A Status Report on Multiphase CFD for Gas-Particles Systems

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OF THE
CHEMICAL REACTION ENGINEERING LABORATORY (CREL)
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Washington University

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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**

www.netl.doe.gov
www.fe.doe.gov

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

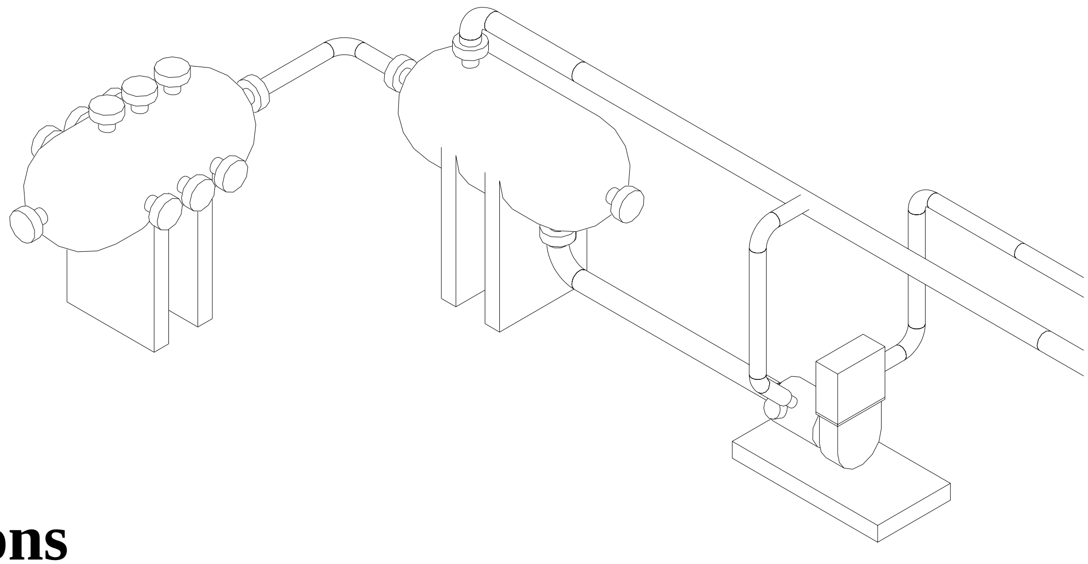
Loop diagrams

Structural

Report generation

Reduce rework

Standards/Specifications



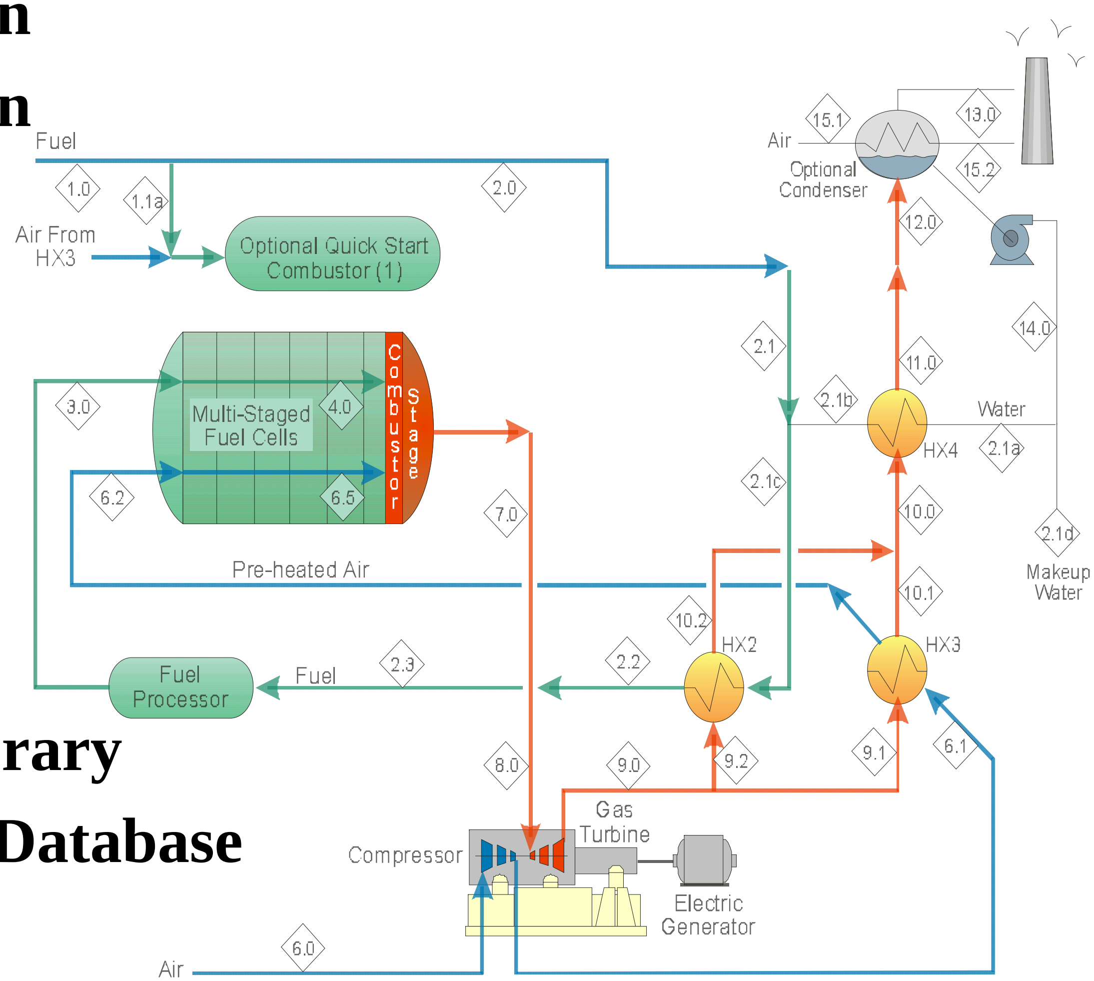
Process Simulation

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

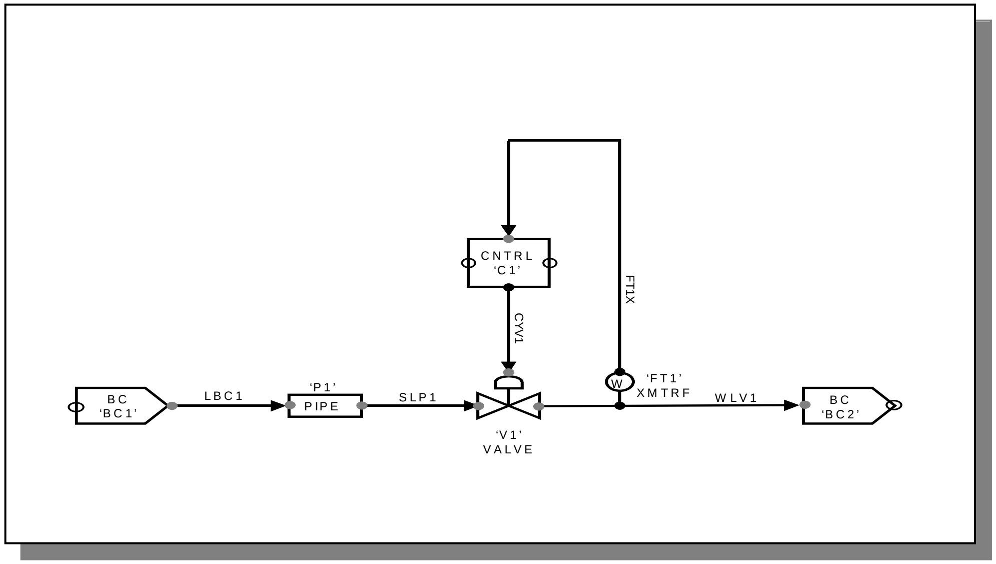
Start Up/Shut Down

Load Following

Transients Upsets

Safety

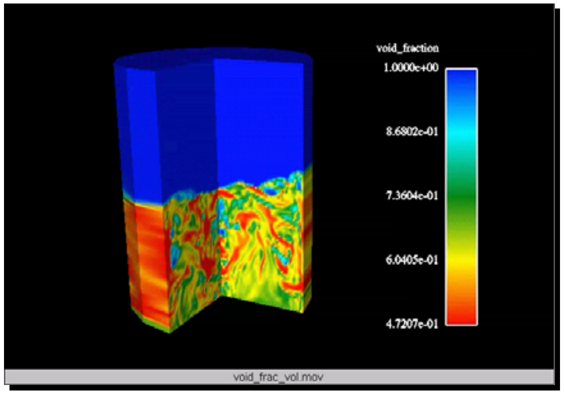
…



Mechanistic Modeling

CFD Simulations

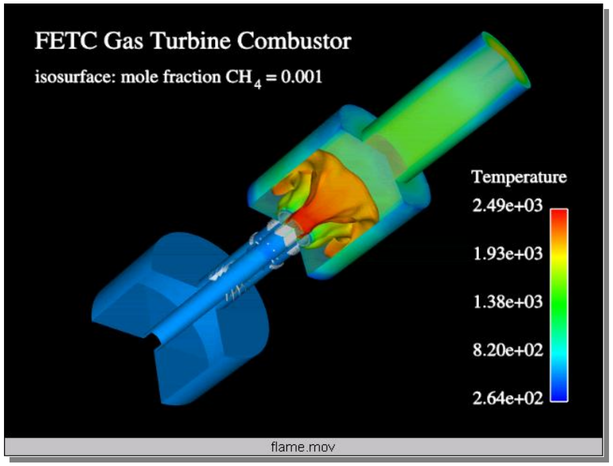
- single/multi-phase
- heat transfer
- chemical reactions



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)

Outline

- Hierarchy of CFD models
- ***Eulerian-Eulerian approach***
- Fundamental set of equations
- Constitutive Laws
- Examples

Local variables

Navier-Stokes eq. for fluid

Newton's Laws for particles

$$\left\{ \int_{V_f} \Downarrow g\, dy^3 \right\}$$

Mean variables

Navier-Stokes-like eqs.

for fluid and granular phases

Outline

- **Hierarchy of CFD models**
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- ***Fundamental set of equations***
- **Constitutive Laws**
- **Examples**

