aytekin Gel (Aeolus Research, Inc.)

- Prof. Sankar Sundaresan (Princeton U.)
- Prof. Rodney Fox (Iowa State U.)

- Dr. Bill Rogers (DOE-FE-NETL)