Introduction to CFD Modeling of Fluidized Beds

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presented at

Coal Gasification Short Course

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Much thanks to Drs. Madhava Syamlal, Thomas O'Brien, David Miller, and Chris Guenther (NETL); Dr. John Turner (ORNL)

Objective

The objective of reactor design is to create the right conditions for reactions. The temperature and reactant species distribution, appropriate residence time and removal of products must be considered. Including the effect of a catalyst may be necessary. A comprehensive understanding of all the competing and interacting mechanisms is required to arrive at better designs and improved processes. In particular, gas-solids reacting flows involve, not only complex interactions of granular materials with gas flow, but also phase-change, heterogeneous and homogeneous reactions, heat and mass transfer. Moreover, the spatial and temporal scales may vary over many orders of magnitude. Thus modeling gas-solid reacting flows requires the integration of the best physics and chemistry models from various science and engineering fields with the most advanced computational algorithms. These algorithms must be scalable to large high-performance computers in order to bear on this important topic.

Except from preface of an *Edited Book on "Computational Gas-Solids Flows and Reacting Systems: Theory, Methods and Practice," May, 2010, Eds.* S. Pannala, M. Syamlal and T. O'Brien,

Your instructor

Dr. Sreekanth Pannala, Ph.D.

- **Senior research staff member at ORNL**
- **Over 15 years of experience in modeling reacting multiphase flows**
- **Active MFIX (http://mfix.netl.doe.gov) developer**
- **Interested in solving complex energy problems using high performance computing, predictive multiscale/multiphysics models**

NETL

OAK RIDGE National Laboratory

Collaborators

Oak Ridge National Laboratory

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Zhaoseng Gao

Multiscale/Multiphysics Modeling for Clean Energy (M3E)
http://www.linkedin.com/groups?gid=1849998

Course Goals

- Basics of reacting multiphase flows
  - Give a broader context in terms of solving energy problems
- Numerical methods
- Code walk through
- Setup cases and carry out simulations with different levels of difficulty
- I will be happy if you can take a paper/design and setup a case in MFIX
- Provide foundation for further learning
  - Learn how to find additional information
  - Learn about advanced capabilities
  - Welcome to contact me @ anytime for further pointers

Outline

- **Day 1**
  - Install Cygwin, MFIX, Paraview
  - Reacting multiphase flows
  - Volume averaged equations, closures, code walk through
- **Day 2**
  - Volume averaged equations, closures, code walk through (contd..)
  - Hands-on training: Hydrodynamics cases
- **Day 3**
  - Hands-on training: Study the effect of grid resolution, numerical schemes etc.
  - Hands-on training: Cartesian grid
- **Day 4**
  - Hands-on training: Add heat and mass transfer, chemical reactions
- **Day 5**
  - Hands-on training: Put all the things learned to a case with hydrodynamics, heat and mass transfer and chemical reactions
  - Close with future pointers

This is tentative and subject to change based on the feedback, pace, etc.,

Format

- Theory, approximations, numerical implementation, code compilation and installation, etc.
- Code-walk through
- Work through examples

I want to teach you how to fish rather than catch the fish for your

I want this course to have extensive discussions so that all of us can learn together

Cygwin

- **What Is Cygwin?**
  - **Cygwin is a Linux-like environment for Windows. It consists of two parts:**
  - **A DLL (cygwin1.dll) which acts as a Linux API emulation layer providing substantial Linux API functionality. A collection of tools which provide Linux look and feel.**
  - **The Cygwin DLL currently works with all recent, commercially released x86 32 bit and 64 bit versions of Windows**

Cygwin Installation

- Download Cygwin (setup.exe) from http://cygwin.org/. A nice summary is available at http://www.physionet.org/physiotools/cygwin/.
  - You can use google translator: http://translate.google.com/# if needed
  - http://translate.google.com/translate?js=y&prev=_t&hl=en&ie=UTF-8&layout=1&eotf=1&u=http%3A%2F%2Fwww.physionet.org%2Fphysiotools%2Fcygwin&sl=auto&tl=pt
- Once downloaded, click on setup.exe
- Choose a download site close to you
- Under devel tab, choose 'gcc4-fortran', 'make', 'gdb'
- Under docs tab, choose 'xpdf' – to view pdf files (optional)
- Under edit, choose 'nedit' or 'gedit' – nedit and gedit are simple editors like note pad but provide syntax coloring, etc. (optional)
- Under Graphics, choose 'gnuplot' and 'ImageMagick' (optional)
- Under X11 (see http://x.cygwin.com/docs/ug/setup-cygwin-x-installing.html), choose whatever is most appropriate for your needs – cygwin can be used as an x-terminal similar to exceed but it is also needed if you want to use nedit, etc. (optional) – xorg-server, xterm
- After you choose the above config options you can proceed with the installation. It might take an hour or so to download and install cygwin.

MFIX Installation

- Download mfix from https://mfix.netl.doe.gov/members/download_develop/mfix.tar.gz
- Place it in your home directory on cygwin. If you installed cygwin at c:\cygwin, the home directory would be c:\cygwin\home\your_user_name
- Open the cygwin terminal – click on the shortcut on the desktop
- If you want X support, just type in ‘startx’ and you should get a new terminal which supports X or using the links Cygwin-x under program menu. If you have any problems, try to follow the steps at: http://x.cygwin.com/docs/ug/setup-cygwin-x-installing.html
- To begin with you will be in your home directory. If you have mfix.tar.gz at that location, at the command prompt, type: tar xzvf mfix.tar.gz – this should create the directory mfix
- From now on you can follow the instructions in the Readme for Linux installations. Here is a quick summary:
  - cd mfix/tutorials/fluidBed1 (just picking this as an example)
  - sh ../../model/make_mfix
  - Choose the default settings for compilation options and for the compiler, chose gfortran (option 2)
  - After the compilation is successful, type ./mfix.exe and this should run the case
  - You could download visit (https://wci.llnl.gov/codes/visit/) or paraview (http://paraview.org/) for windows and use it to visualize the data generated directly

Email to mfix-help@mfix.netl.doe.gov or access this mailing list

Modeling and Simulation Terminology

- **Model**
  - **mathematical representation of physical phenomena**
- **Method**
  - **numerical algorithms (discretization, solution methods, etc.)**
- **Code**
  - **software implementation**
- **Simulation**
  - **use of code to perform analysis / design**
  - **requires tight integration with *experiments***
  - **must provide information on inherent *uncertainties***
- **Goal is deep understanding of phenomena**
  - **true predictive capability is by-product**
  - **successful prediction can be achieved with inadequate (or even incorrect) model(s)**

Goals of Predictive Modeling and Simulation

- **Increased safety**
  - improved understanding of underlying physical phenomena
    - geometric effects
    - coupled effects previously studied separately
  - more accurate analysis of both normal operation and accident scenarios
- **Reduced cost**
  - rapid screening and prototyping
    - exploration of materials and geometries
  - fewer, more targeted experiments
  - improved manufacturing processes
  - reduced margins
    - dramatically improved quantification of uncertainties
- **Improved decision-making**
  - risk mitigation, identification of issues/problems that could lead to failure

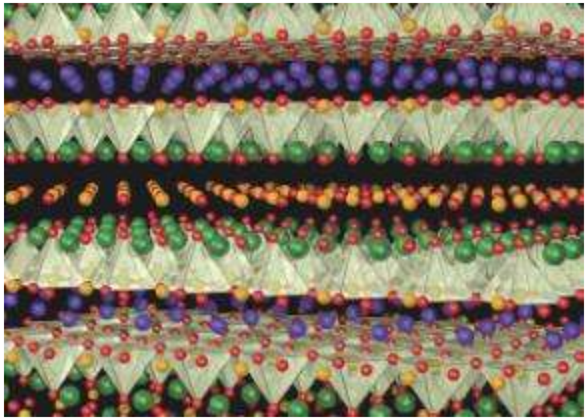
Advantages of open-source technology

- Access to the entire source code
  - more extensible
    - not limited to user defined modules
  - potentially more rapid contributions
    - Linux, Apache, Emacs, Firefox, Thunderbird are great examples
  - cost
    - can be an advantage for Universities, small companies
- Leverage investments from other DOE programs
  - robust and accurate numerical algorithms
  - more easily adapt to new architectures
- Develop new techniques to perform multiscale / multiphysics coupling seamlessly
  - not available in any commercial software
- Successful algorithms and models can be adopted by commercial companies

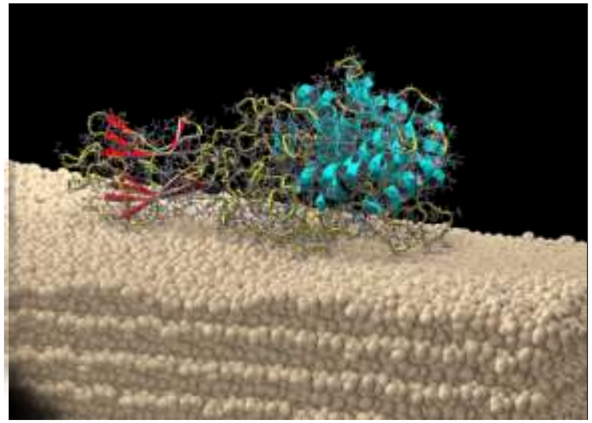
Outline of introduction

- Overview of computational science at Oak Ridge National Laboratory
- The need for clean energy
- Multiscale/multiphysics simulations for energy systems
  - Coal/biomass pyrolysis/gasification
  - Fluidized bed CVD coater for nuclear fuel particles
  - Batteries
- Current set of models used at various scales
- Example simulation results
  - Fluidized bed CVD coater for nuclear fuel particles
- Importance of multiphysics coupling
- Compound wavelet matrix method (CWM), dynamic CWM, time parallel CWM
- Opportunities/Challenges/Summary

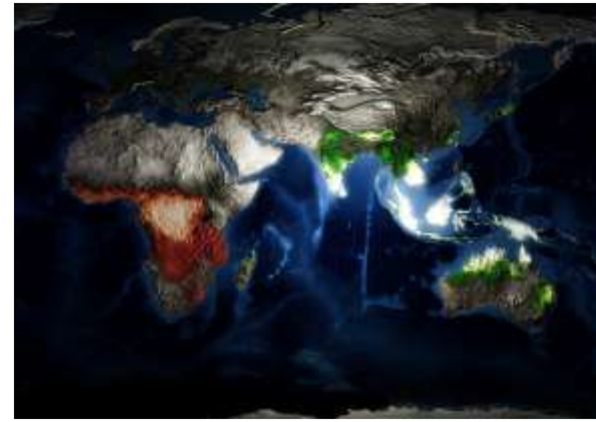
Advancing Scientific Discovery



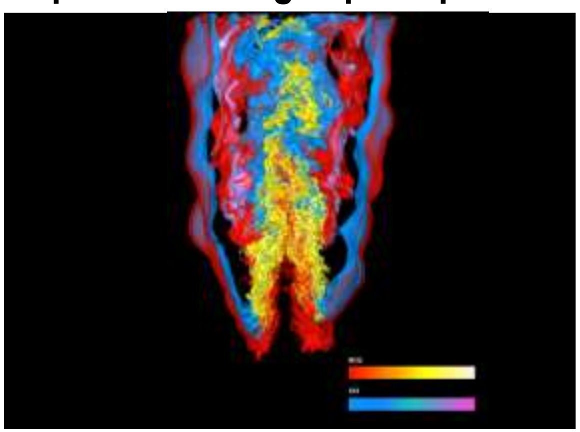
Resolved decades-long controversy about validity of 2D Hubbard model in predicting behavior of high-temperature superconducting cuprate planes



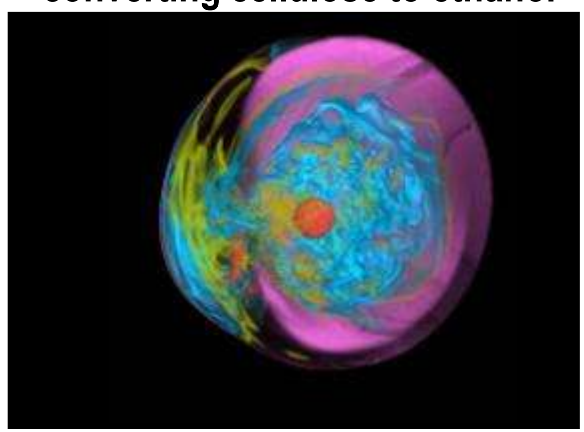
300K-atom models of cellulase enzyme on cellulose substrate reveal interior enzyme vibrations that influence reaction rates converting cellulose to ethanol



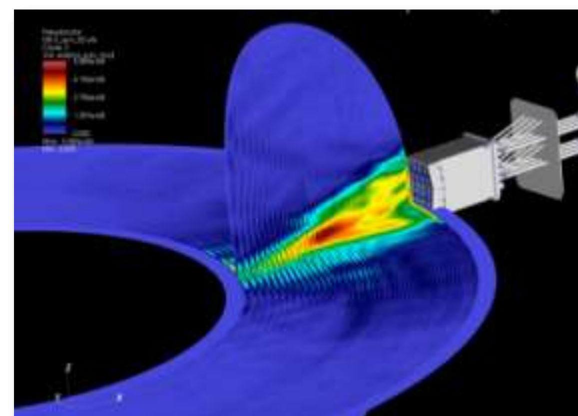
Addition and intercomparison of carbon-land models in new climate model is resolving key processes for carbon sources & sinks



Turbulence chemistry revealed in study of lifted turbulent H_2/air jet flames in ignitive coflow relevant to diesel engines and gas turbines



Instability of supernova shocks was discovered directly through simulation and core collapse pulsar mechanism was explained



Providing increasing assurance that RF power will effectively heat ITER

Courtesy: Doug Kothe (ORNL)

Some Science Drivers

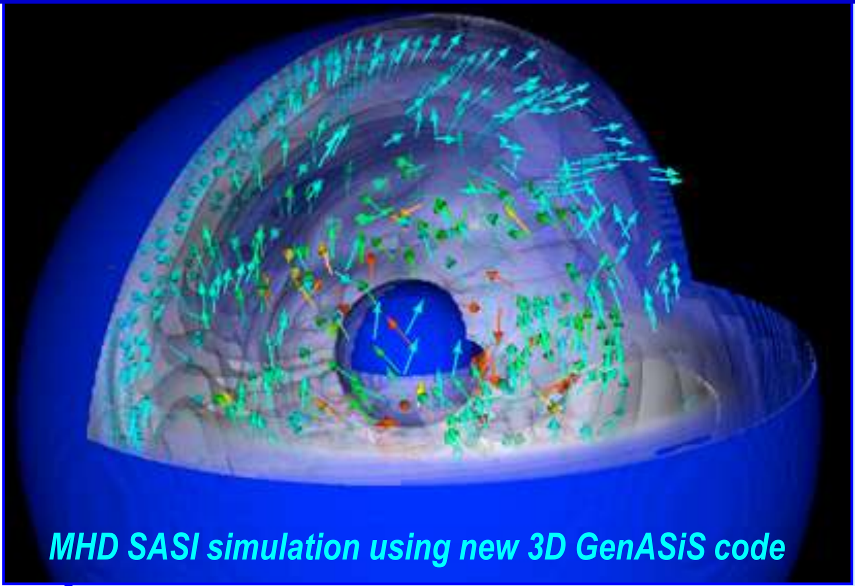
Science Domains	Science and Engineering Driver
Accelerator Physics	Optimize a new low-loss cavity design for the ILC
Astrophysics	Explosion mechanism of core-collapse supernovae and Type Ia supernovae
Biology	Can efficient ethanol production offset the current oil and gasoline crisis?
Chemistry	Catalytic transformation of hydrocarbons; clean energy & hydrogen production and storage
Climate	Predict future climates based on scenarios of anthropogenic emissions
Combustion	Developing cleaner-burning, more efficient devices for combustion.
Fusion	Plasma turbulent fluctuations in ITER must be understood and controlled
High Energy Physics	Find the Higgs particles thought to be responsible for mass, and find evidence of supersymmetry
Nanoscience	Designing high temperature superconductors, magnetic nanoparticles for ultra high density storage
Nuclear Energy	Can all aspects of the nuclear fuel cycle be designed virtually? Reactor core, radio-chemical separations reprocessing, fuel rod performance, repository
Nuclear Physics	How are we going to describe nuclei whose fundamental properties we cannot measure?

The OLCF Transition to Operations plan is accelerating readiness while emphasizing the science case for Leadership Systems.