E-E Multiphase Model Equations

Continuity Equations

Chemical Rates

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

Momentum Equations

$$\frac{\partial}{\partial t}(\varepsilon_m \rho_m \vec{v}_m) + \nabla \cdot (\varepsilon_m \rho_m \vec{v}_m \vec{v}_m) = \nabla \cdot \overline{\overline{S}}_m$$

Stresses

$$+\sum_{l=1}^{M} \vec{I}_{ml}$$

Interaction Term

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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

$$\frac{\partial}{\partial t}(\varepsilon_m \rho_m h_m) + \nabla \cdot (\varepsilon_m \rho_m h_m \vec{u}_m) = \varepsilon_m \left(\frac{\partial p_m}{\partial t} + \vec{u}_m \cdot \nabla p_m \right) + \overline{\overline{S}} : \nabla \vec{u}_m + S_m$$

$$- \nabla \cdot \vec{q}_m + \sum_{l=1}^{M} \left(\gamma_{ml} (T_l - T_m) + R_{ml} h_{ml} \right)$$

Outline

- **Hierarchy of CFD models**
- **Eulerian-Eulerian approach**
- **Fundamental set of equations**
- *Constitutive Laws:*

closure – dependence on mean variables

- **Examples**

Constitutive Laws: Phase Interaction

- **Bouyancy**
- **Drag**
- **Lift**
- **…**

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

F_{ml} is:

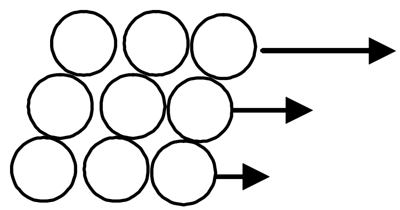
1) empirical

2) function of: velocity, voidage, …

Constitutive Laws: Granular Stresses

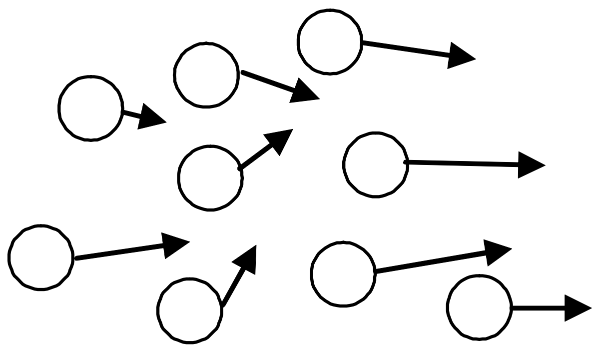
Plastic flow

- 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

$$\overline{\overline{S}}_{sm} = \begin{cases} -P_{sm}^{p}\,\overline{\overline{I}} + \overline{\overline{\tau}}_{sm}^{\,p} & \text{if } \varepsilon_g \le \varepsilon_g^{*} \\ -P_{sm}^{v}\,\overline{\overline{I}} + \overline{\overline{\tau}}_{sm}^{\,v} & \text{if } \varepsilon_g > \varepsilon_g^{*} \end{cases}$$

Plastic Regime
(Schaeffer – 1987)

Viscous Regime
(Lun et al. – 1984)

Multiphase Model - Granular Stress
Viscous Regime

Granular Pressure

Granular Temperature

$$P_{sm}^{v} = K_{1m}\,\varepsilon_{sm}^{2}\,\Theta_{m}$$

$$K_{1m} = 2\left(1 + e_{mm}\right)\rho_{sm}\,g_{0_{mm}}$$

Shear Stress

$$\overline{\overline{\tau}}_{sm}^{v} = 2\,\mu_{sm}^{v}\,\overline{\overline{D}}_{sm} + \lambda_{sm}^{v}\,\mathrm{tr}\left(\overline{\overline{D}}_{sm}\right)\overline{\overline{I}}$$

$$\lambda_{sm}^{v} = K_{2m}\,\varepsilon_{sm}\sqrt{\Theta_{m}}$$

$$K_{2m} = \frac{4\,d_{pm}\,\rho_{sm}\left(1 + e_{mm}\right)\varepsilon_{sm}\,g_{0_{mm}}}{3\sqrt{\pi}} - \frac{2}{3}K_{3m}$$

Multiphase Model - Granular Stress
Plastic Regime

$$P_{sm}^{p} = \varepsilon_{sm} P^{*}$$

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

Pressure

$$\overline{\overline{\tau}}_{s1}^{\,p} = 2\,\mu_{s1}^{p}\,\overline{\overline{D}}_{s1}$$

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

Shear Stress

$$I_{2D} = \frac{1}{6}\left[(D_{s11} - D_{s22})^{2} + (D_{s22} - D_{s33})^{2} + (D_{s33} - D_{s11})^{2}\right] + D_{s12}^{2} + D_{s23}^{2} + D_{s31}^{2}$$

Second Invariant of the Deviator of the Strain Rate Tensor

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- ***Examples***

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, O_3, SiH_4, SiHCl3, CH_4,$TiCl_4$, $-CH_2-$

MFDRC - NETL MFIX Code

- MFIX - Multiphase Granular Flow Code

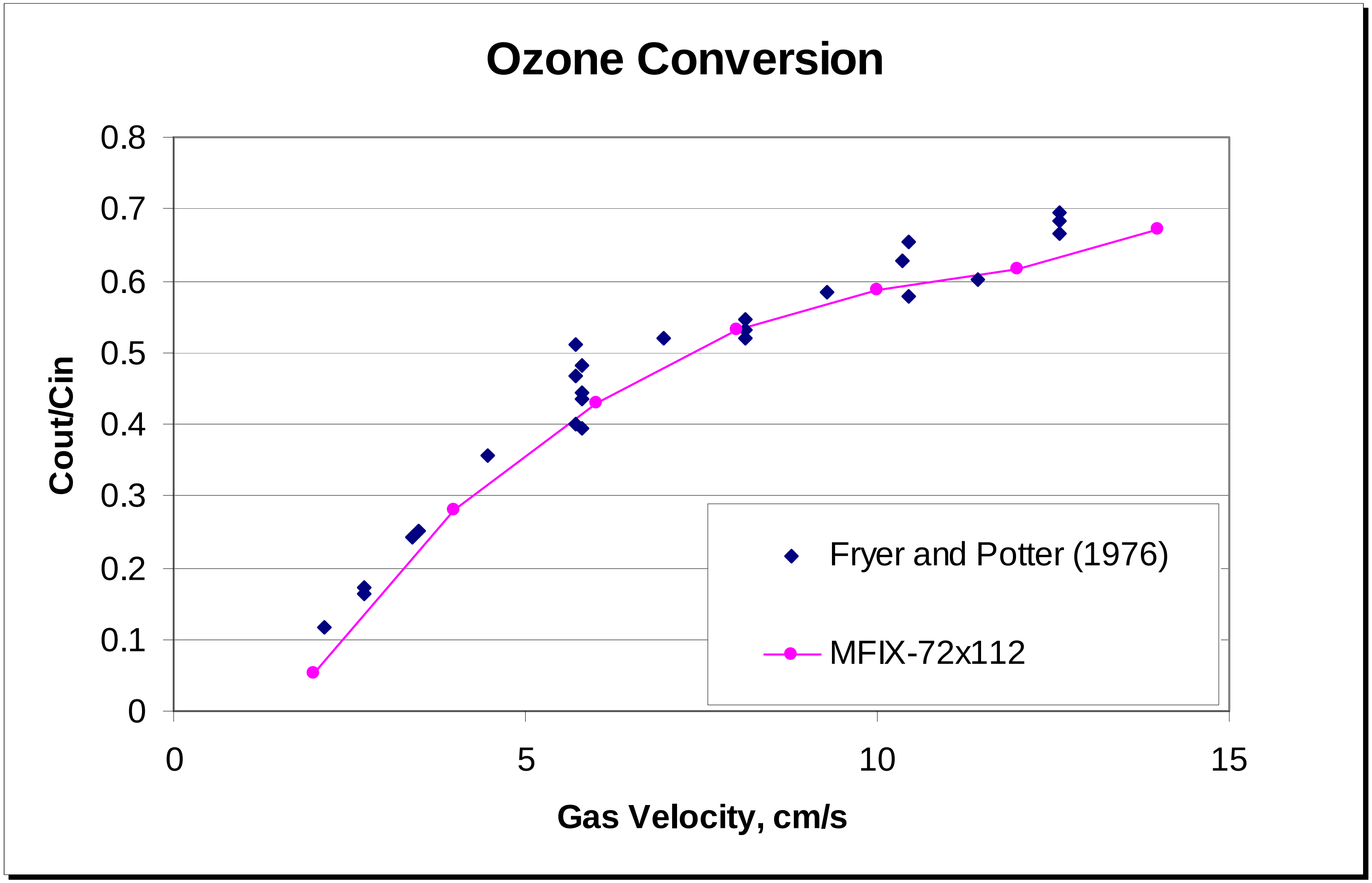
MFIX Application - Ozone Decomposition

- Fryer and Potter (1976)
- 117 mm, 2650 kg/m^3 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

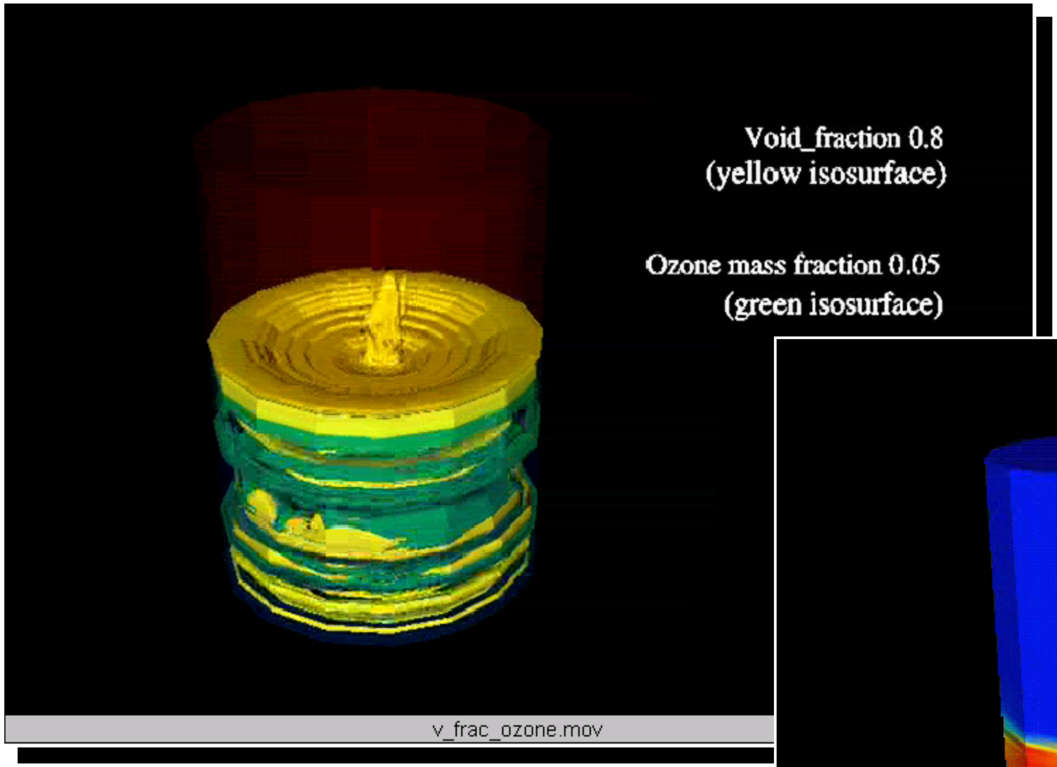
$$O_3 \rightarrow 1.5\ O_2$$

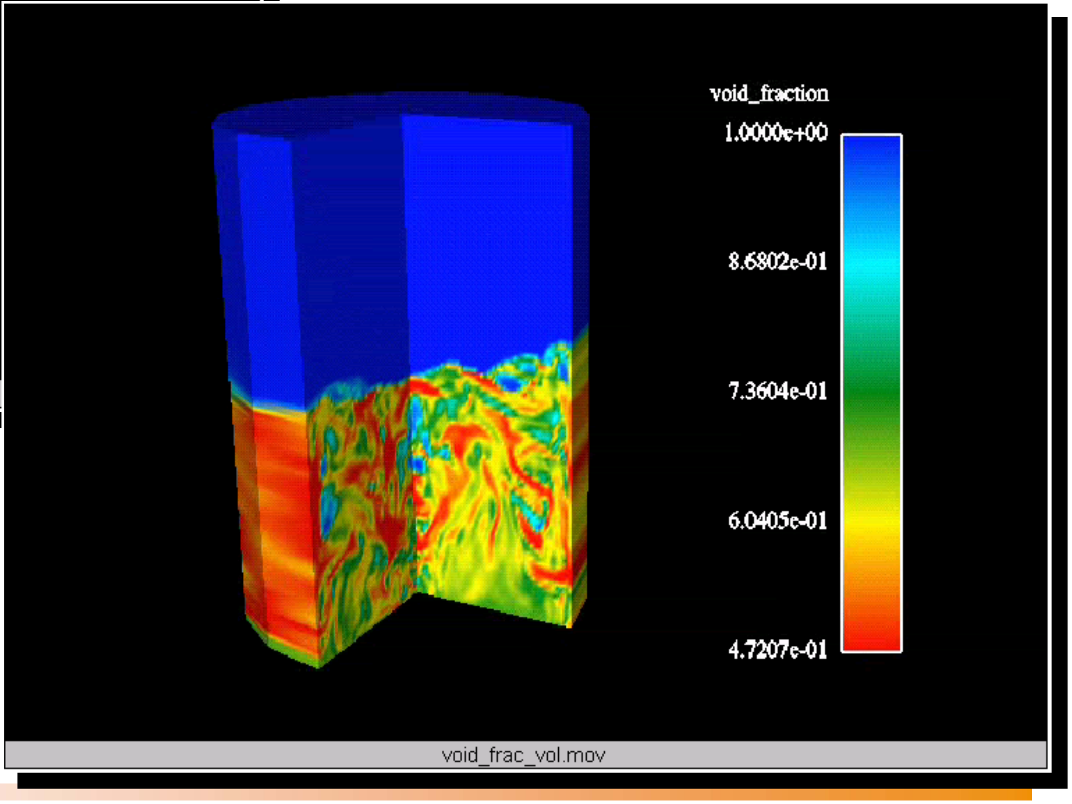
- Catalyzed by sand impregnated with iron oxide