Courtesy: Doug Kothe (ORNL)

Discovering the Elusive Core Collapse Supernova Explosion Mechanism

Researchers glean unprecedented insight into the shock waves that blow apart a 10- to 20-solar mass star



Researchers can now simulate ~1 second after 'post-bounce'. Petascale systems will allow longer simulations: tens of seconds after the explosion and will allow inclusion of neglected yet important physics such as magnetic fields.

- **Achieved longer run simulations and, 0.8 seconds after explosion, saw the initial shock wave revived by turbulence of in-falling material**
- **CHIMERA used to investigate multiple stellar models, effect of both Newtonian and Einsteinian gravity, and impact of recently discovered subatomic physics**
  - **>12K cores used in current 3D simulations**
- **Current 3D spatial resolution**
  - **78x156x312 (Chimera)**
  - **256x256x256 (Genasis)**

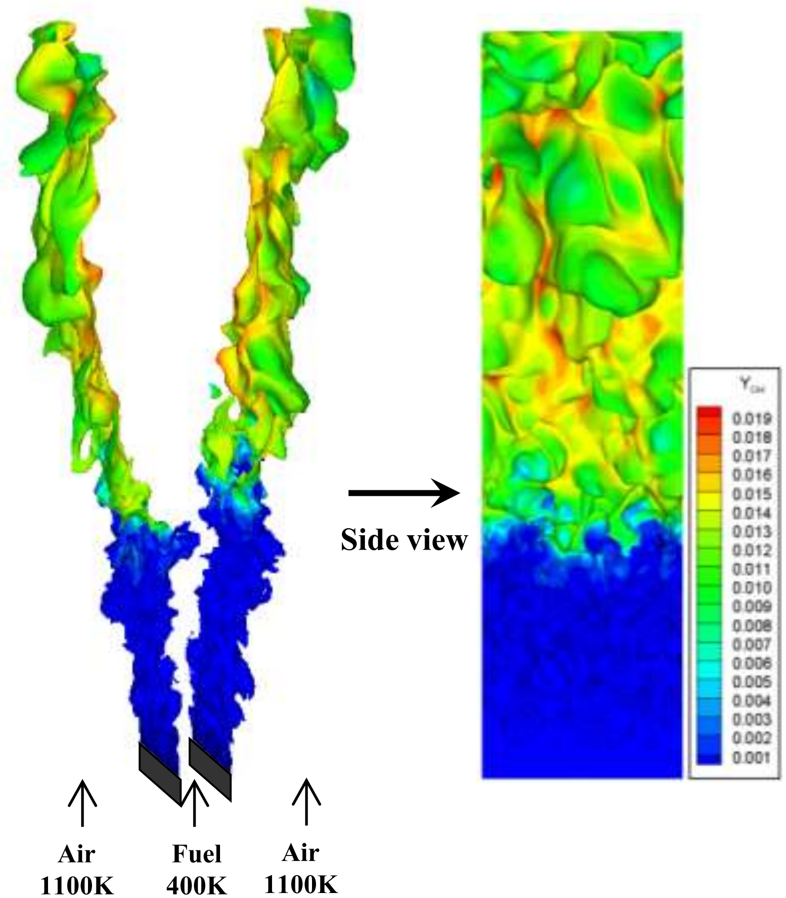
LCF liaison contributions
- **Implementing efficient, collective I/O**
- **Pencil decomposition of 3D flow algorithm**
- **Preconditioning of the neutrino transport equation**

Ref: Tony Mezzacappa (ORNL)

Courtesy: Doug Kothe (ORNL)

New Results in Flame Stabilization in an Auto-Ignitive Jet

- First fully-resolved simulation of a 3D lifted flame in heated co-flow with detailed chemistry
- Lifted flames occur in diesel engines and gas turbine combustors
  - Flame stabilized against fuel jet and recirculating hot gases
- Direct numerical simulation of a lifted flame in heated co-flow
  - ~1 billion grid points and 14 degrees of freedom per grid point
  - H_2/Air detailed chemistry
  - Jet Reynolds number = 11,000
  - Largest DNS at the highest Reynolds number
  - 2.5M hours on Jaguar at the LCF
- Simulation reveals source of stabilization
  - Upstream auto-ignition
  - Vorticity generation at flame base due to baroclinic torque



Instantaneous OH radical concentration on a stoichiometric mixture fraction iso-surface shows flame lift-off

LCF liaison contributions
- **Cray X1E loop vectorization of S3D**
- **Identified and fixed X1E MPI bottleneck**
- **Lagrangian tracers; I/O rework with NW University**
- **Jaguar scaling studies helped to identify processors burdened by memory corrections**

Ref: Jackie Chen (ORNL)

Courtesy: Doug Kothe (ORNL)

Dramatic increases in computational hardware capabilities will continue.

2004
Cray X1
3 TF

2005
Cray XT3
Single-core
26 TF

2006
Cray XT3
Dual-core
54 TF

2007
Cray XT4
119 TF

2008
Cray XT4
Quad-core
166 TF

Cray XT4
Quad-core
263 TF

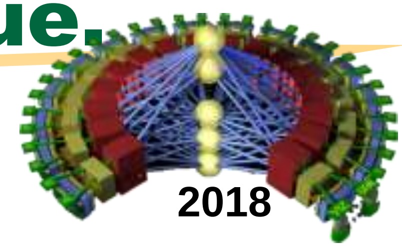
2009
Cray “Baker”
6-core, dual-socket SMP
~1000 TF
100TB, 2.5PB

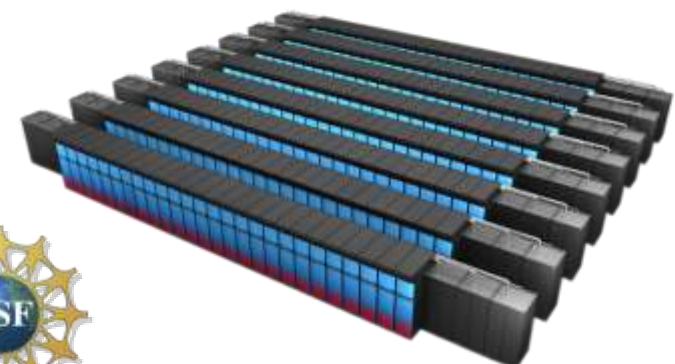
Cray “Baker”
6-core, dual-socket SMP
~2600TF
300 TB, 10PB

2011
OLCF-3 / DARPA
20 PF

2015
Future system
100–250 PF

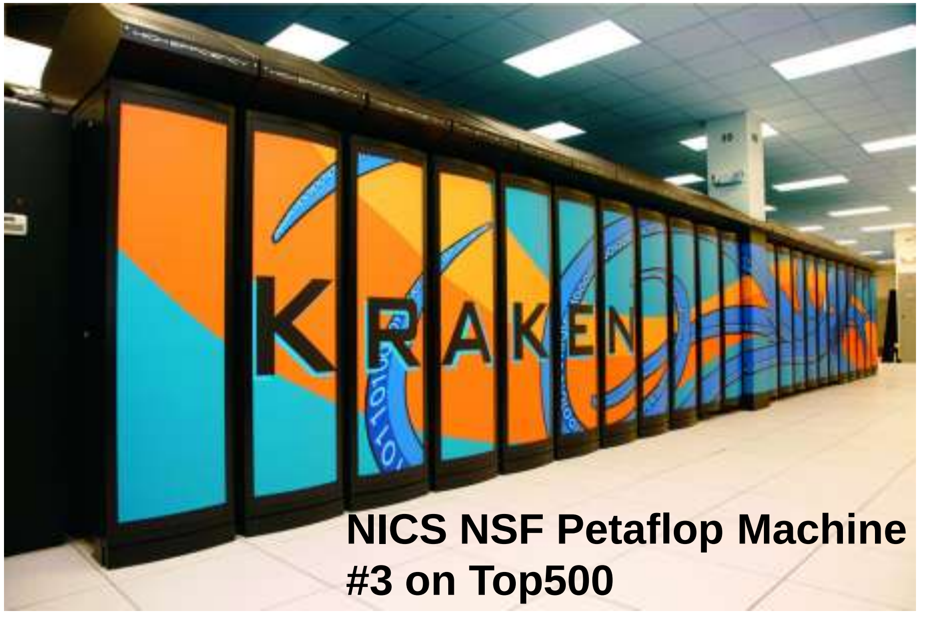
2018
Future system
1000 PF
(1 EF)





DOE's Leadership Computing Facilities are providing resources to industry, academia, and other national labs.

Jaguar Cray XT5
#1 on Top 500 list
2.332 Petaflop/s peak performance
1.759 PF/s sustained performance
37,376 AMD Opteron processors (6-core, 2.6 GHz)
224,256 total compute cores
362 TB total system memory



NICS NSF Petaflop Machine
#3 on Top500

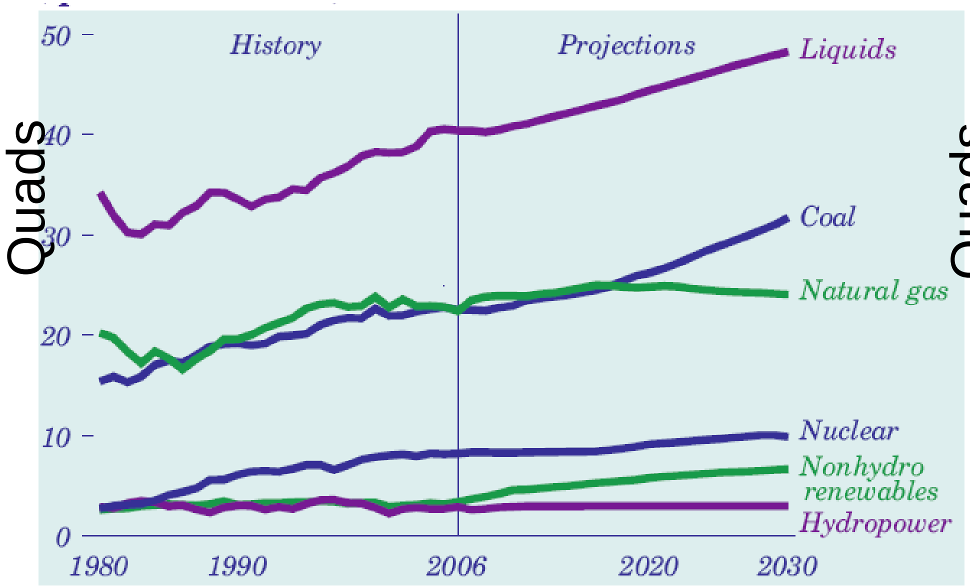
ORNL provides leadership computing to INCITE program and director's discretionary allocation, NSF allocations through NICS – a way for industry / academia / national labs to get access

NEED FOR CLEAN ENERGY

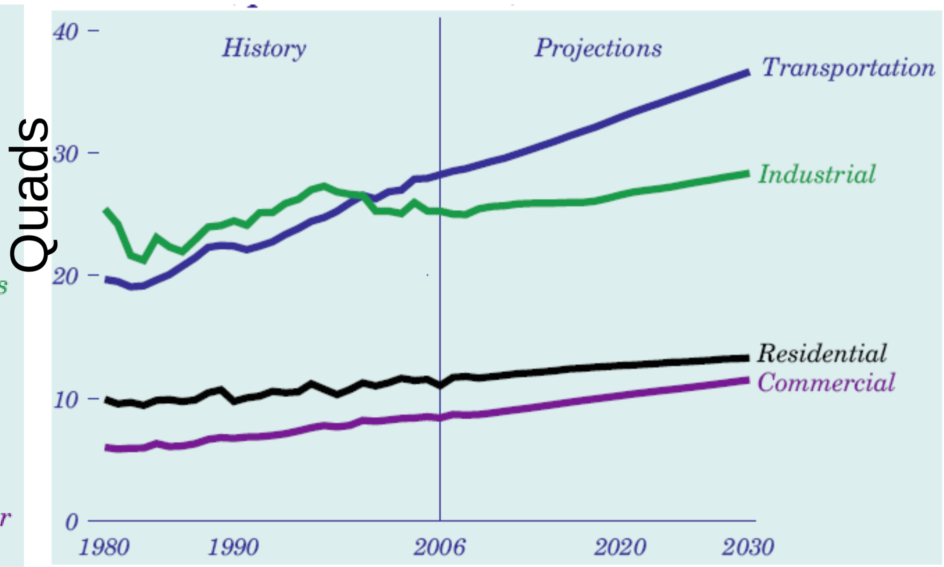
The Nation that Leads in Clean Energy Will Lead Global Economy

- President Obama at MIT on Friday, Oct. 23, 2009
  - The world is now engaged in a peaceful competition to determine the technologies that will power the 21st century. From China to India, from Japan to Germany, nations everywhere are racing to develop new ways to producing and use energy.
  - According to Pentagon, Energy Security is #1 National Security
- Clean/alternative energy is best response to petro-dictatorship and in enabling world peace
  - paraphrasing Thomas Friedman, NY Times Columnist

Energy Trends



Energy consumption by Fuel



Energy consumption by Sector

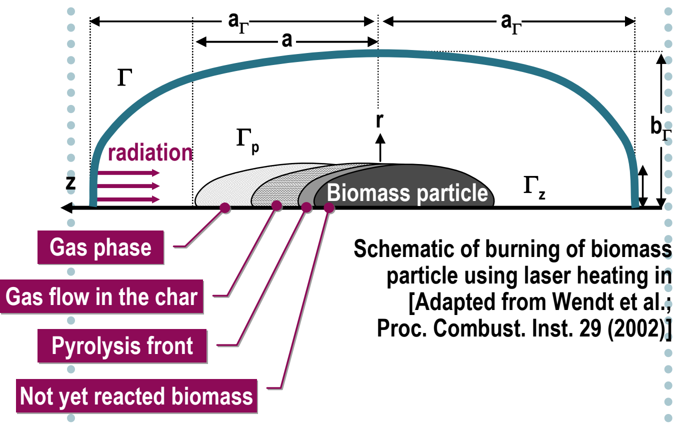
If we want to change these alarming trends (double by 2050 and triple by 2100 for the World), it is critical to make key investments today and simulation science can/should play a big role

Source: Annual Energy Outlook 2008, Early Release

SOME EXAMPLES, CURRENT STATE-OF-THE-ART

Coal/Biomass gasification

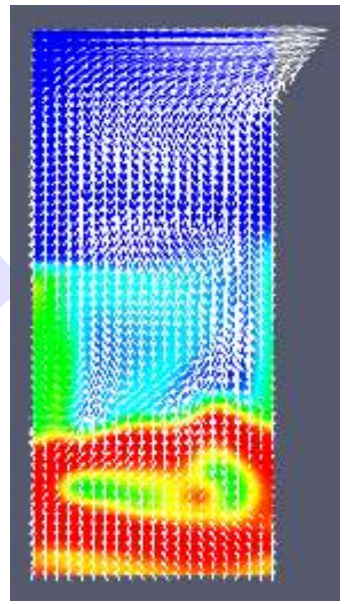
Coal/Biomass Particle (small scale)



Schematic of burning of biomass particle using laser heating in [Adapted from Wendt et al.; Proc. Combust. Inst. 29 (2002)]

- ~ mm particles
- Complex flow: gas phase, gas phase in char, pyrolysis front, unreacted biomass
- Wide range of species
- Surface processes at nm length scale and ns time scales

Coal/Biomass Gasifier/Pyrolyzer (device scale)



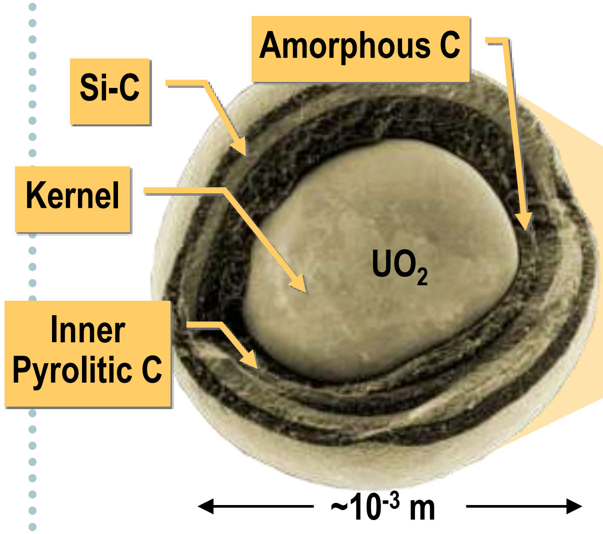
- ~ m in size
- Gasification/pyrolysis at high temperatures (~1000°C) in reactor with large residence times ~10 s
- Coal/Biomass particles cycle thru wide range of conditions where complex chemistry occurs

- Design challenge: Maintain optimal temperatures, species, residence times in each zone to attain right gasification/pyrolysis
- Truly multiscale problem: ~O(13) time scales, ~O(10) length scales
- Materials challenge: Design/understand material properties for the biomass pellets/particles at μm/nm scale
  - Size
  - Porosity
  - Integrity
  - Composition
  - Binders?