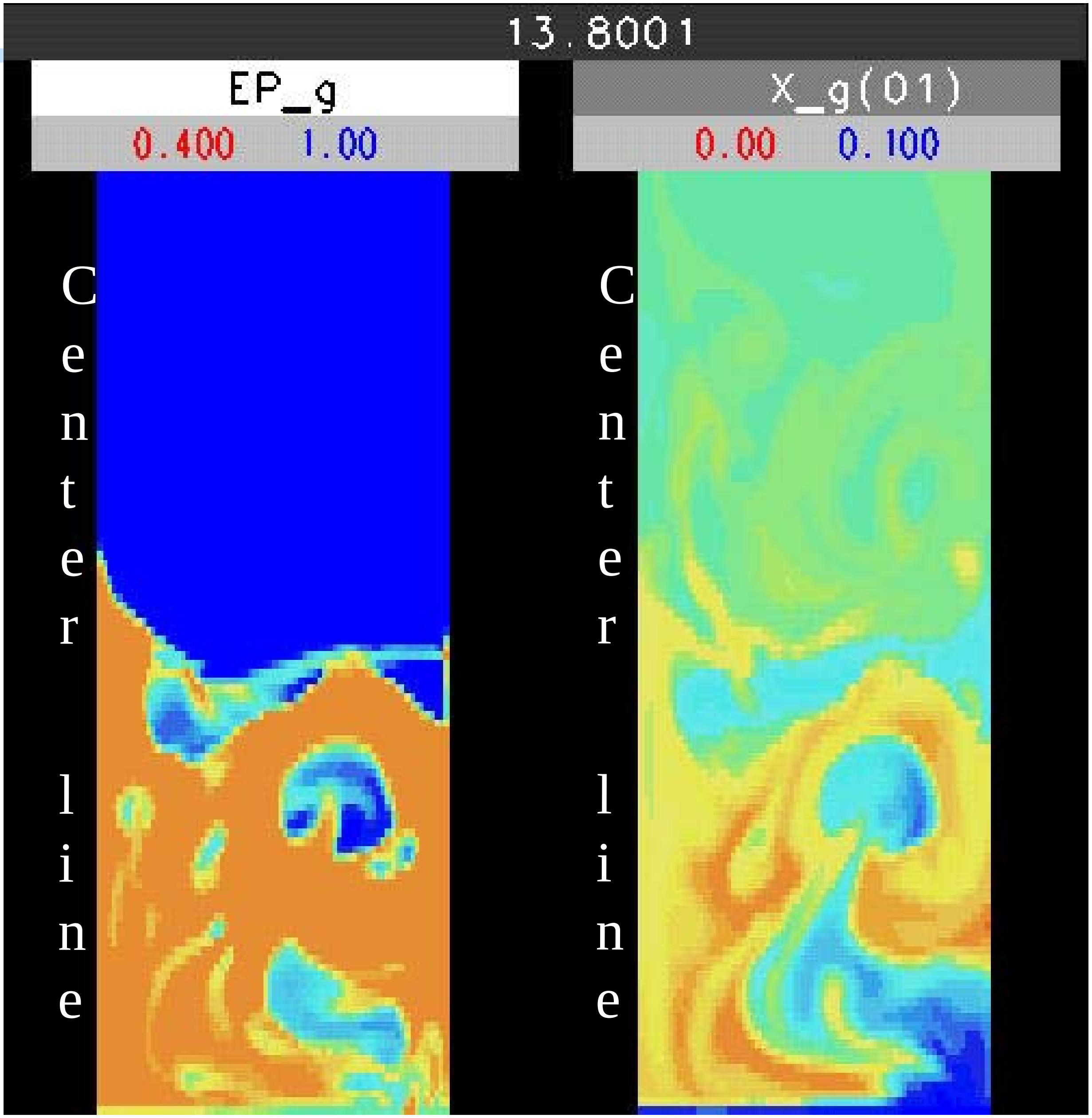
MFIX Code - Ozone Decomposition



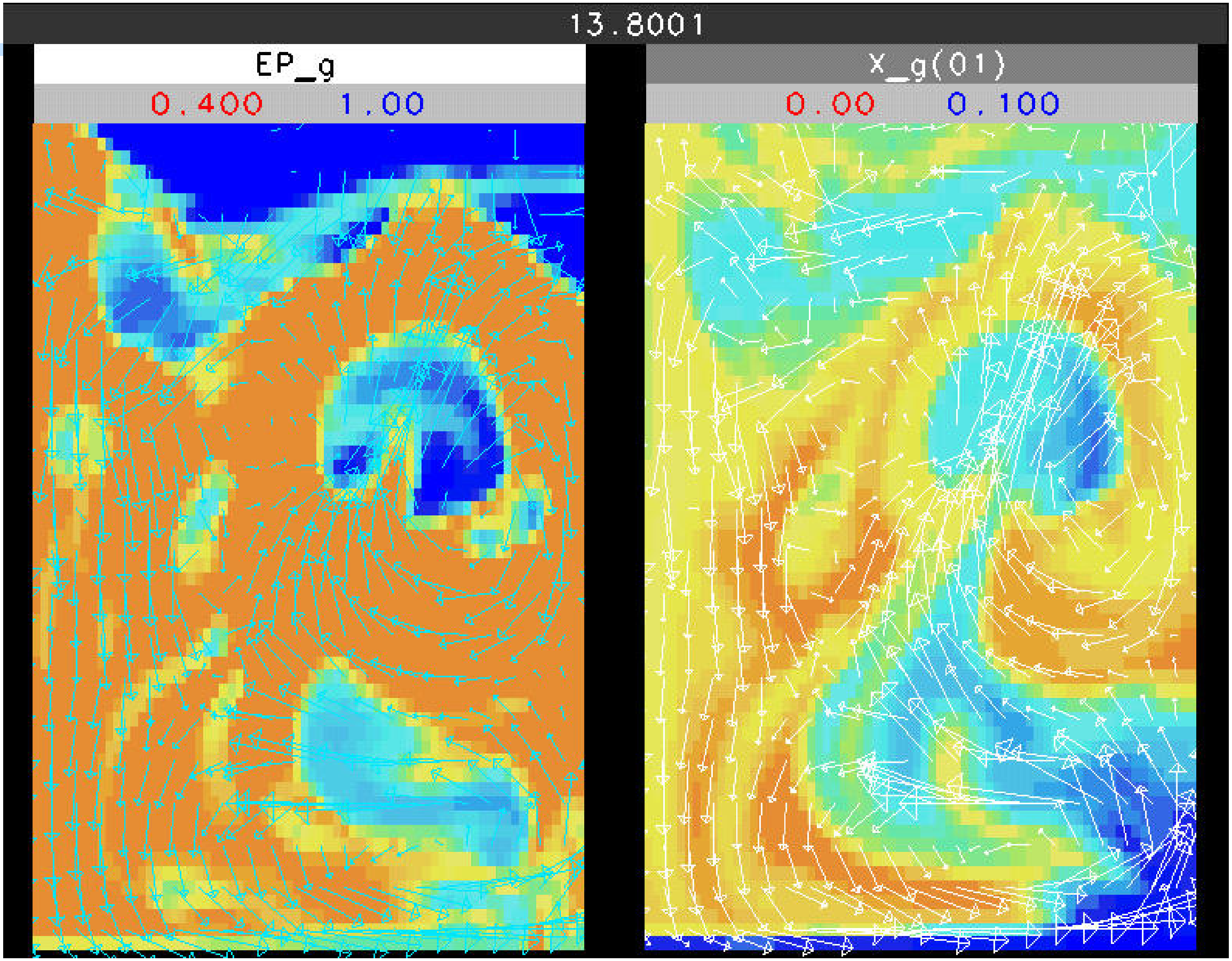
MFIX Code - Ozone Decomposition

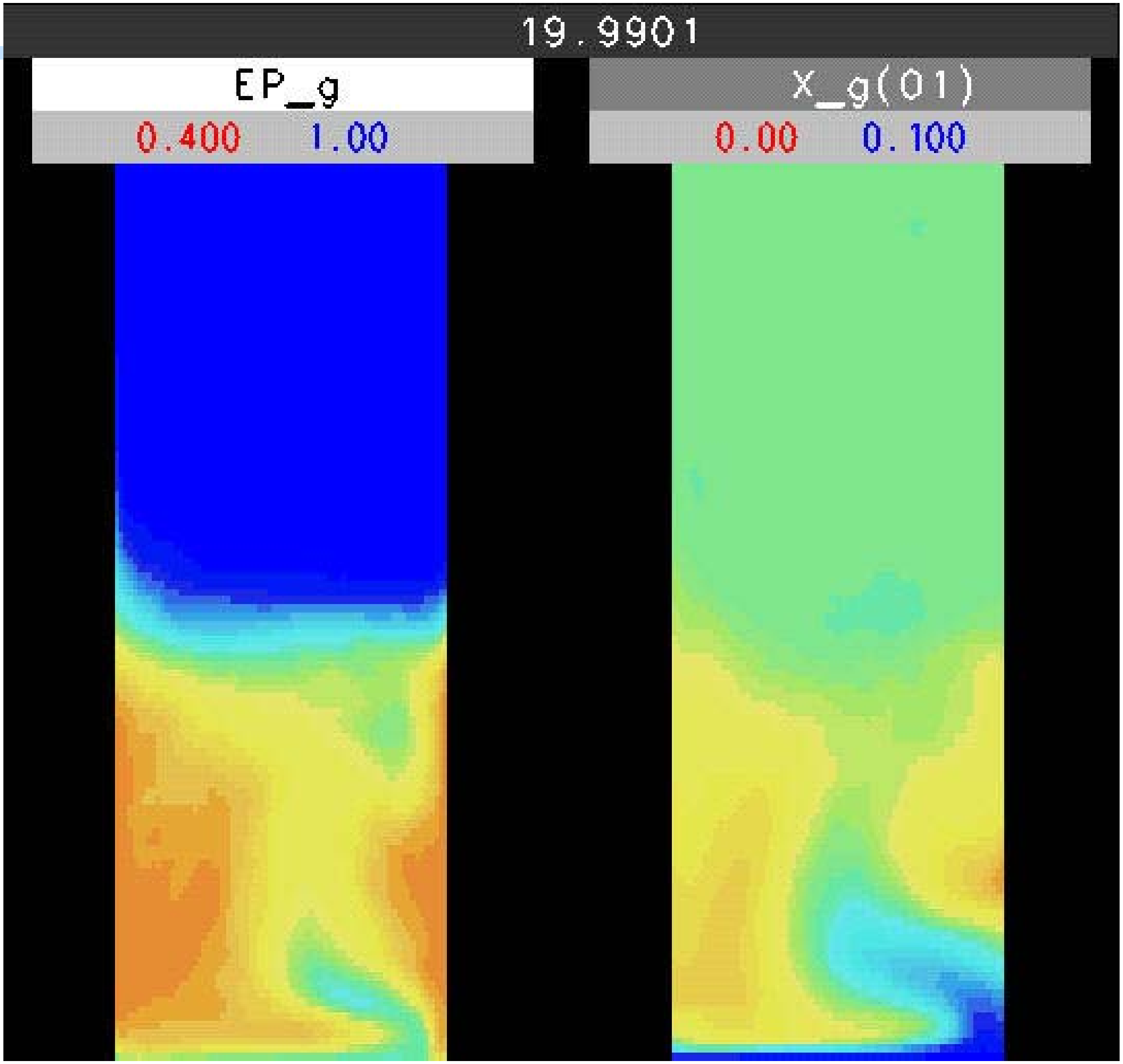






U = 8 cm/s; Hmf = 11.5 cm


13.8001
EP_g
0.400 1.00
X_g(01)
0.00 0.100


19.9901
EP_g
0.400 1.00
X_g(01)
0.00 0.100

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

Chem. Eng. Sci., *50*, 3615-3624, 1995

- Part II: Theoretical Analysis and Modeling"

Chem. Eng. Sci., *50*, 3625-3635, 1995

Hydrogenation of $SiCl_4$

"Investigation of the Hydrochlorination of $SiCl_4$"
Final Report JPL Contract No. 9506061, 1981-1983
J. Y. P. Mui, Solarelectronics, Inc.

Process for the hydrochlorination of $SiCl_4$ with H_2 to form $SiHCl_3$ in a fluidized bed of Si (m.g.)

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

$$3\,SiCl_4 + 2\,H_2 + Si \Leftrightarrow 4\,SiHCl_3$$

Hydrogenation of SiCl4

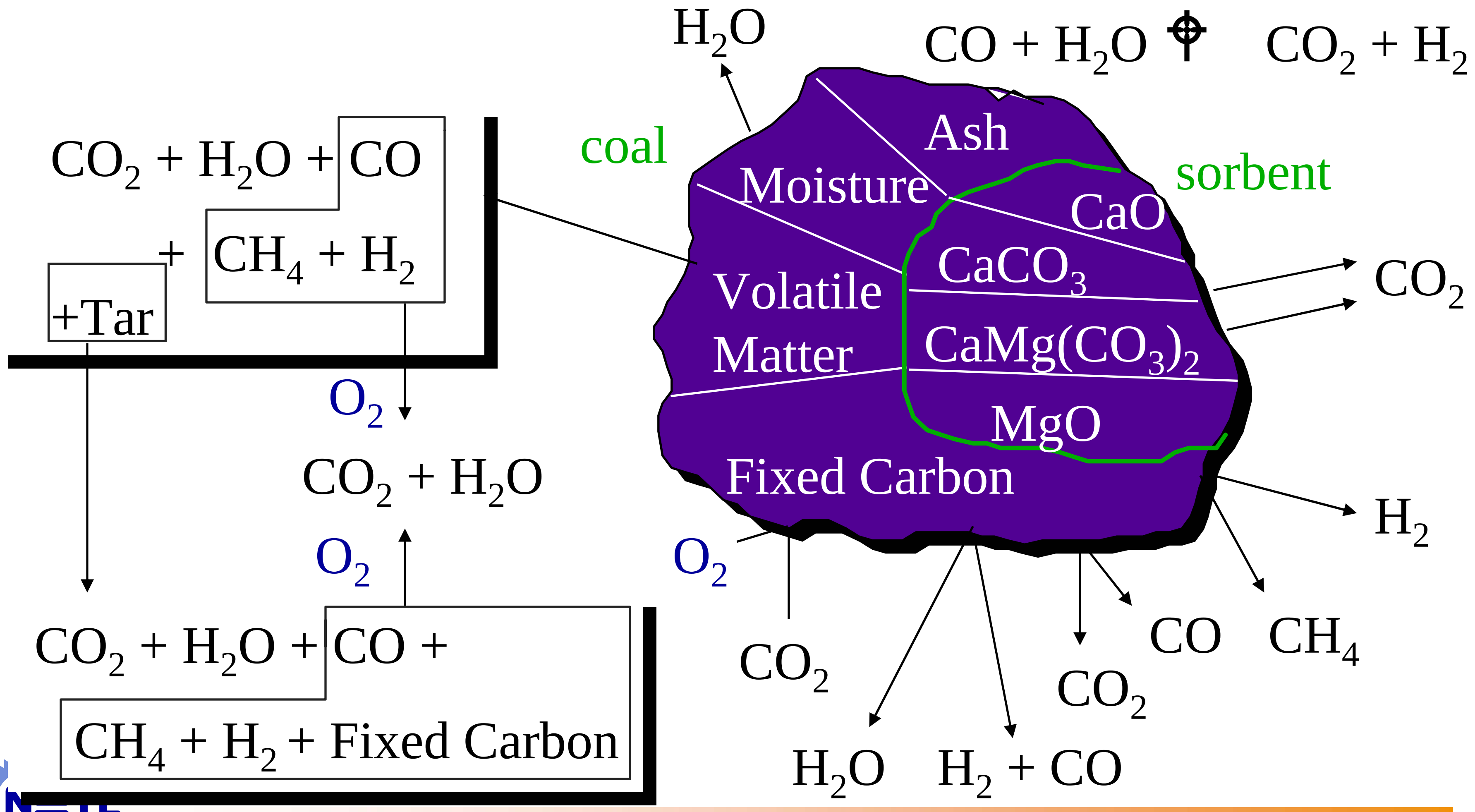
$$"3\,SiCl_4 + 2\,H_2 + Si \Leftrightarrow 4\,SiHCl_3"$$

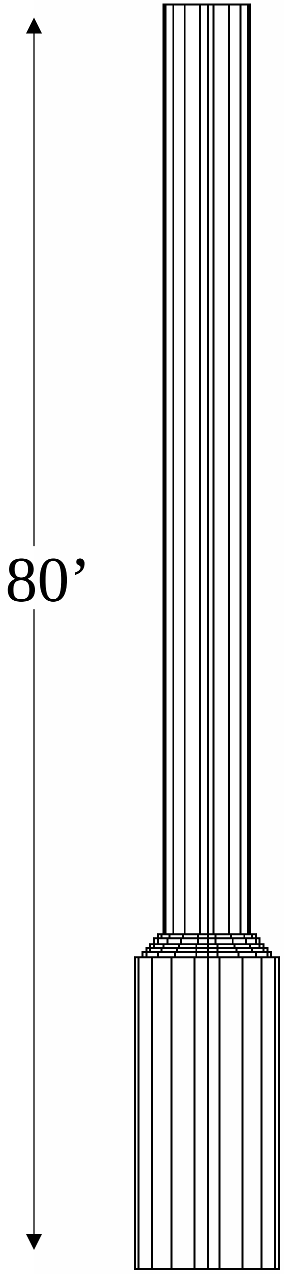
$$SiCl_4 \xrightarrow{Cu\text{-}Si} SiCl_2$$

$$\left[SiCl_2 \rightarrow \left\{ \begin{array}{l} \xrightarrow{H_2} SiH_2Cl_2 \\ \rightarrow \end{array} \right\} \right] \xrightarrow{HCl} SiHCl_3$$

$$-Si-Cu-Cl- \xrightarrow{H_2} -Si-Cu- + HCl$$

Coal Gasification: Carbonizer Chemistry



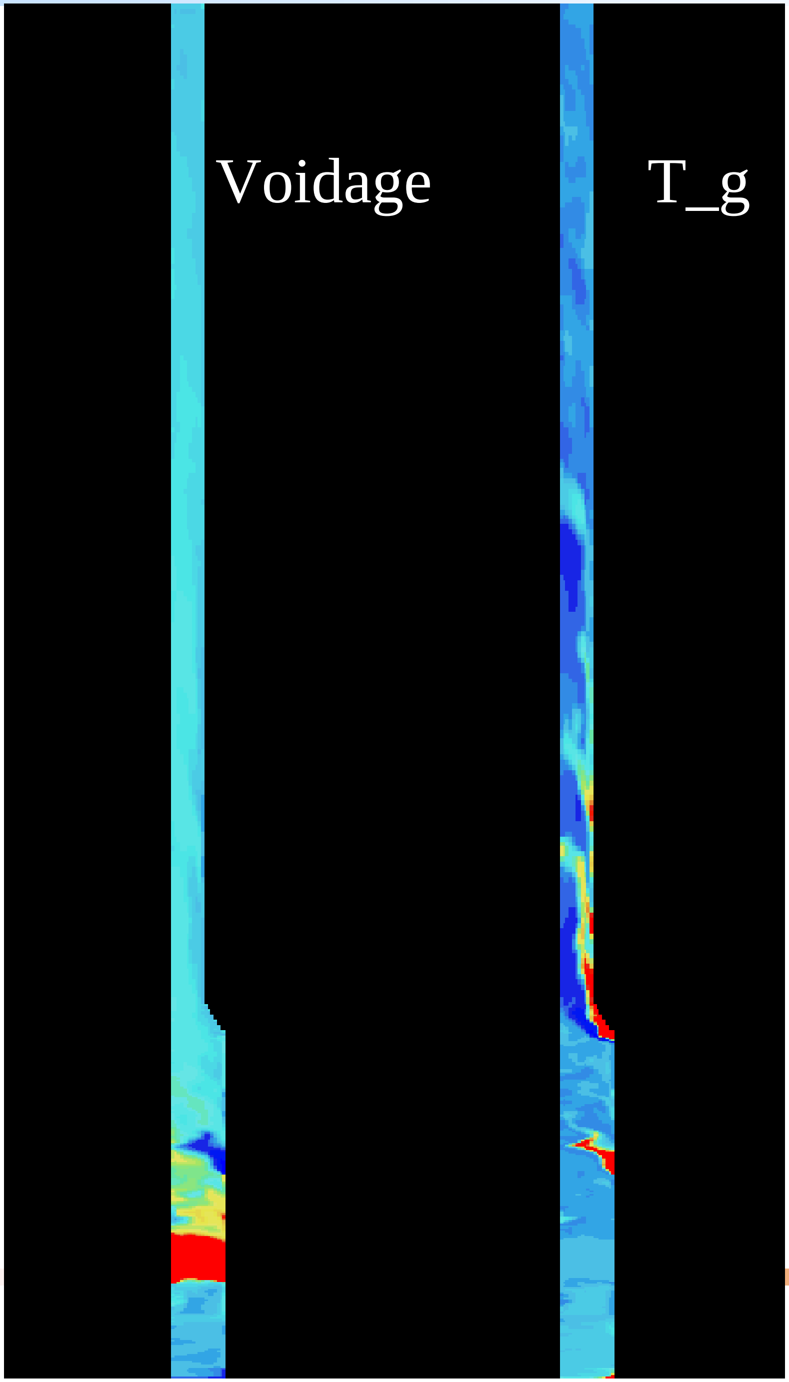


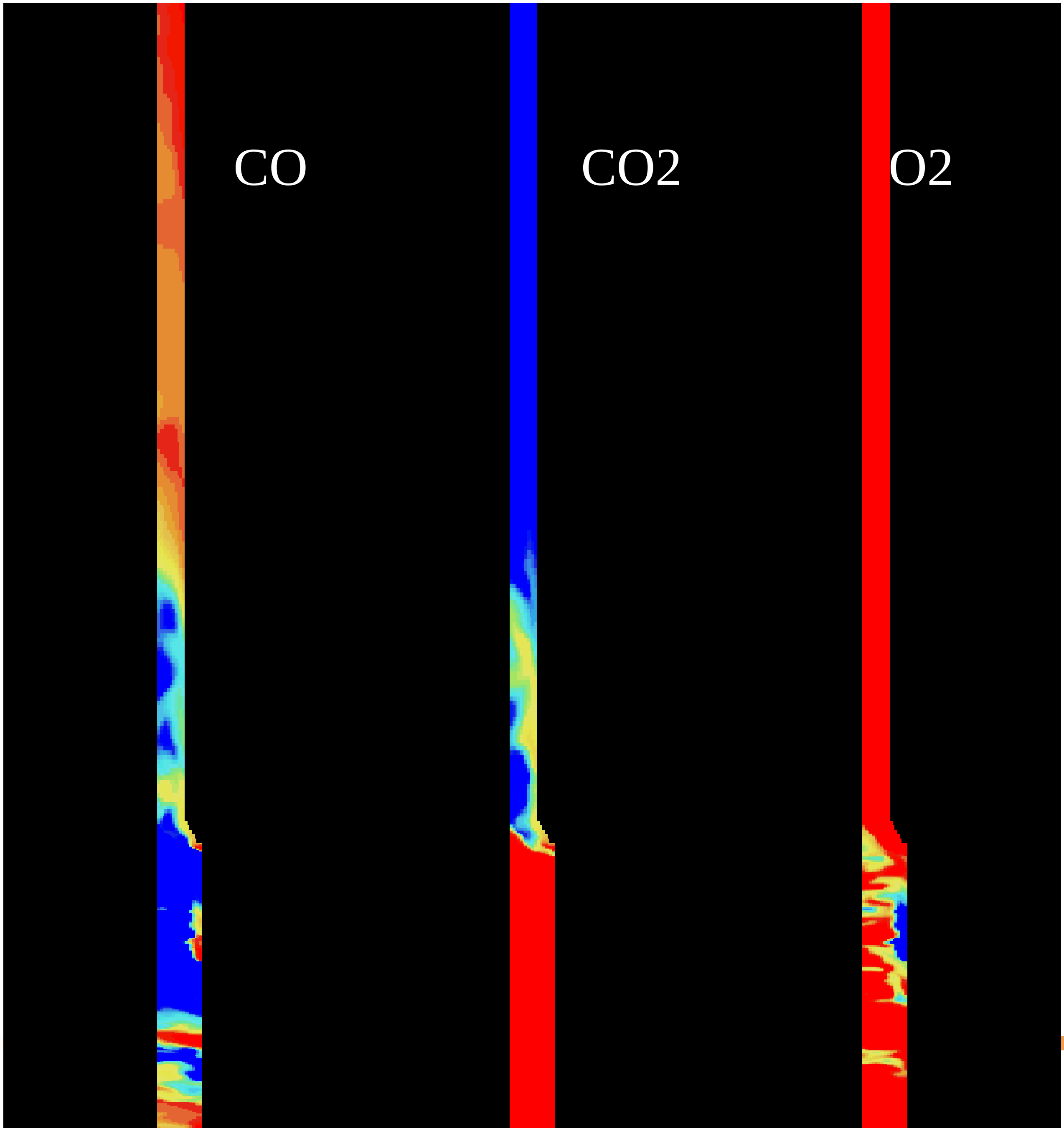
Power Systems Development Facility Kellogg, Brown & Root Transport Reactor