SP et al. (CFD in CRE, 2008; Chapter in a ACS Book)

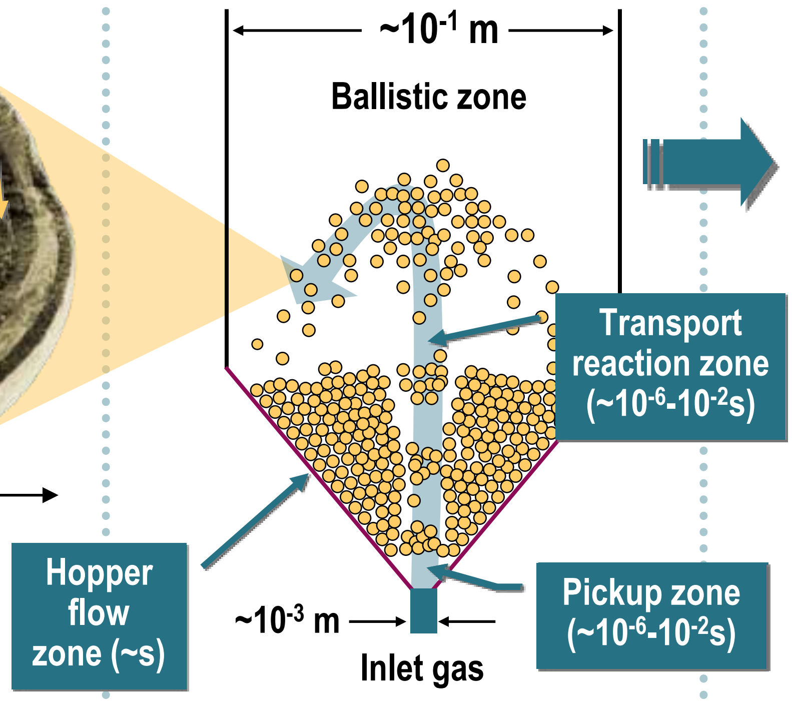
Nuclear fuel coating process

Coated fuel particle (small scale)



- 0.5- to 1-mm particles
- Coating encapsulates fission products
- Failure rate < 1 in 10^5
- Quality depends on surface processes at nm length scale and ns time scales

Spouted bed coater (device scale)



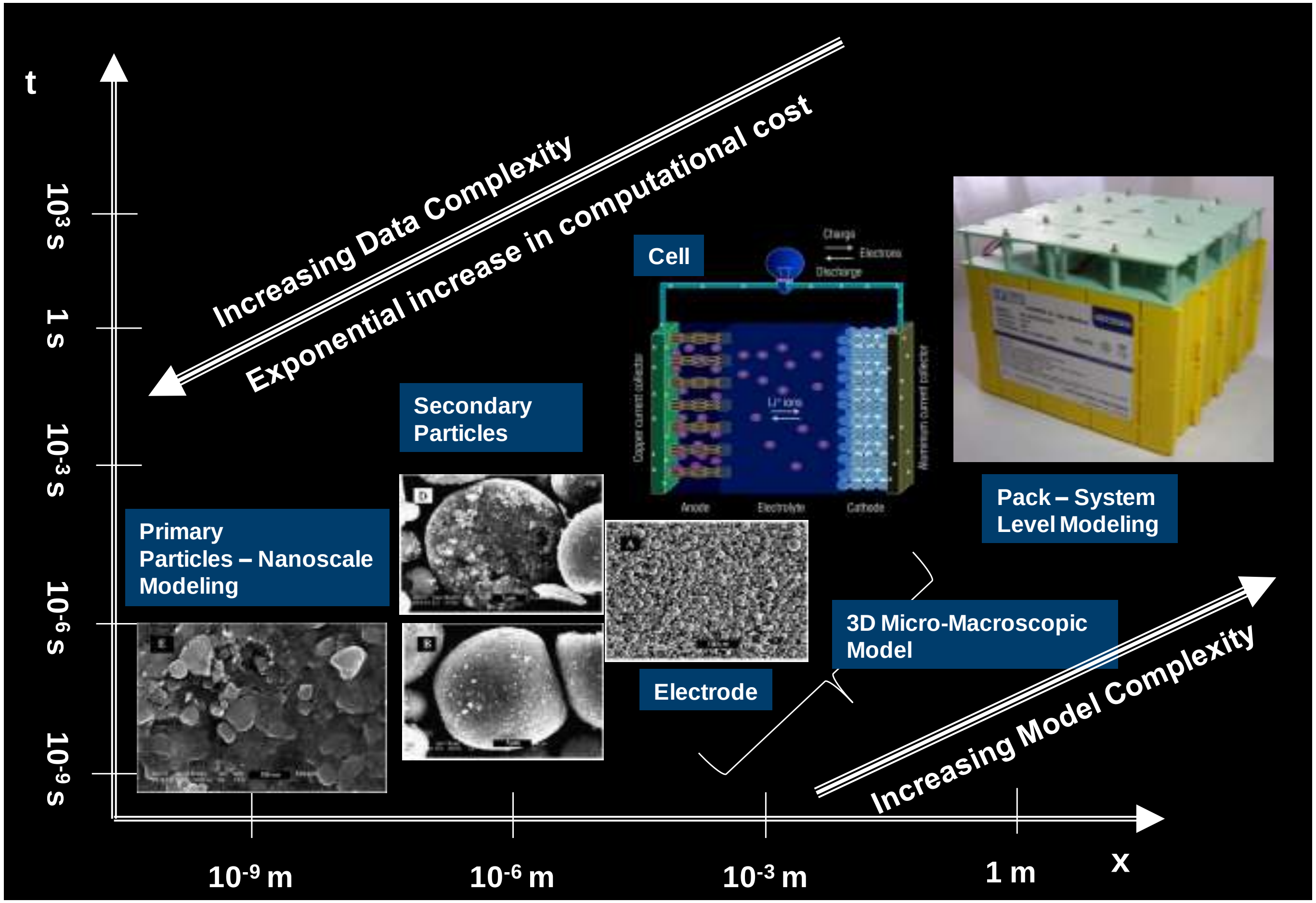
- Coating at high temperature (1300–1500°C) in batch spouted bed reactor for ~10^4 s
- Particles cycle thru deposition and annealing zones where complex chemistry occurs

- Design challenge: Maintain optimal temperatures, species, residence times in each zone to attain right microstructure of coating layers at nm scale
- Truly multiscale problem: ~O(13) time scales, ~O(8) length scales

Needs innovative multiscale algorithms along with peta-/exascale computing

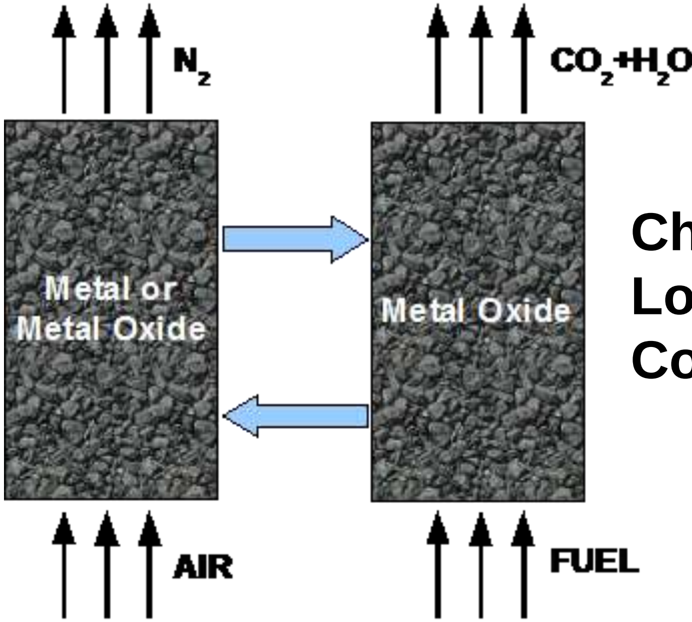
Pannala et al. (CVD, 2007), ORNL/CF-06/06, ORNL/TM-2006/520, ORNL/CF-05/14, ORNL/CF-05/13, ORNL Technical Report for INL MPO 00056009

Batteries are complex, multi-scale dynamical systems



Need to integrate models at various scales from Atomistic to Micro-Macroscopic Models to System level modeling and include several physics – species transport, energy transport, electrochemical reactions, and mechanics

Other Applications



Chemical Looping Combustion

- Similar to hemoglobin in our blood
- Higher efficiency with lower entropy losses
- No thermal NOx
- Separated CO2 stream for sequestration
- Potential carbon-negative technology if used with biomass
- Challenges
  - Catalysts with fast oxidation and reduction
  - Material durability
  - Cost

Carbon Nanotubes, Nanofibers and Nanostructures	▪ Light weight and high strength ▪ Supercapacitors ▪ Challenges about bulk production with desired chirality, diameter, number of walls etc.
Thin film Si deposition on powders and Si production	▪ Modify material properties (strength, corrosion resistance, tribology etc.) ▪ Reduce cost for PVs
Reactive flows through fibrous media	▪ Light weight, low-cost and high-strength composites ▪ Fuel cell components

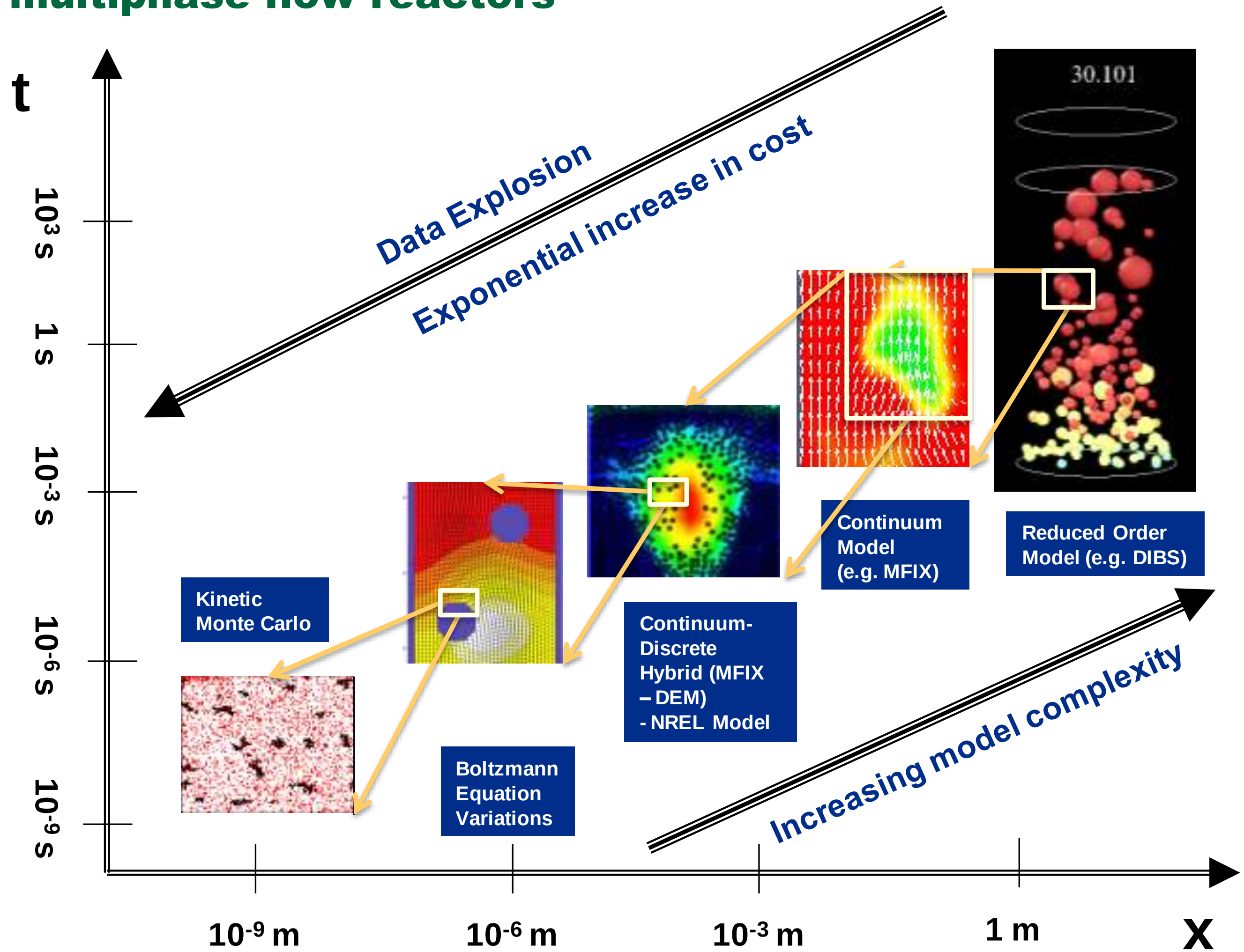
SP and Wood (J. Nanosci. Nanotech., 2004)
Wood, SP et al. (PRB, 2007)

What is being done and what can be done differently…

- **New technologies take decades**
  - **Lab scale → pilot scale → production scale**
  - **Resistance to adopting new ideas**
  - **Current models have limited quantitative predictability/credibility**
  - **Cultural barrier**
- **Why we need to do things differently**
  - **Energy crisis is current and growing**
  - **We need tomorrow’s technology today**
  - **Economic opportunity**
- **What can be done differently**
  - **Development of integrated and scalable Multiscale/Multiphysics (MSMP) predictive models**
  - **Component and lab-scale experiments targeted to validate computational models**
  - **Integrate lab scale experiments along with simulations to design new plants and devices**

Multiphysics heterogeneous chemically reacting flows for energy systems

Goal: Building a suite of models for unprecedented capability to simulate multiphase flow reactors



- Through support from various DOE offices (FE, EERE, and NE) we have developed suite of models for unprecedented capability to simulate heterogeneous chemically reacting flows
- Hybrid methods to couple two physical models (e.g. MFIX DEM)
- Uncertainty quantification to probe only quantities of interest at smaller scales

SP et al., *Edited Book on "Computational Gas-Solids Flows and Reacting Systems: Theory, Methods and Practice," May, 2010.*

NETL

OAK RIDGE National Laboratory

Depending on need, there is a range of fluid bed modeling approaches

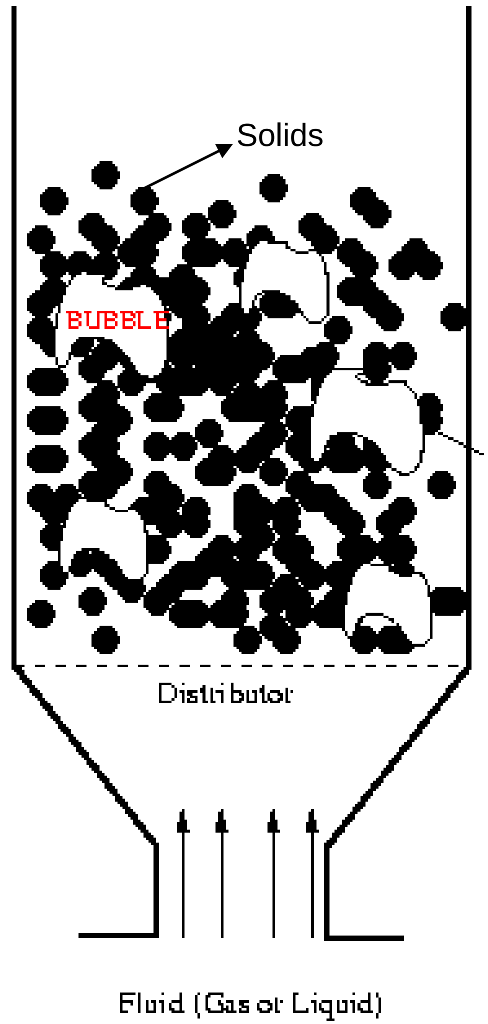
- **Low-Order Bubble/Circulation Model**
  - Bubbles/circulation modeled with simple interaction rules, correlations
  - Solution based on integration of ODE's
  - Fast, near-real time
- **Detailed MFIX 3D Model**
  - Interspersed continuum model for both gas and solids
  - Solution of Navier-Stokes equations using computational grid
  - Slower, more detailed
- **DES (Discrete Element Simulation)**
  - MD kind of simulation for granular particles
  - Slower, detailed for particles
- **MFIX-DES (MFIX coupled with DES)**
  - Continuum approach for gas phase and DES for solids