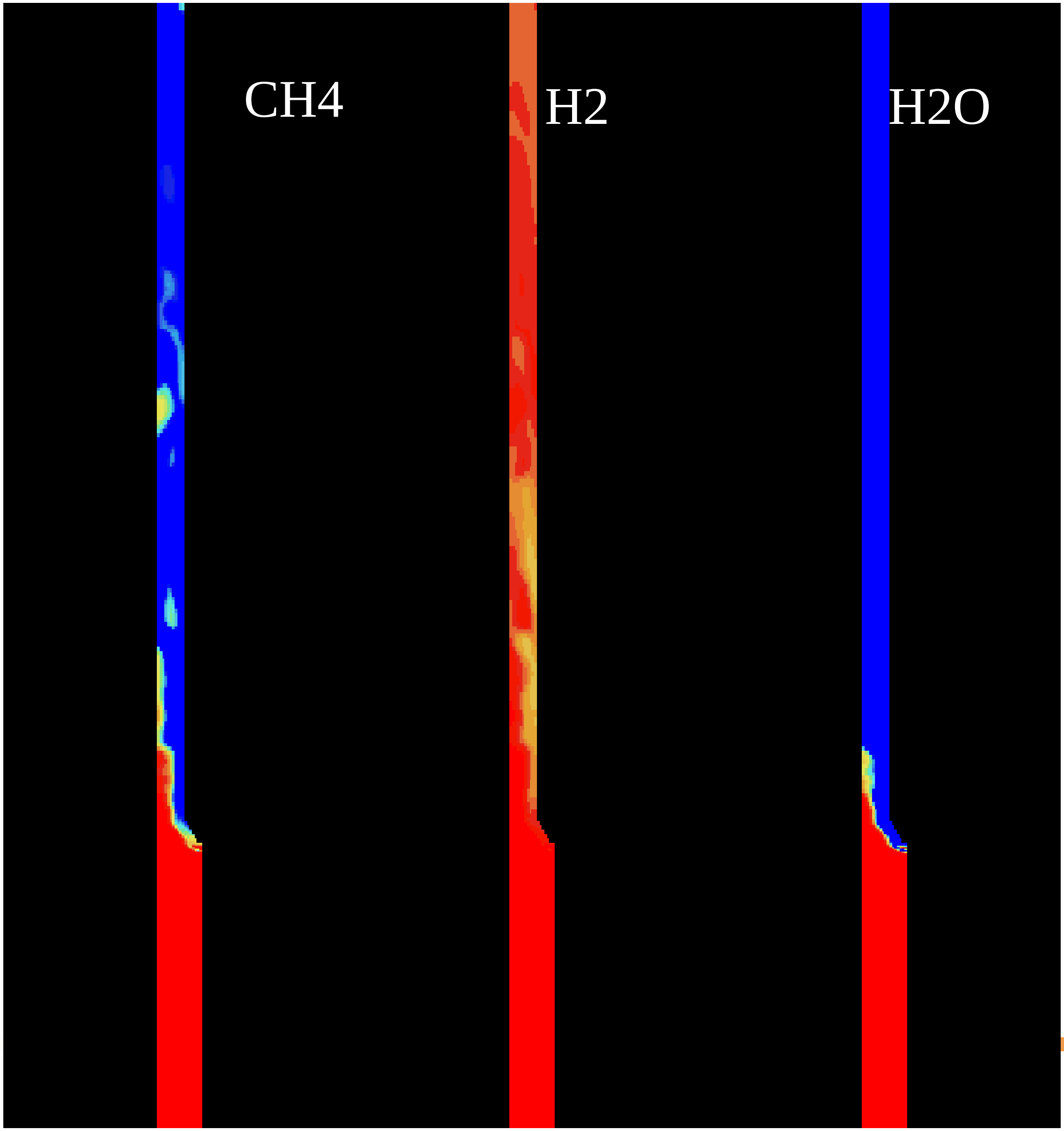
- Transient, 3-D cylindrical coordinated
  >250K computational cells

- 8 gas species: O_2, CO, CO_2, CH_4, H_2, H_2O,
  N_2, Tar
  4 solid species: Ash, Volatile Matter,
  Moisture, Fixed Carbon

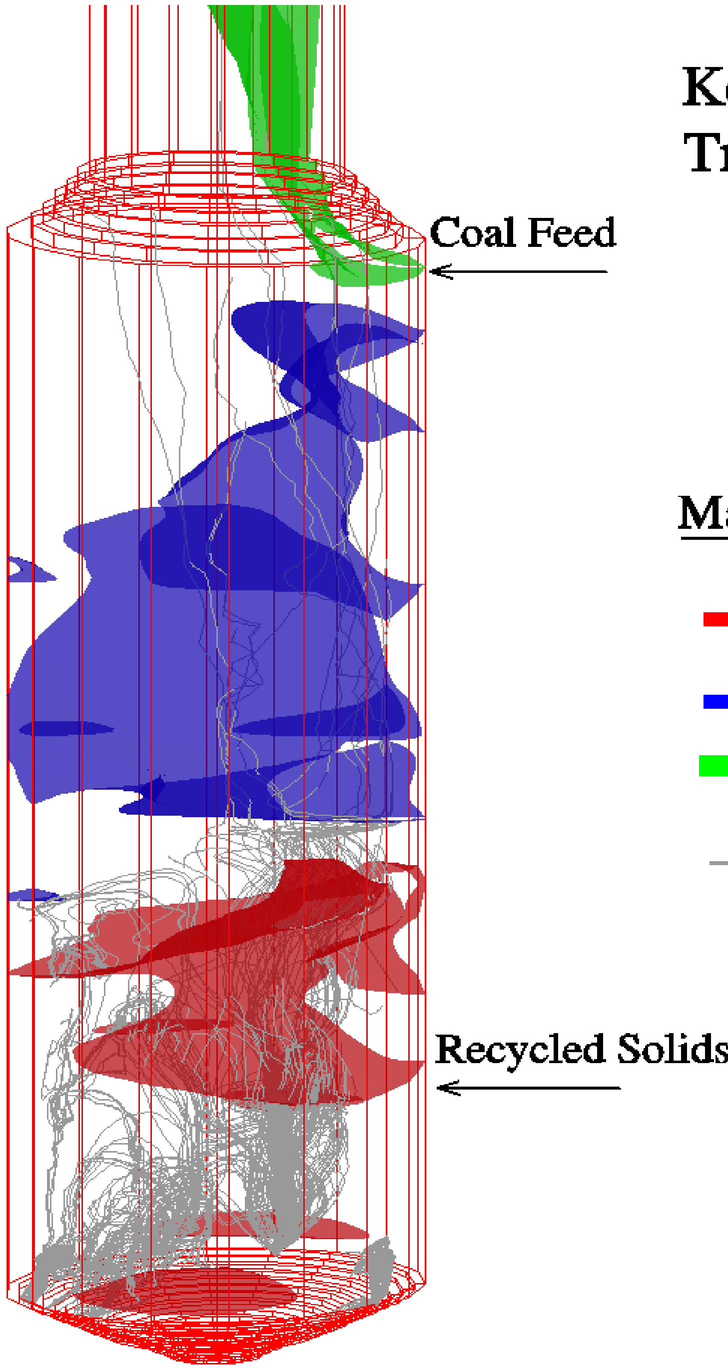
- Parallel runs at Pittsburgh Super Computing Center (PSC)
  < week CPU time ~ 10 seconds of simulation


Voidage
T_g


CO
CO2
O2


CH4
H2
H2O

Kellogg Brown and Root, Inc.
Transport Gasifier



Mass Fractions of Gas and Solids

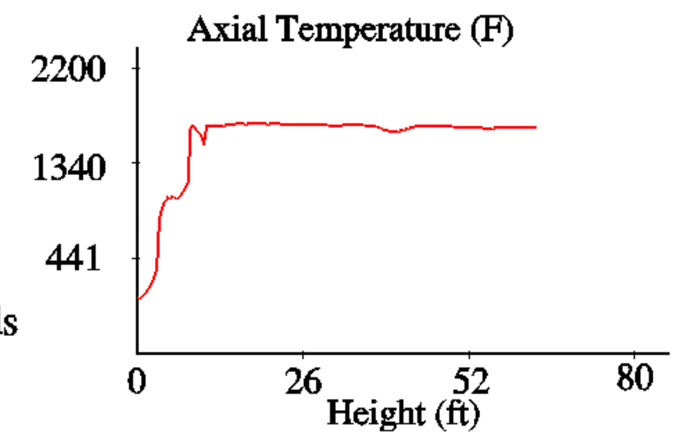
- Oxygen (20%)
- Oxygen (2%)
- Coal (1-2%)
- Solid Pathlines

Kellogg Brown and Root, Inc. Transport Gasifier

Isosurface Void Fraction

Gas Temperature (F)

- 1675 (red)
- 1241 (green)
- 808 (blue)



Simulations using PC Coal Lab# to determine yields and composition of volatile matter