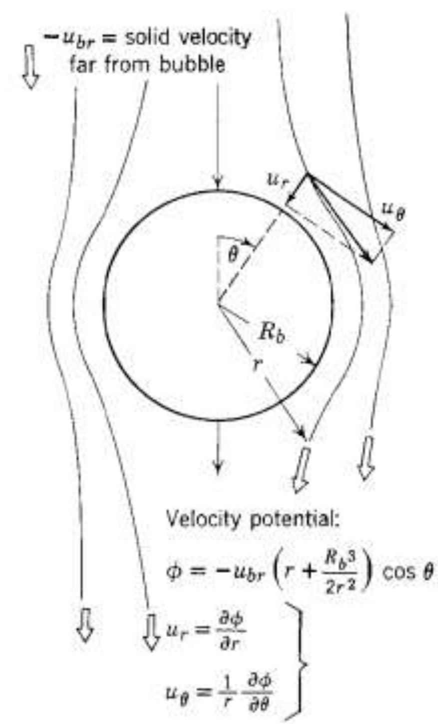
Heat & mass transfer, chemical kinetics, particle evolution can be incorporated in all of above

REDUCED ORDER MODELS

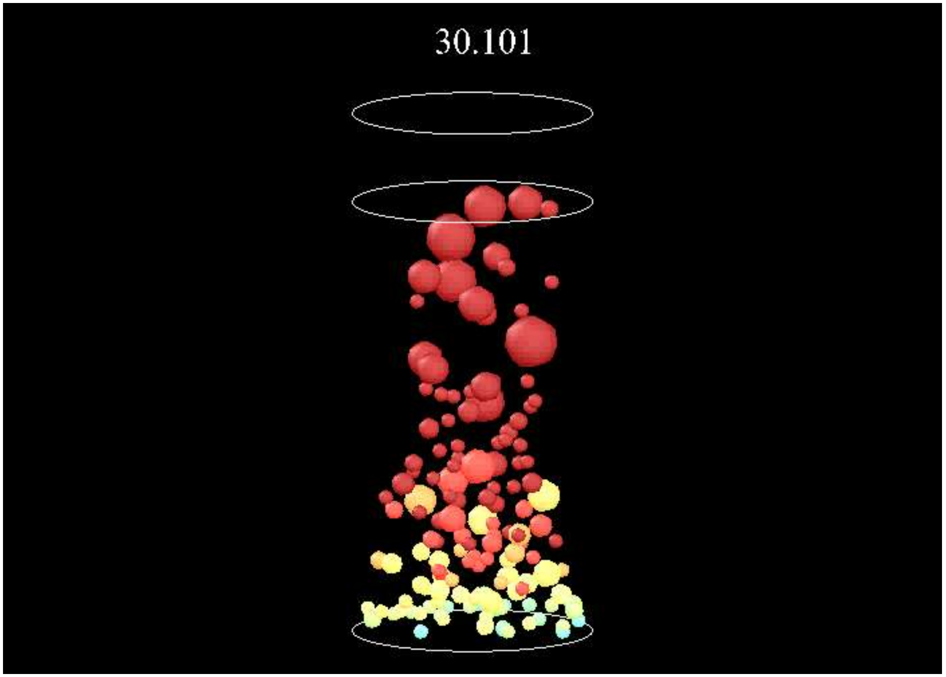
The ORNL/NETL DIBS code is an example of a low-order bubble/circulation model

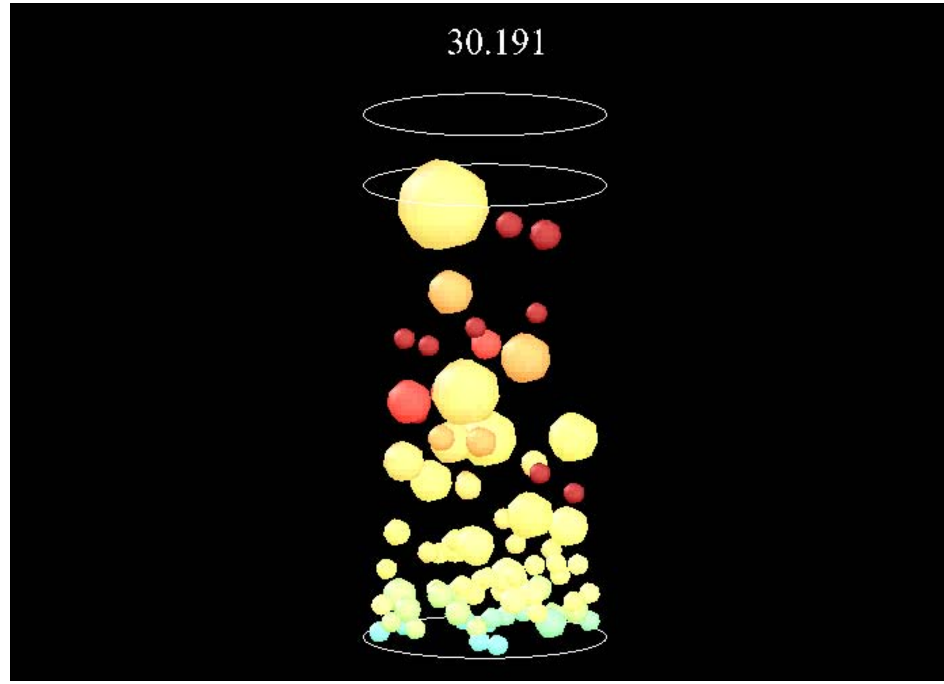
- **Applies to bubbling beds**
- **Gas distributed between emulsion and bubble phases**
- **Davidson & Harrison bubbles corrected for experimentally observed pair interactions**
  - **Trailing bubble accelerates toward leading bubble**
  - **Bubbles coalesce when they collide**
- **Each bubble is tracked individually and progress of local gas-exchange and reaction accounted for**
- **Progress of emulsion gas reactions tracked**
- **Bulk motion of emulsion solids and global solids properties tracked**
- **Objective is to quantify mixing, contact time, and local chemical reaction rates between gas and solids to produce overall conversion of reactants**





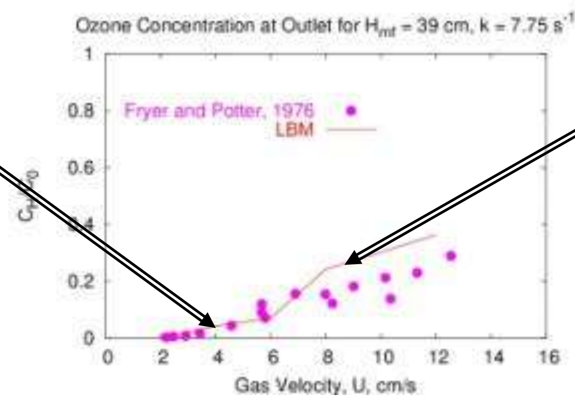
An advantage of the DIBS code is that it reveals global mixing patterns and runs in near real time





H = 40 cm, k = 7.75/s & U = 4.0 cm/s

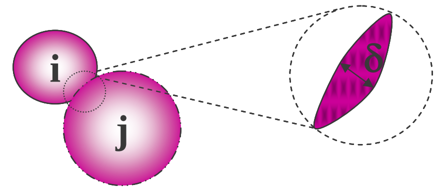
H = 40 cm, k = 7.75/s & U = 8.6 cm/s

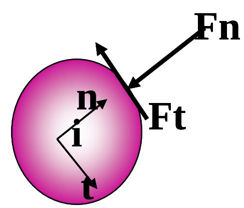


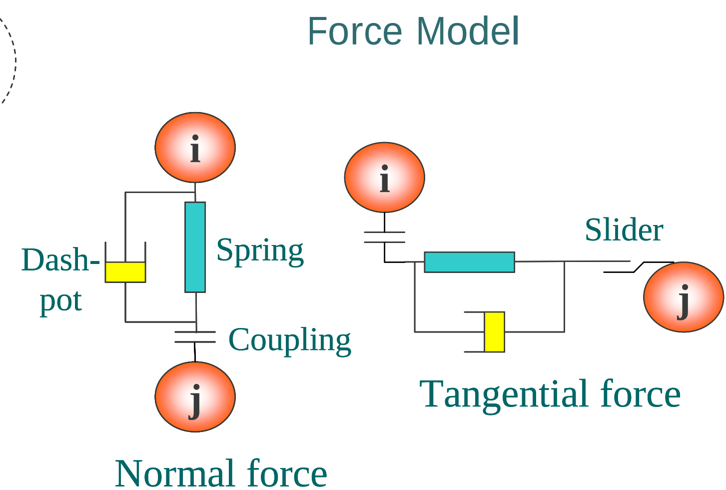
DISCRETE ELEMENT MODEL

Discrete element codes are based on the most fundamental description of particle motion

- **Soft sphere model admitting spherical particles of varying sizes**
  - **Based on model of Cundall and Strack**
- **Efficient search algorithms developed**
  - **N^2 search (for reference only)**
  - **Non-binary search (NBS) for particles of similar size**
  - **Quadtree/Octree for particles of different sizes**







Governing Equations

$$\dot{\vec{v}}_s = \frac{\vec{F}}{m} + g \qquad \vec{F} = \vec{f}_C + \vec{f}_D \qquad \vec{f}_{Ci} = \sum_j \left(\vec{f}_{Cnij} + \vec{f}_{Ctij}\right)$$

$$\vec{f}_{Cni} = -k\vec{\delta}_{nij} - \eta\vec{v}_{nij} \qquad \vec{f}_{Cti} = -k\vec{\delta}_{tij} - \eta\vec{v}_{tij}$$

$$\vec{v}_n = \left(\vec{v}_r \bullet \vec{n}\right)\vec{n} \qquad \vec{v}_t = \vec{v}_r - \vec{v}_n + r\left(\vec{\omega}_i + \vec{\omega}_j\right) \times \vec{n}$$

$$\left|\vec{f}_{Ctij}\right| \triangleright \mu_f \left|\vec{f}_{Cnij}\right| \qquad \vec{f}_{Ctij} = -\mu_f \left|\vec{f}_{Cnij}\right| \vec{t}_{ij} \qquad \vec{t}_{ij} = \frac{\vec{v}_{tij}}{\left|\vec{v}_{tij}\right|}$$

$$\dot{\vec{\omega}} = \frac{\vec{T}_C}{I} \qquad \vec{T}_{Ci} = \sum_j \left(r\vec{n}_{ij} \times \vec{f}_{Ctij}\right)$$

2D Fluidized Bed with a Central Jet

Fluidization by air

X/d = 37.5; Y/d = 250

$U_{superficial}$ = 1.8m/s

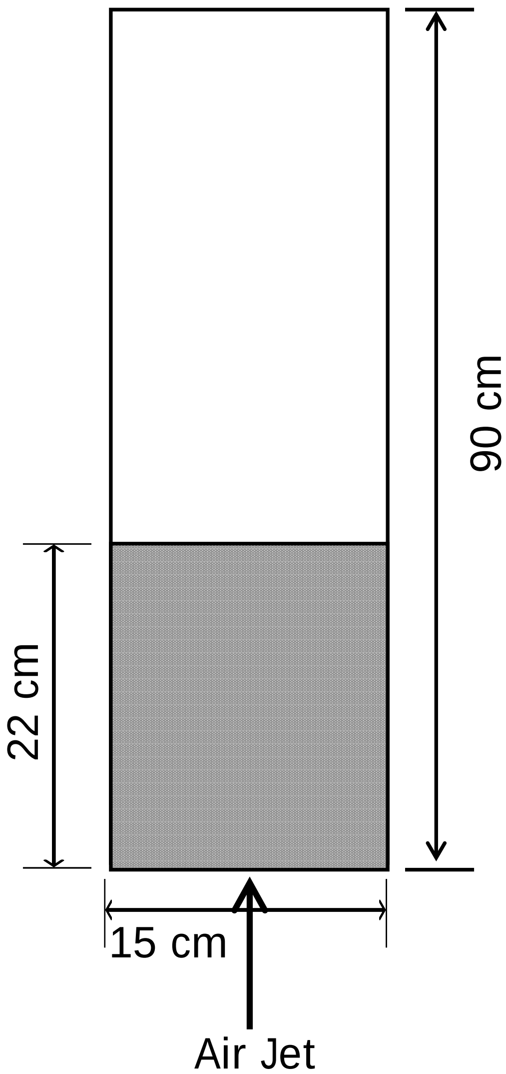
$U_{central\text{-}jet}$ = 4.2m/s

Particles

N = 2400

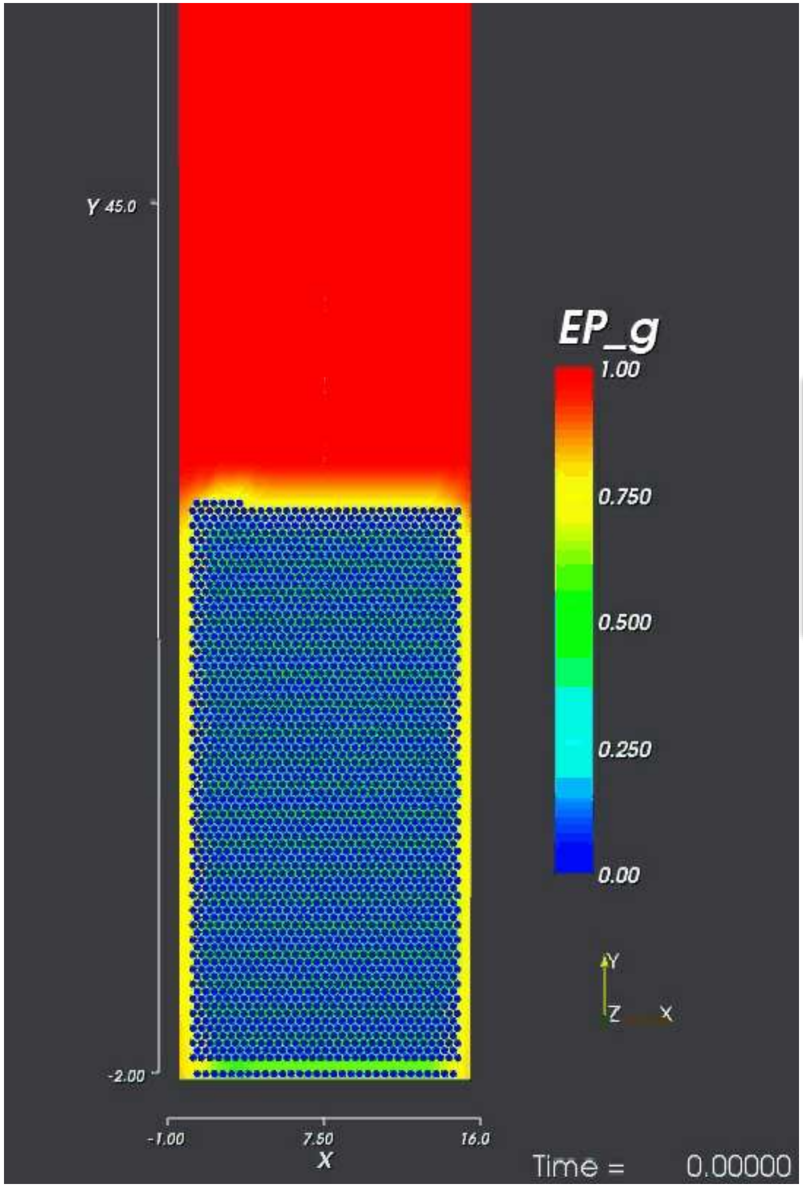
d = 4mm

Density = 2700 kg/m^3



Tsuji et al. Powder Tech 1993

Results



Need to perform detailed validation against Tsuji's paper

MACROSCALE CFD SIMULATIONS

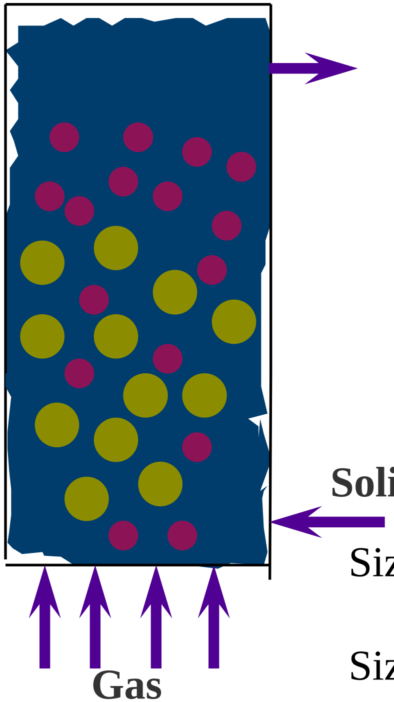
MFIX simulation package

- **General multiphase flow CFD code which couples hydrodynamics, heat & mass transfer and chemical reactions**
- **SMP, DMP and Hybrid Parallel code which runs on many platforms including Beowulf clusters**
- **Open-source code and collaborative environment (http://www.mfix.org or http://mfix.netl.doe.gov)**
- **Over 2000 researchers from over 500 institutions around the world**