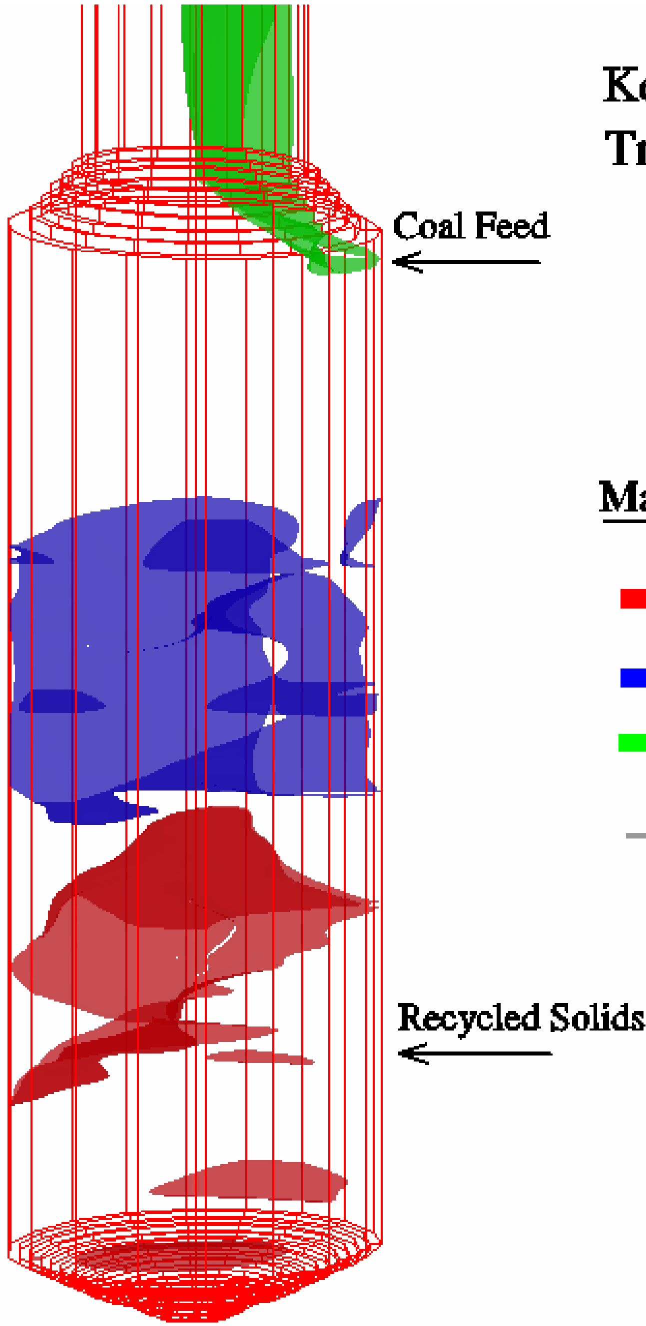
Powder River Basin Coal

- air and oxygen blown
- with/without lower mixing zone

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

#Niksa Energy Associates

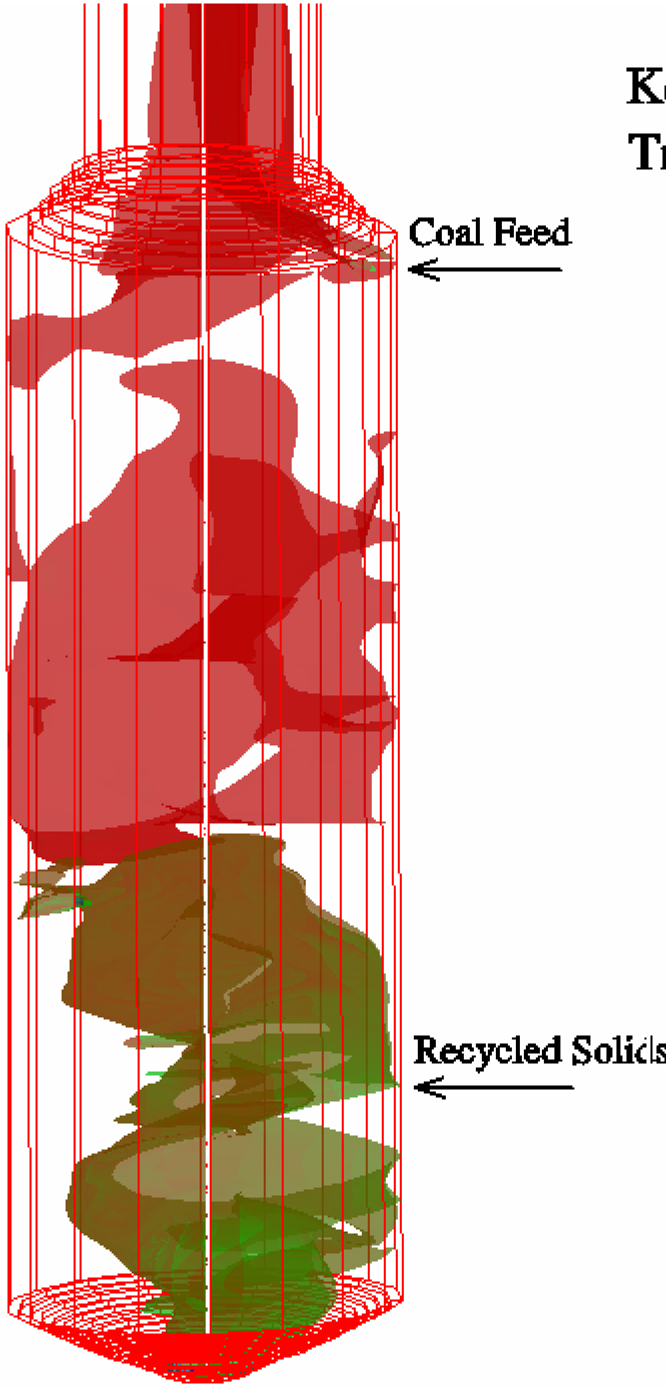
Kellogg Brown and Root, Inc.
Transport Gasifier

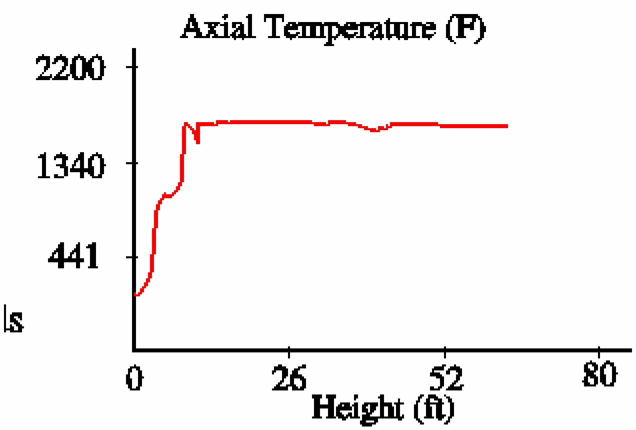


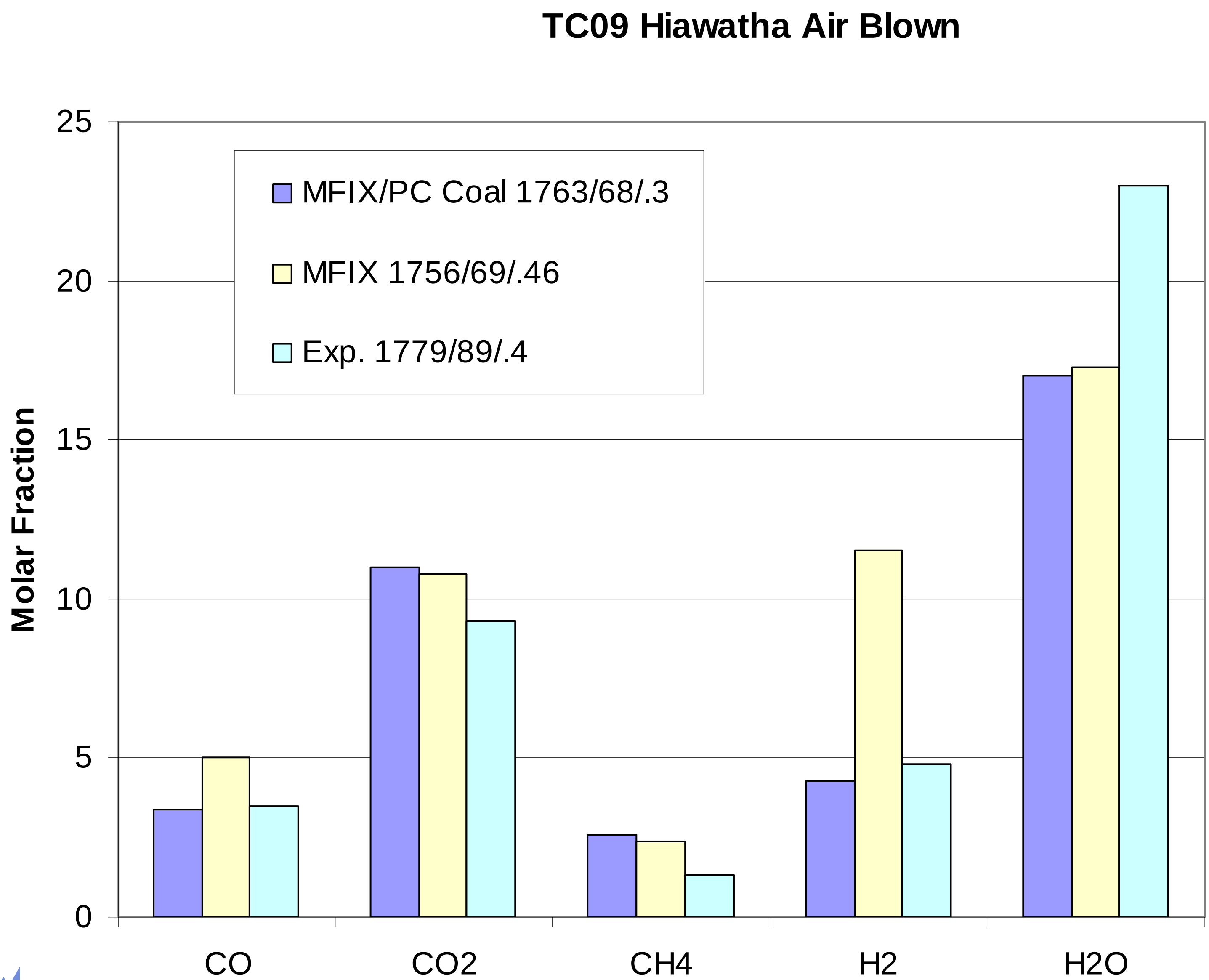
Mass Fractions of Gas and Solids

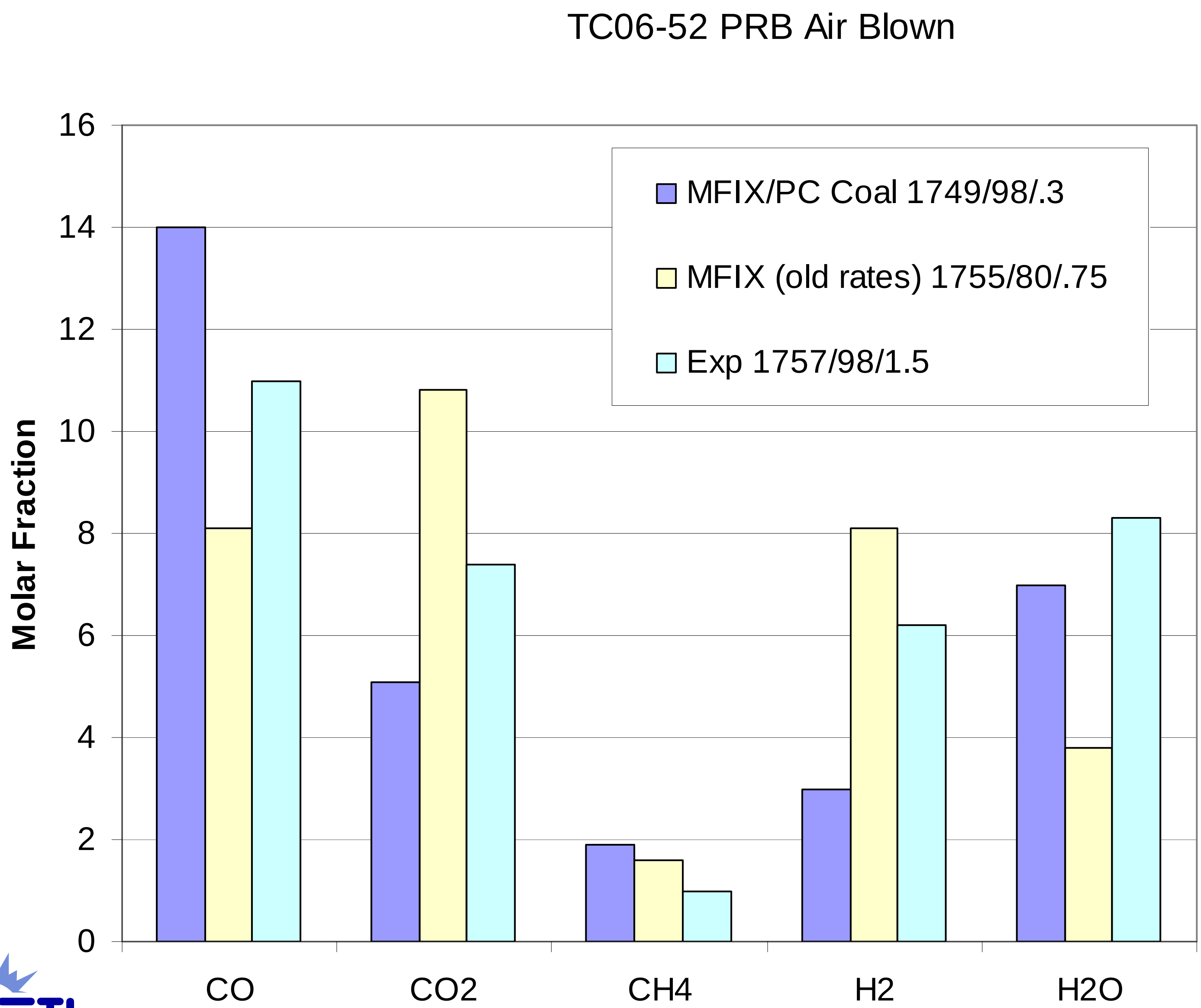
- Oxygen (20%)
- Oxygen (2%)
- Fixed Carbon (2%)
- Solid Pathlines

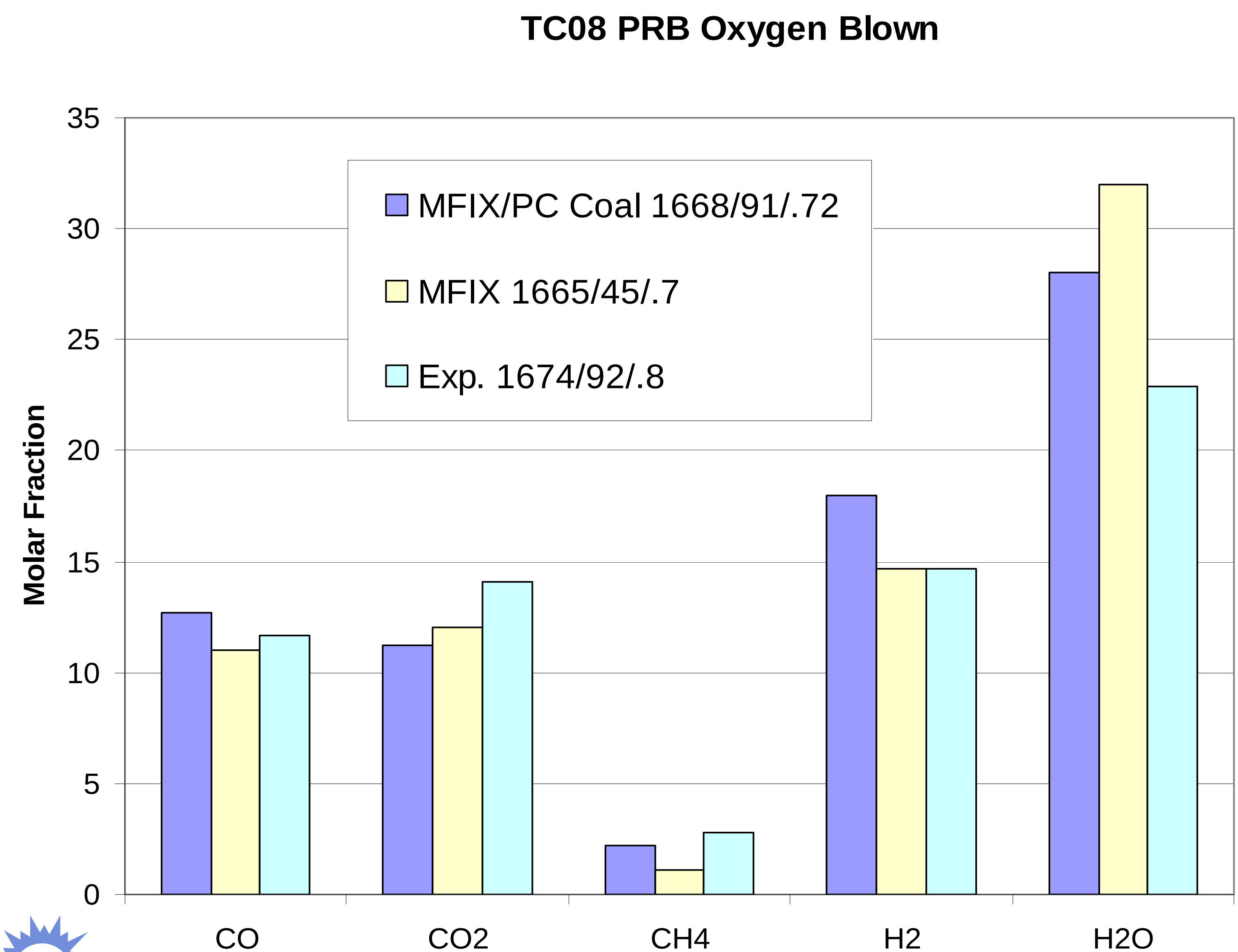
Kellogg Brown and Root, Inc.
Transport Gasifier



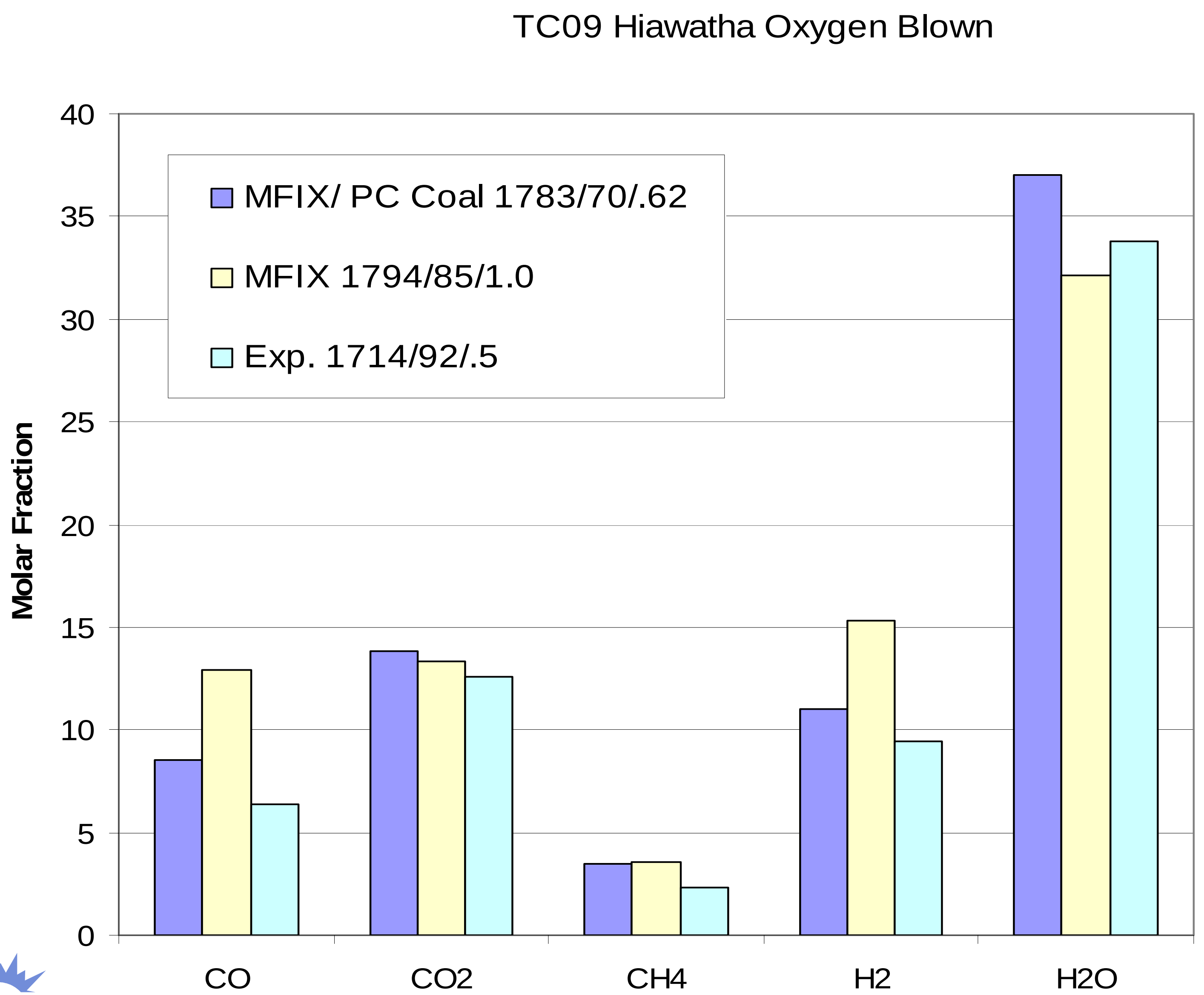



TC09 Hiawatha Air Blown
Molar Fraction
0
5
10
15
20
25
MFIX/PC Coal 1763/68/.3
MFIX 1756/69/.46
Exp. 1779/89/.4
CO
CO2
CH4
H2
H2O


TC06-52 PRB Air Blown
Molar Fraction
0
2
4
6
8
10
12
14
16
CO
CO2
CH4
H2
H2O
MFIX/PC Coal 1749/98/.3
MFIX (old rates) 1755/80/.75
Exp 1757/98/1.5



TC08 PRB Oxygen Blown
Molar Fraction
35
30
25
20
15
10
5
0
MFIX/PC Coal 1668/91/.72
MFIX 1665/45/.7
Exp. 1674/92/.8
CO
CO2
CH4
H2
H2O



TC09 Hiawatha Oxygen Blown
Molar Fraction
0
5
10
15
20
25
30
35
40
MFIX/ PC Coal 1783/70/.62
MFIX 1794/85/1.0
Exp. 1714/92/.5
CO
CO2
CH4
H2
H2O

MFIX Code: General Description www.mfix.org

(**M**ultiphase **F**low with **I**nterphase e**X**changes)

- 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

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- Prof. Rodney Fox (Iowa State U.)

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