R&D 100

2007

Multiphase formulation



- **Two Phases**

  Fluid

  Solids

- **Three phases**

  Fluid

  Solids - 1

  Solids - 2

Size 1

Size 2

- **Details of flow field and particle interaction have been averaged out.**
- **Account for the information lost due to averaging through the use of *constitutive equations***

Continuity Equation

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

Momentum Equation

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

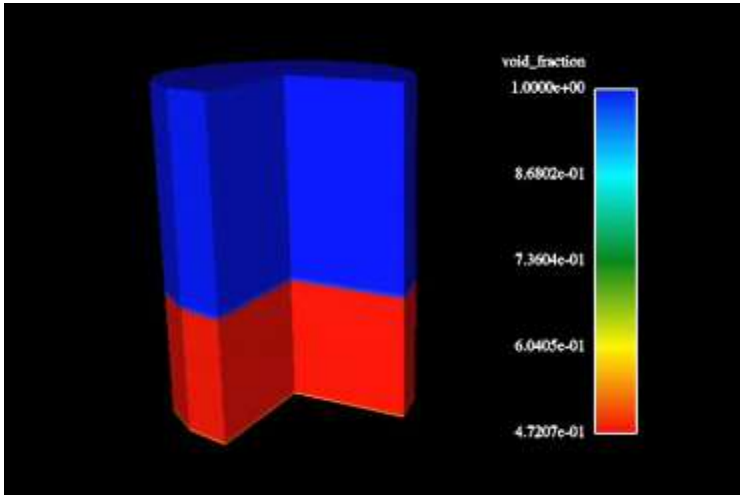
Stresses

Interaction Term

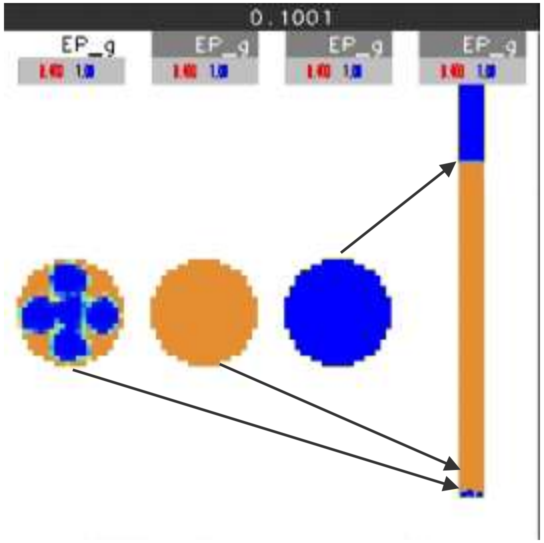
Granular Stresses are modeled by the kinetic theory of granular material in the viscous regime and plasticity theory in the plastic regime

Drag law describes the interaction between the gas and the particles

The MFIX code is an example of a more detailed CFD-type of model



Ozone Reactor (Void Fraction)



Silane Reactor

Square Circulating Fluidized Bed

Instantaneous snapshots of voidage surface (=0.85). Indicates the core-annulus flow and the solids flowing down at the walls (used MAVIS for visualization).

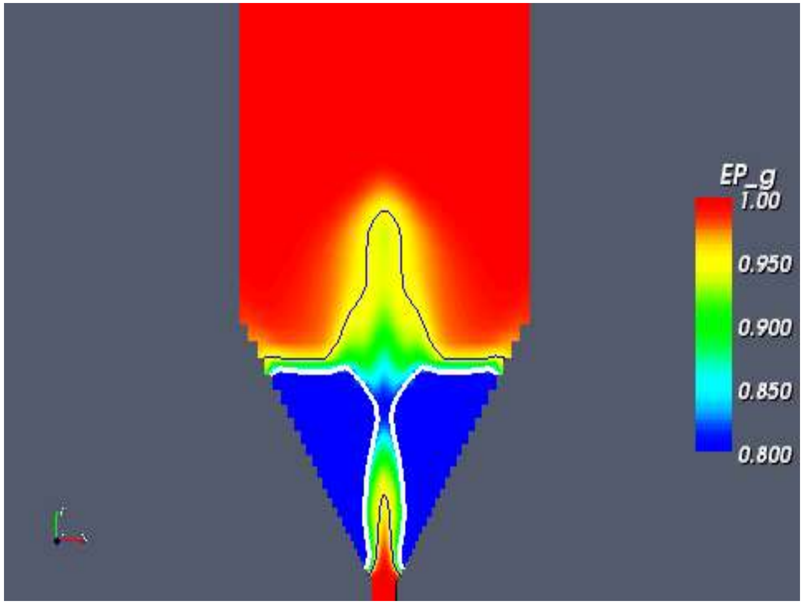
FLUIDIZED BED CVD COATER FOR NUCLEAR FUEL PARTICLES

Simulation objectives:

- **Demonstrate simulations with *sufficient detail* to capture known effects of coater operation and design on quality**
- **Develop analytical tools that aid coater scale-up and design**
- **Develop improved nuclear fuel coaters with unprecedented levels of product quality**
- **Develop improved fundamental understanding of the controlling mechanisms for both C and SiC chemical vapor deposition**
- **Develop improved fundamental understanding of the dynamics of spouted bed reactors**

Observation (1): MFIX is able to simulate general circulation & flow patterns of UTK and ORNL experiments

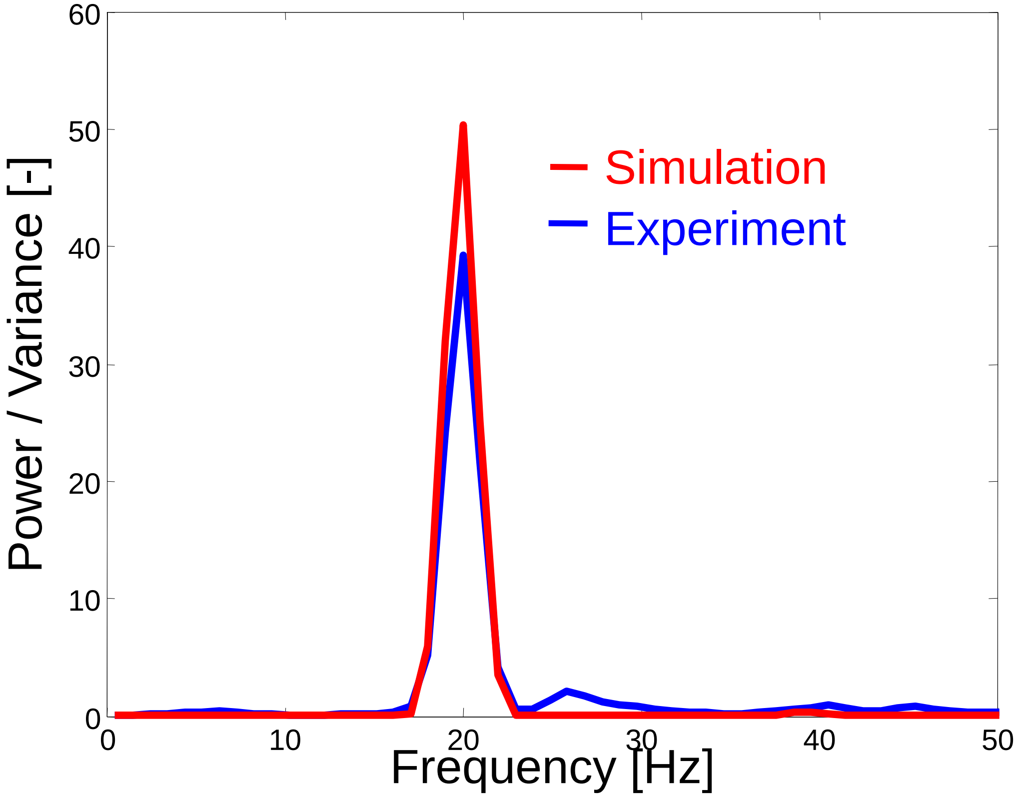
Ambient UTK experiment, 500 μm ZrO_2 at V_g=12m/s



Simulation

- **Correctly predicts major flow zones**
- **Some hydrodynamic parameters need 'tuning' based on experiments**
  - Coefficient of restitution (solids-solids, solids-wall friction)
  - Solids internal angle of friction (solids flowability)
  - Solids stress formulation
  - Drag Correlation
  - Boundary conditions (e.g. specularity coefficient)

Observation (2): MFIX can predict correct dynamic time scales



500 μm ZrO_2 at 300 K in air for UTK 2-inch mockup

Gas pulsations are directly measurable

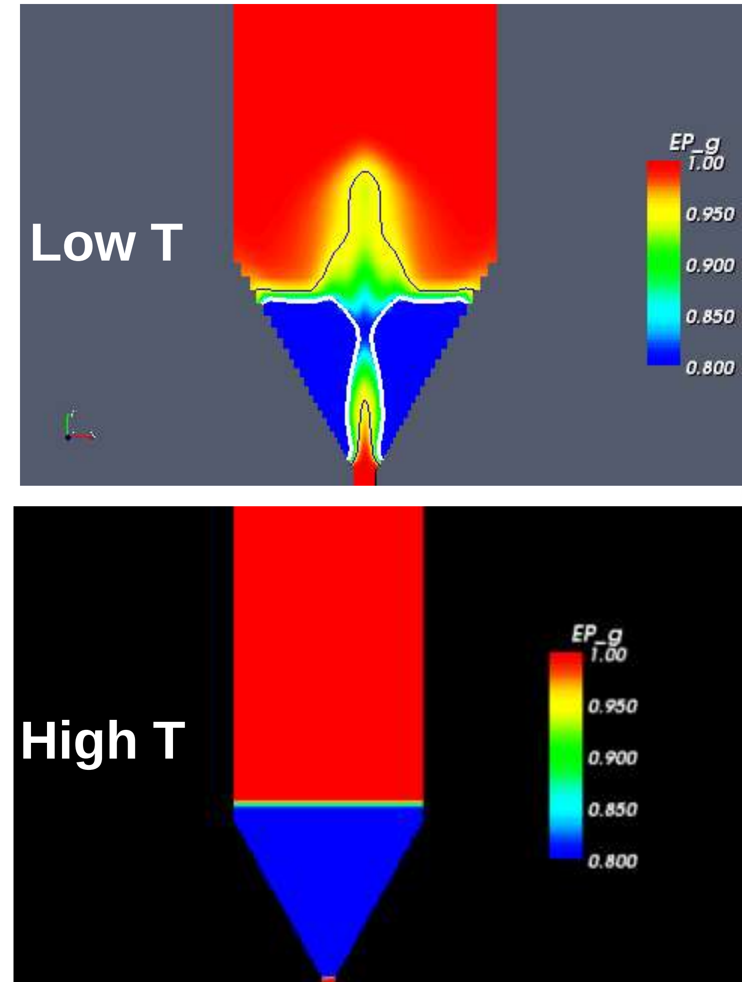
Pulsations contain important information on solids circulation

The circulation times also relate to particle-coating gas contact time

Observation (3): Standard heat transfer correlations in MFIX appear to work well for this application

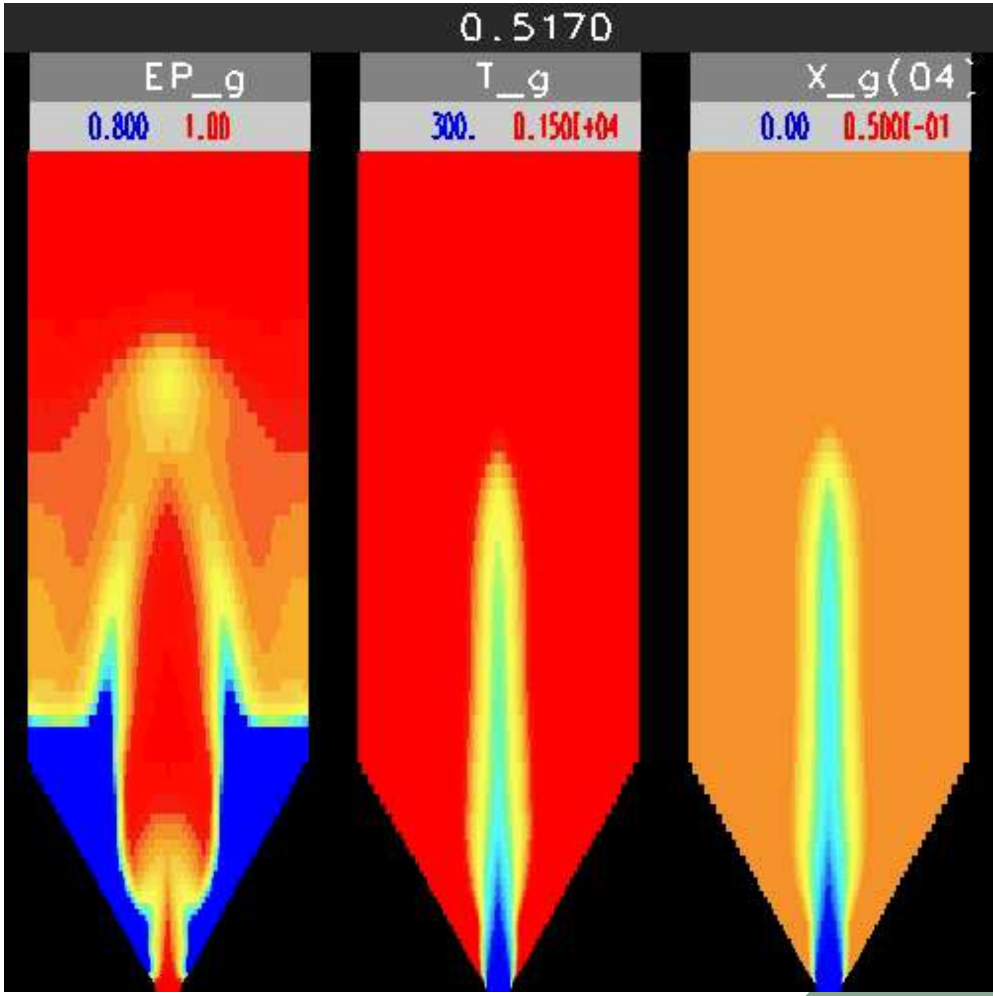
- **Gunn (1978) heat & mass transfer correlations used**
- **Large effects of temperature due to**
  - **Density and viscosity change**
  - **Sudden radial and axial expansion**
- **Two different example cases**
  - **500 μm ZrO2 in 30.06 m/s air at 298 K**
  - **536 μm buffer coated UCO in 14.6 m/s Argon/Acetylene/Propylene mixture at 1523K**
- **Jet expansion is much more dramatic at higher T**
- **At higher T, spouting also becomes more vigorous and pulsation frequency drops by ~1/2**
- **Consistent with experiments**
  - **indicates proper coupling between heat transfer and hydrodynamics**

Void Fraction



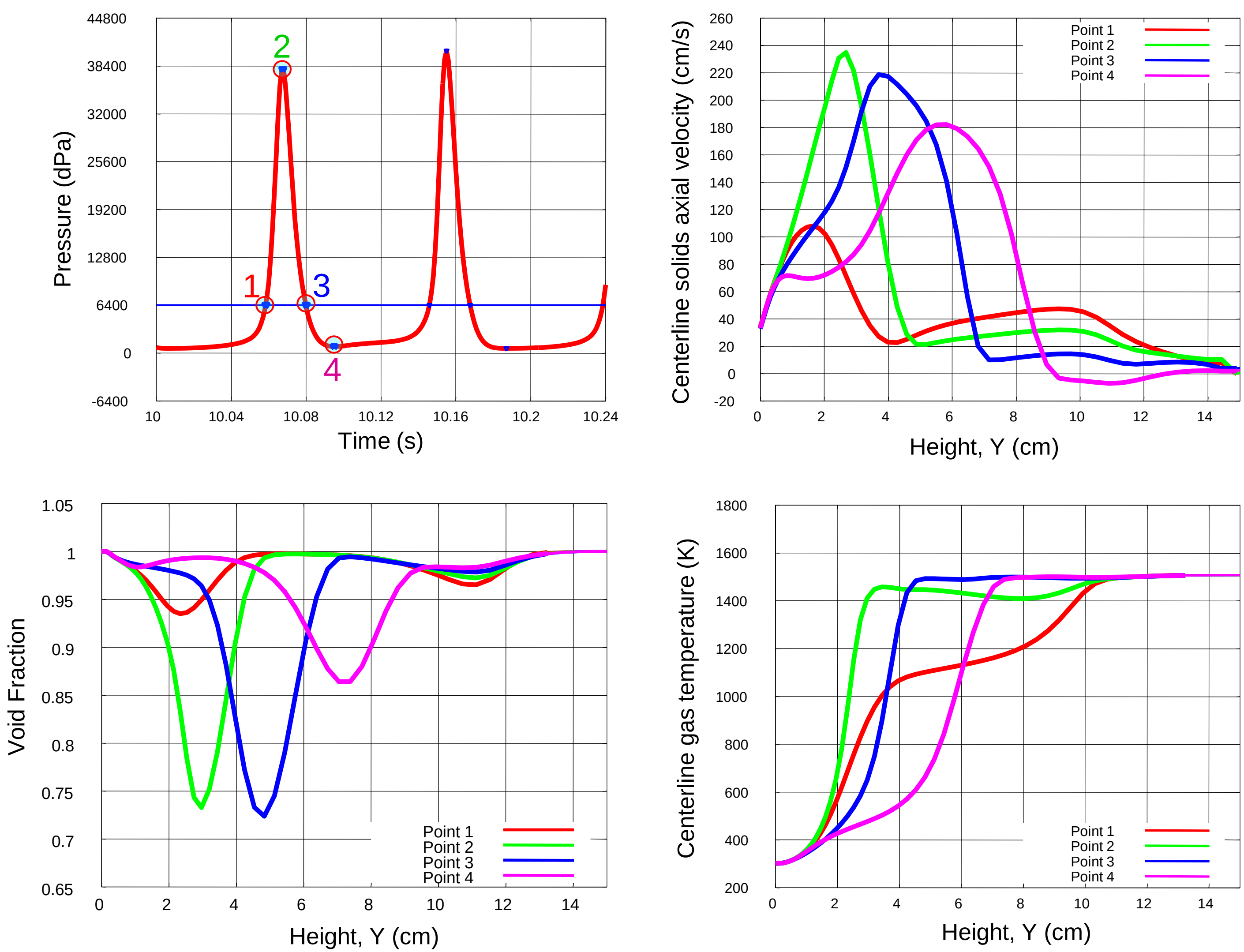
Observation (4): We see very high spatial & temporal gradients at coating conditions

Void Fraction, Gas Temperature, H_2 mass fraction



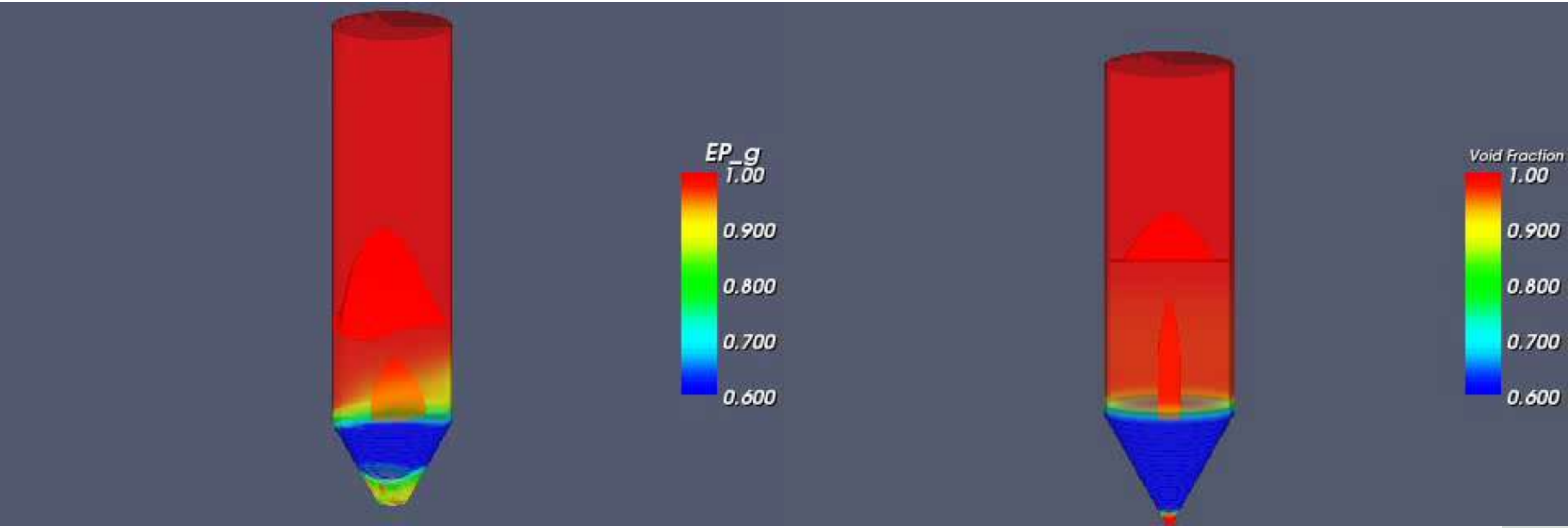
- **Experimental observations indicate core zone is the most important (location of 'snow' formation during C deposition)**
- **Inlet gas heats very quickly to furnace temperature with solids (unlike pure gas flow)**
- **Very large absolute fluctuations in velocities, temperatures & concentrations during pulsation cycle**
- **Characteristics of these gradients, fluctuations expected to be major factors for design, scaling**

Observation (5): Considerable variations in the core in time as well as space



Observation (6): Injector design very critical to overall spouting behavior

Side View (Translucent)
[Contour surface corresponds to 0.99 void fraction]
Similar to peering into a glass bed with marbles



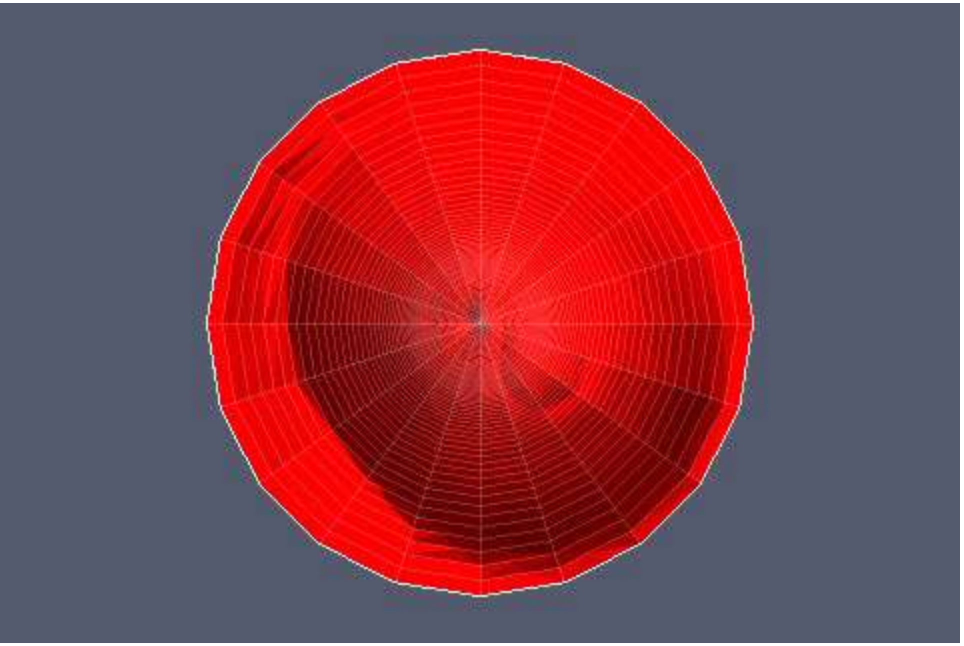
3D Multi-hole (6 holes: 1 + 5)

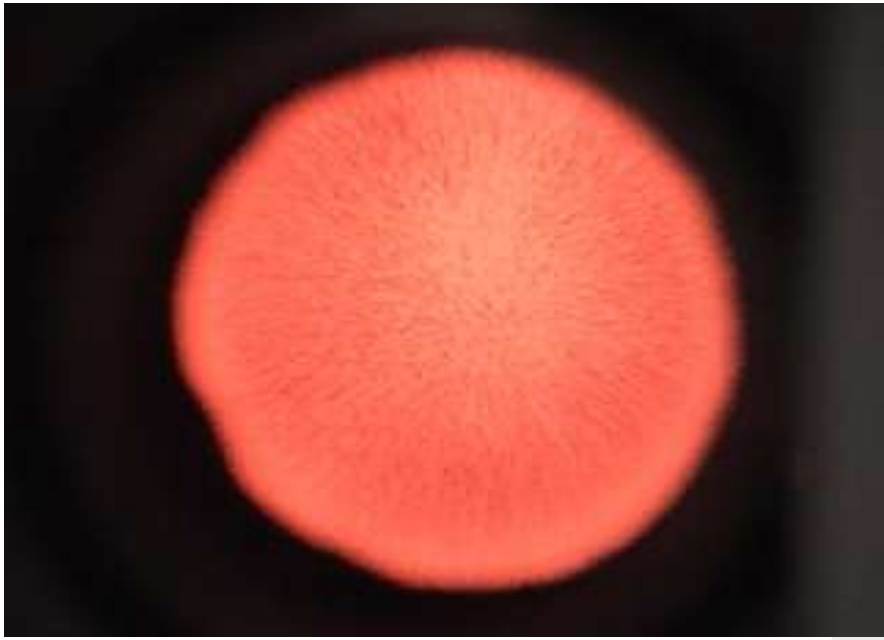
Reference NUCO IPyC condition

3D Single-hole

Observation (7): MFIX simulation predicts surface 'sloshing' observed in experiments

Top View





Simulations (Void Fraction = 0.99)

Experiments

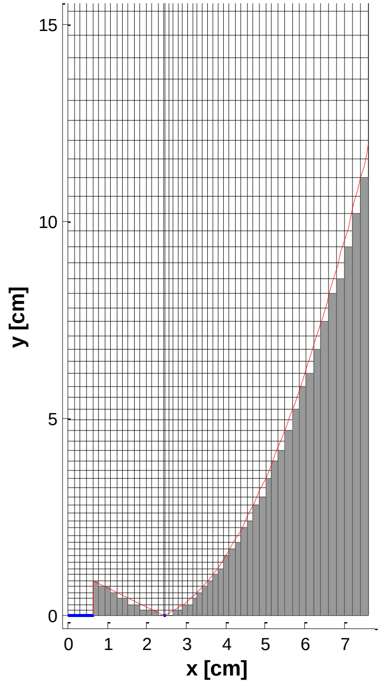
FLUIDIZED BED CVD COATER FOR NUCLEAR FUEL PARTICLES – *SCALE-UP*

Discriminating characteristics (DCs) have been proposed as generic quantitative indicators

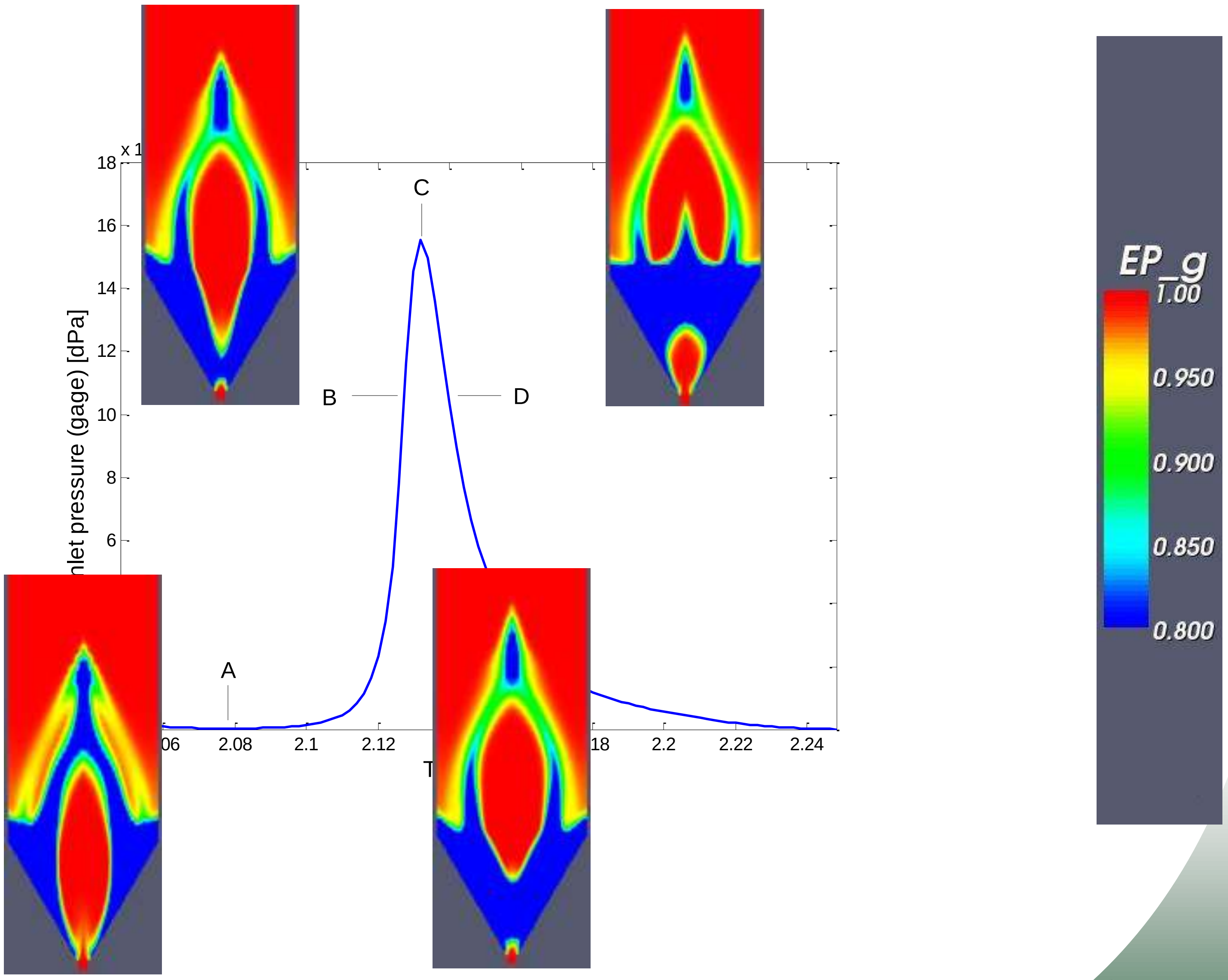
Discriminating Characteristic	Multi-hole	Single-hole	Comments
Dimensionless Solids Circulation Time (DSCT)	20.75	35.34	40% reduction
Ballistic Particle Profile (BPP) (10%) (cm)	8.56	10.97	Significant reduction in fountain height
Net Solids Impact Rate (NSIR)(g/s)	32.77	17.83	90% increase in wall impacts
Core Diameter (CD) (cm)	2.96	2.18	Significant increase in core diameter
Gas Velocity at center line at initial bed height (VG@CH) (cm/s)	346	949	Significant decrease in gas velocity
Solids Velocity at center line at initial bed height VS@CH (cm/s)	39.8	80.4	
Gas T at center line at initial bed height TG@CH (K)	1371	1000	Gas heats up quickly
Solids T at center line at initial bed height TS@CH (K)	1516	1486	
H2 concentration at center line at initial bed height H2@CH	0.0393	0.0243	Significant product formation at bed height
Acetylene concentration at center line at initial bed height C2H2@CH	0.0221	0.0788	Significant decrease in the reactant species
Propylene concentration at center line at initial bed height C3H6@CH	0.0179	0.0639	Significant decrease in the reactant species
GRADT (K/cm)	857.87	249.37	Huge difference in the gas heat-up rate
T@GRADT (K)	434.5	461.9	
Y@GRADT (cm)	0.25	1.382	Gas heats up very close to the inlet

Geometries and gas distributors

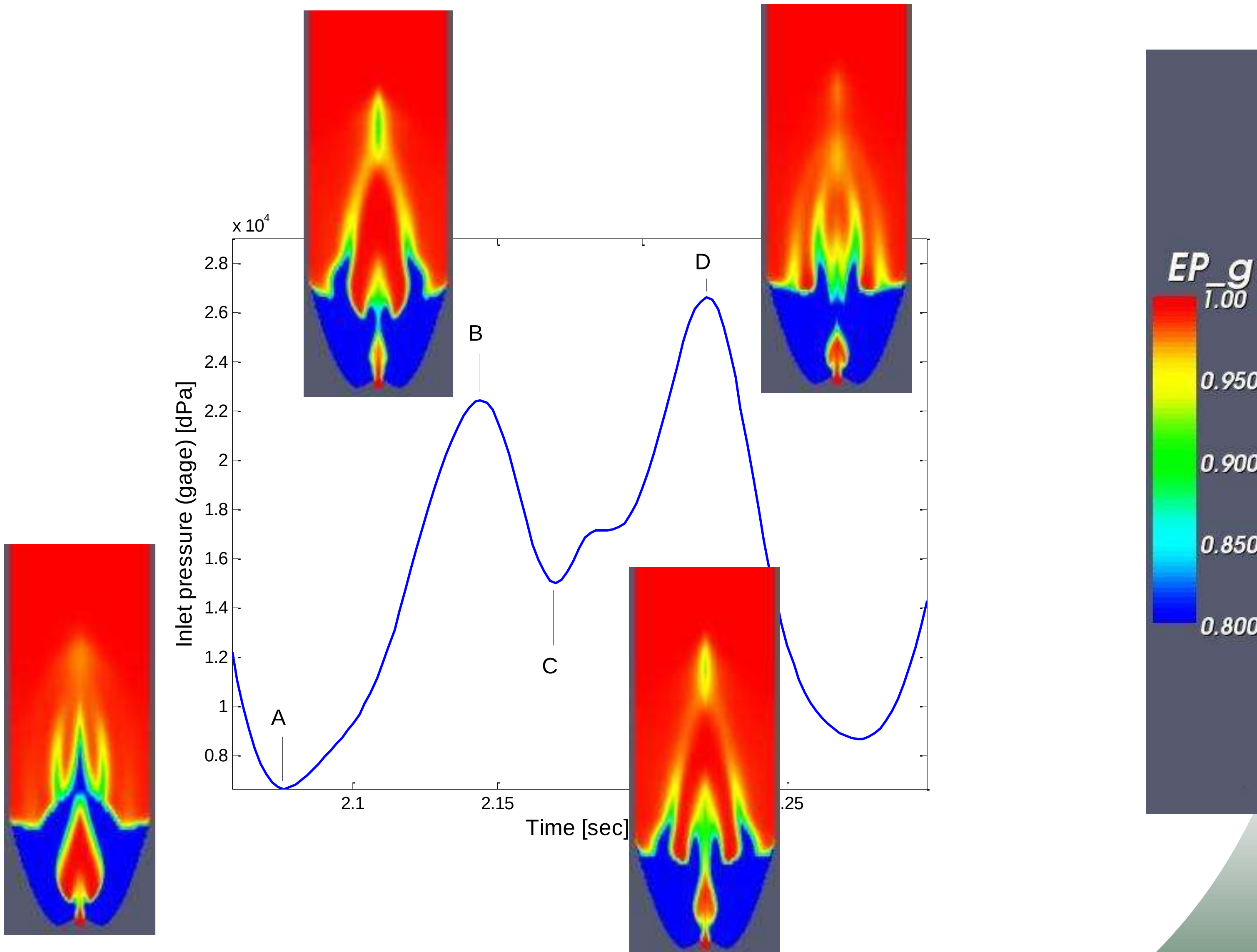
Run	Geometry	Distributor	Diluent gas partition Center | ring	Total gas mass flow rate [kg/hr]
1	Cardioid	Ring+center	0.908 | 0.092	10.7
2	Cardioid	Ring+center	0.938 | 0.062	16.1
3A	Cardioid	Multiport	0.908 | 0.092	10.7
3B	Cardioid	Multiport	0.908 | 0.092	10.7
4	Cardioid	Multiport	0.908 | 0.092	10.7
5	Cone	Center	N/A	10.7



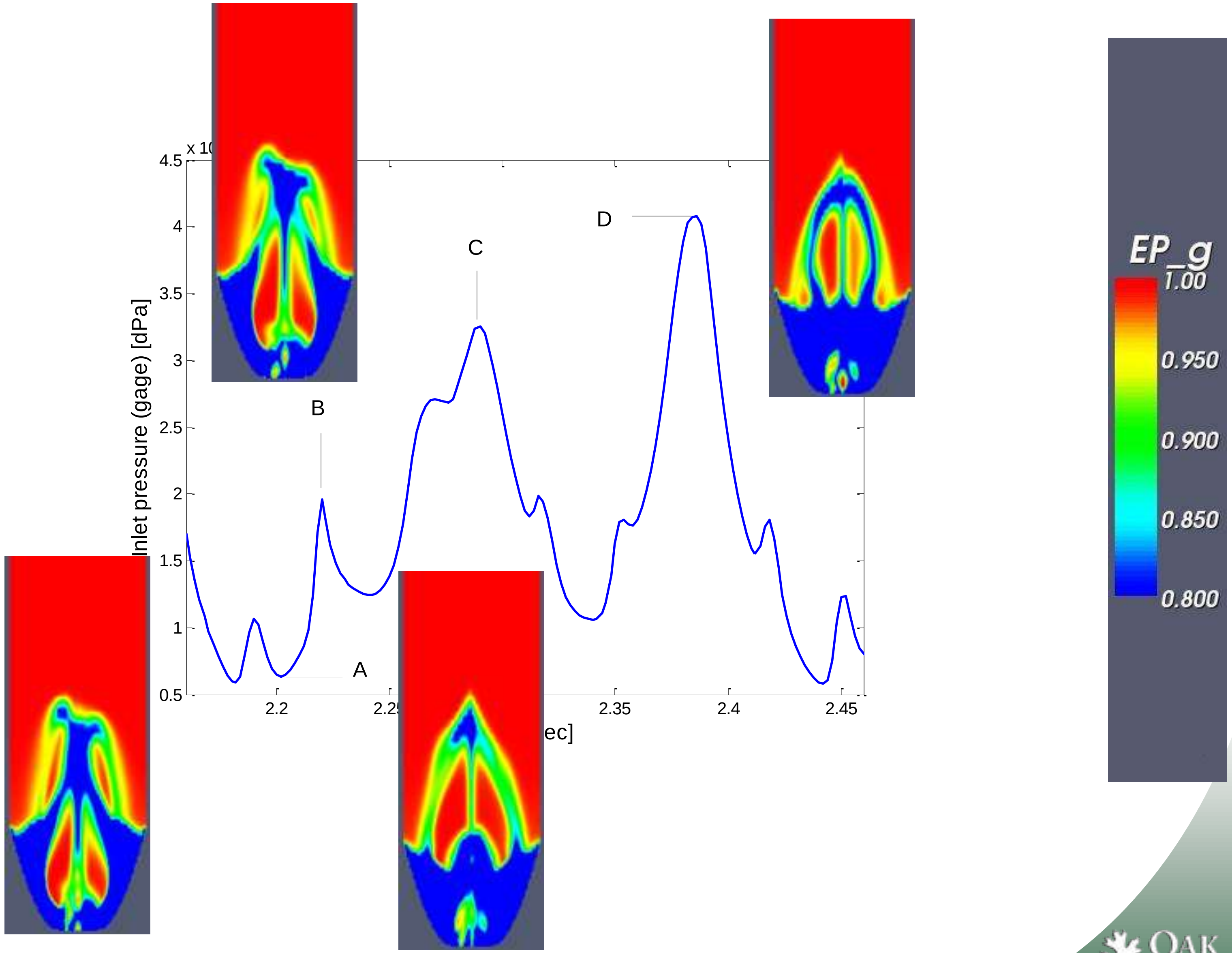
Reference cone design



Ring + center (Design #1)



Multiport injector (Design #3)

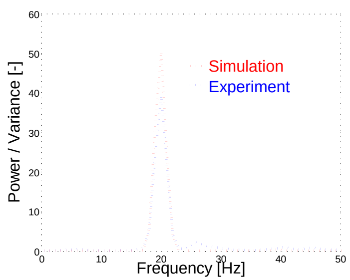


Conclusions from FBCVD scale-up studies

- Cardioid chalice with the multi-port design appears to have the best gas-solids mixing and heat transfer rates
  - Conical spouted beds cannot be scaled from 2” to 6”
  - Impact of swirl is minimal
  - Coater hydrodynamics and heat transfer are only minimally affected by mass transfer and chemical reactions.
- Design time reduced by order of magnitude at a fraction of cost

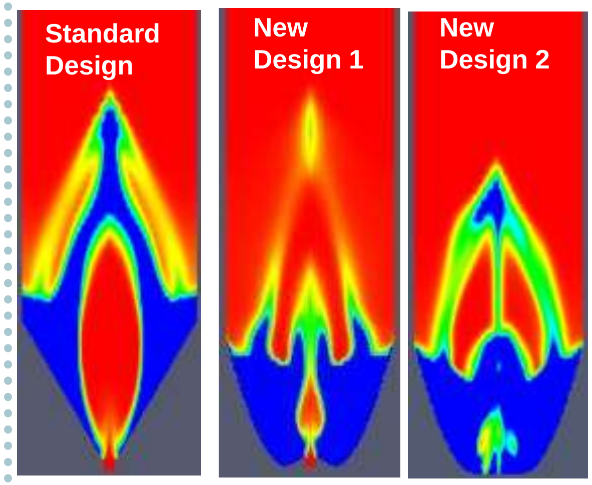
FBCVD Coater Scale-up Success

Validation (laboratory scale)



- Validated the code with available data from cold-flow and hot-furnace experiments
- Determined over 20 discriminating characteristics of importance to the coating process (e.g. particle residence time in the coating zone)

Evaluation (production scale)



- Explored four different designs
- Evaluated them based on the discriminating characteristics (DCs) as it is impossible to match all the non-dimensional parameters
- Cardioid chalice with the multi-port design appeared to have the best gas-solids mixing and heat transfer rates based on the DCs

- The production scale coater was built at BWXT, Lynchburg, VA
- After some initial fine-tuning, the coater is now being used to coat nuclear fuel particles for the DOE NE's advanced gas-cooled reactor program

Drastic reduction in design cycle time: What would have otherwise taken ~ 2 decades or so to arrive at a new coater design only took ~ 2 years with a validated CFD model

Art of making fuel particles has become science

Pannala et al. (CVD, 2007), ORNL/CF-06/06, ORNL/TM-2006/520, ORNL/CF-05/14, ORNL/CF-05/13, ORNL Technical Report for INL MPO 00056009

MULTISCALE/MULTIPHYSICS COUPLING

So what needs to be done for multiphysics coupling?

- **Can we rewrite the equations or the solution methods so that only *relevant* information is propagated upward from fine- to coarse-scales (upscaling) and coarse- to fine-scales (downscaling) in a tightly coupled fashion?**
  - **New mathematics, theory and analysis**
  - **Unification of governing equations across several scales**
    - **Lattice based methods across all scales?**
  - **Long-term**
- **If that is not possible, can we take the information from different methods and perform this in a posteriori fashion with various degrees of coupling?**
  - **Interpolation and extrapolation between the regions**
    - **Typical multiphysics coupling approach: FSI, BEM-Level Set, Inviscid/Viscous-BL for external aerodynamics, fluid-particle/droplet etc.**
    - **Usually invoked as a boundary condition or a source term**
    - **This is done almost implicitly in various methods we already use: grid stretching, multiblock, AMR, Adaptive basis**
  - **One can do better by transferring higher order statistics rather than just averages**
    - **Use stochastic processes to transfer the information**
      - **Use UO process to drive a stationary isotropic turbulence problem**

General Problem Definition

$$\dot{\mathbf{y}}_c = \mathbf{g}(\mathbf{x}, t, \mathbf{y}_c), \;\; \mathbf{y}_c(\mathbf{x}, 0) = \mathbf{y}_0(\mathbf{x}), \quad \mathbf{x} \in \mathcal{B}, \;\; t \in [0, T]$$

$$\dot{\mathbf{y}}_f = \mathbf{f}(\mathbf{x}, t, \mathbf{y}_f), \;\; \mathbf{y}_f(\mathbf{x}, 0) = \mathbf{y}_0(\mathbf{x}), \quad \mathrm{x} \in \mathcal{B}, \;\; t \in [0, T].$$

where **g** describes the coarse field, **f** describes the fine field

- We seek solution of the form

$$\mathbf{y}(\mathbf{x}, t) = \Phi\left[\mathbf{y}_c(\mathbf{x}, t), \mathbf{y}_f(\mathbf{x}, t)\right]$$

- Map takes the solution of the coarse-field over the entire domain and the fine-field over a subset of the domain to obtain a good approximation to y_f.
- The algorithms should be amenable to parallel implementation in both space and time

CWM (Compound Wavelet Matrix) and dCWM (dynamic CWM) Algorithms

CWM

Given: $\mathbf{y}_c(t)$ and $\mathbf{y}_f(\tau)$ with $t \in [0, T]$ and $\tau \in [0, T_f]$
Compute wavelet transforms: $\mathbf{y}_c^W = \mathcal{W}[\mathbf{y}_c(t)]$ and $\mathbf{y}_f^W = \mathcal{W}[\mathbf{y}_f(\tau)]$
Apply window filter: $\mathbf{y}_c^{H \circ W} = \mathcal{H}_{(a,b)}[\mathbf{y}_c^W]$ and $\mathbf{y}_f^{H \circ W} = \mathcal{H}_{(b,c)}[\mathbf{y}_f^W]$
Compute CWM: $\mathbf{y}_{CWM} = \mathbf{y}_c^{H \circ W} \oplus \mathbf{y}_f^{H \circ W}$
Compute inverse wavelet transform: $\mathbf{y}(t) = \mathcal{W}^{-1}[\mathbf{y}_{CWM}]$

$$\mathcal{H}_{(a,b)}(s) = \begin{cases} 1 \text{ if } a < s < b \\ 0 \quad \text{otherwise} \end{cases}$$

dCWM

for $n = 0$ to $N - 1$ **do**
  Given: $\mathbf{y}_c(t)$ and $\mathbf{y}_f(\tau)$ with $t \in [T_n, T_{n+1}]$ and $\tau \in [T_n, T_n + \delta T_f]$
  Compute wavelet transforms: $\mathbf{y}_c^W = \mathcal{W}[\mathbf{y}_c(t)]$ and $\mathbf{y}_f^W = \mathcal{W}[\mathbf{y}_f(\tau)]$
  Apply window filter: $\mathbf{y}_c^{H \circ W} = \mathcal{H}_{(a,b)}[\mathbf{y}_c^W]$ and $\mathbf{y}_f^{H \circ W} = \mathcal{H}_{(b,c)}[\mathbf{y}_f^W]$
  Compute dCWM: $\mathbf{y}_{dCWM} = \mathbf{y}_c^{H \circ W} \oplus \mathbf{y}_f^{H \circ W}$
  Compute inverse wavelet transform: $\mathbf{y}(t) = \mathcal{W}^{-1}[\mathbf{y}_{dCWM}]$
end for

SP with Frantziskonis et al. (IJMCE, 2006 & 2008)
SP with Mishra et al. (IJCRE, 2008)
SP with Mishra et al. (LNCS, 2008)
SP with Muralidharan et al. (PRE, 2008)

Compound Wavelet Matrix – Graphical Representation

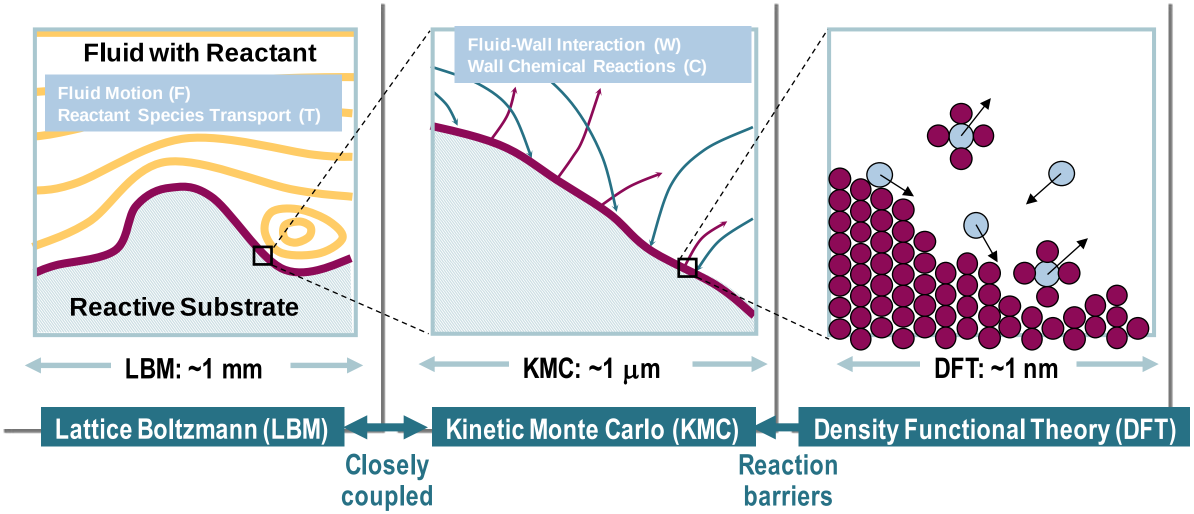
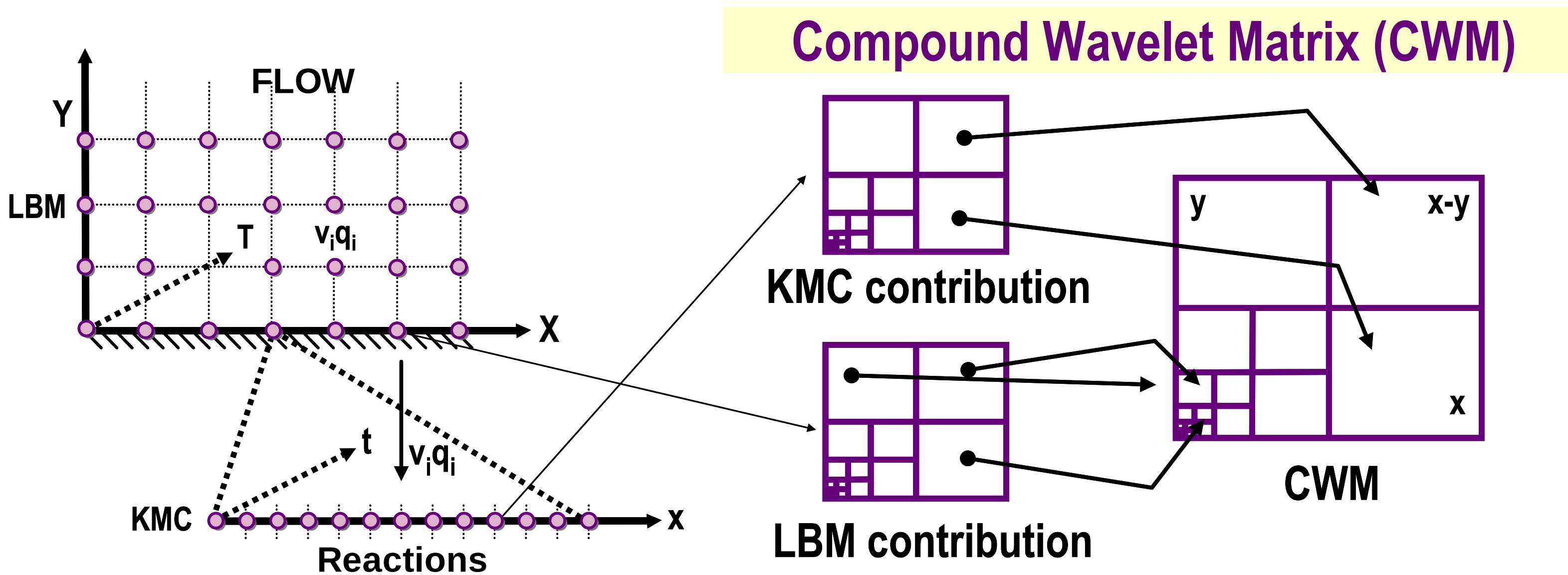
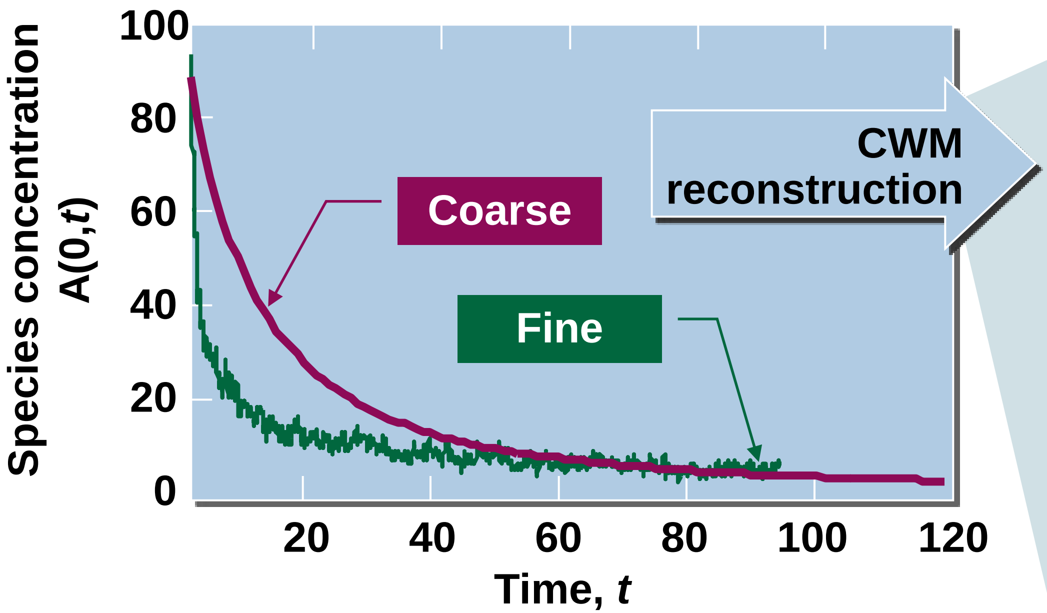


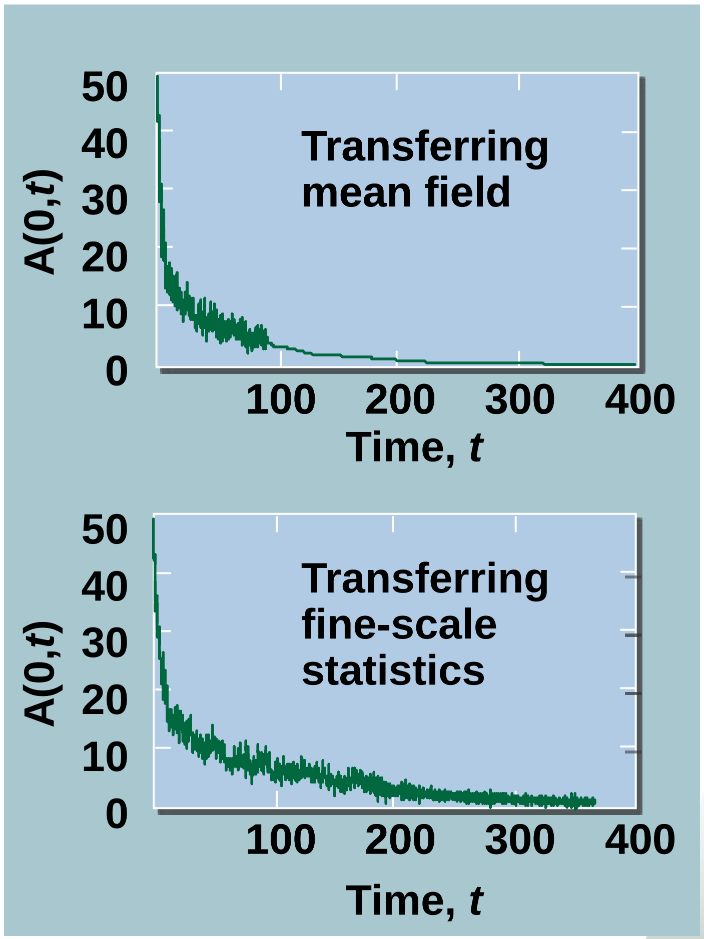
Figure adapted from Succi et al., *Computing in Science and Engineering*, **3(6)**, 26, 2001



Procedure: Perform upscaling and downscaling using CWM

Results from a prototype reaction diffusion problem



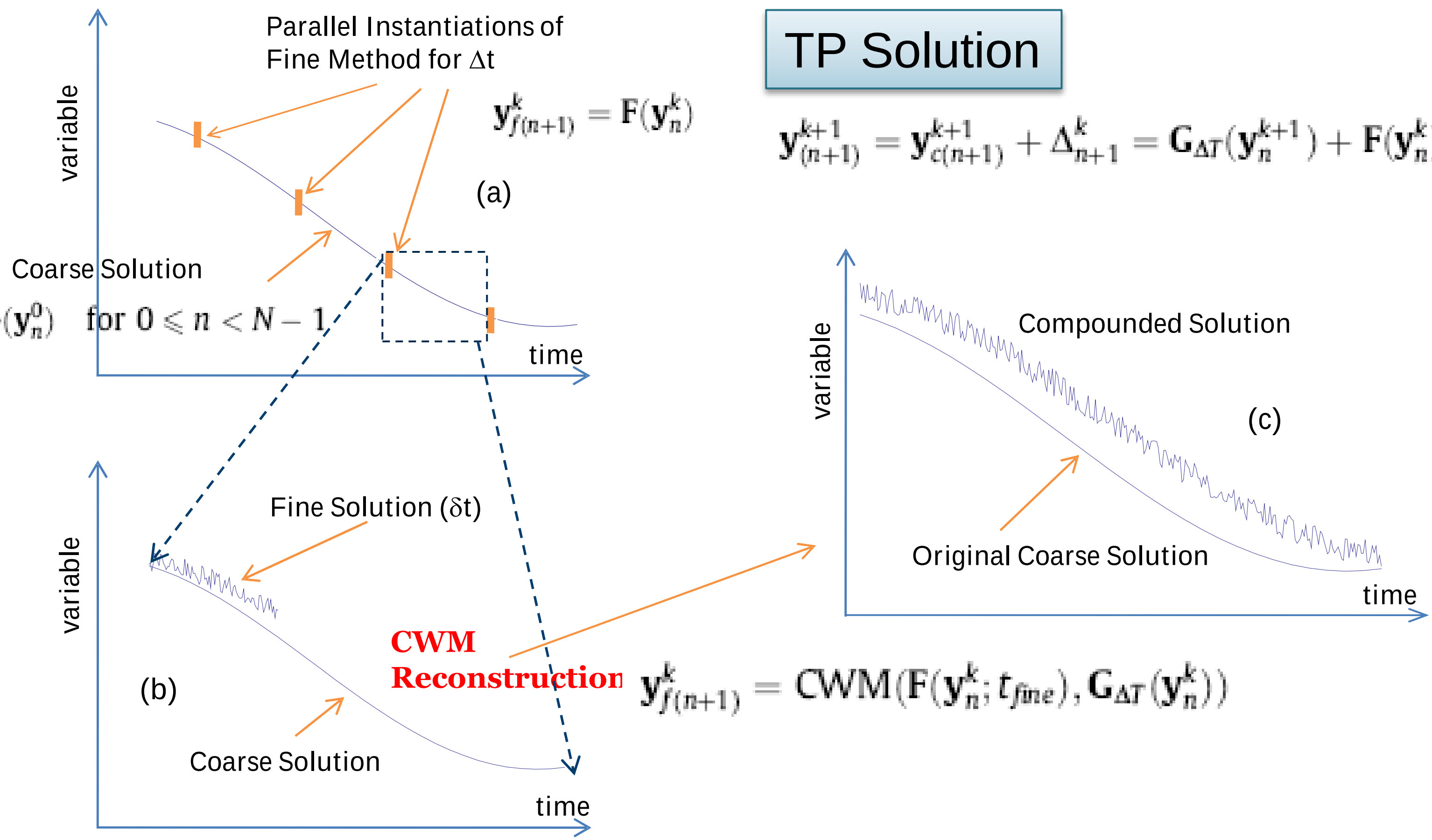


- Successfully applied CWM strategy for coupling reaction/diffusion system
- A unique way to bridge temporal and spatial scales for MSMP simulations

SP with Frantziskonis et al. (IJMCE, 2006 & 2008)
SP with Mishra et al. (IJCRE, 2008)

SP with Mishra et al. (LNCS, 2008)
SP with Muralidharan et al. (PRE, 2008)

tpCWM (Time Parallel CWM)



$$\mathbf{y}^{k}_{f(n+1)} = \mathbf{F}(\mathbf{y}^{k}_{n})$$

$$\mathbf{y}^{0}_{n+1} = \mathbf{G}_{\Delta T}(\mathbf{y}^{0}_{n}) \quad \text{for } 0 \leqslant n < N-1$$

$$\mathbf{y}^{k}_{f(n+1)} = \mathrm{CWM}(\mathbf{F}(\mathbf{y}^{k}_{n}; t_{fine}), \mathbf{G}_{\Delta T}(\mathbf{y}^{k}_{n}))$$

TP Solution

$$\mathbf{y}^{k+1}_{(n+1)} = \mathbf{y}^{k+1}_{c(n+1)} + \Delta^{k}_{n+1} = \mathbf{G}_{\Delta T}(\mathbf{y}^{k+1}_{n}) + \mathbf{F}(\mathbf{y}^{k}_{n}) - \mathbf{G}_{\Delta T}(\mathbf{y}^{k}_{n})$$

tpCWM Solution

$$\mathbf{y}^{k+1}_{(n+1)} = \mathbf{y}^{k+1}_{c(n+1)} + \Delta^{k}_{n+1} = \mathbf{G}_{\Delta T}(\mathbf{y}^{k+1}_{n}) + \mathrm{CWM}(\mathbf{F}(\mathbf{y}^{k}_{n}; t_{fine}), \mathbf{G}_{\Delta T}(\mathbf{y}^{k}_{n})) - \mathbf{G}_{\Delta T}(\mathbf{y}^{k}_{n})$$

tpCWM applied to Lotka-Volterra predator-prey equations

$$X + Y_1 \xrightarrow{\alpha} 2Y_1$$

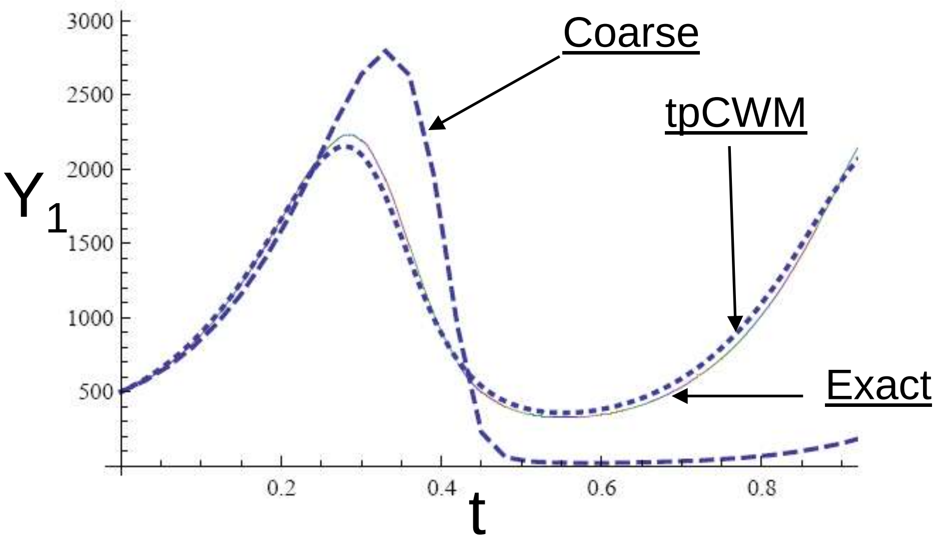
$$Y_1 + Y_2 \xrightarrow{\beta} 2Y_2$$

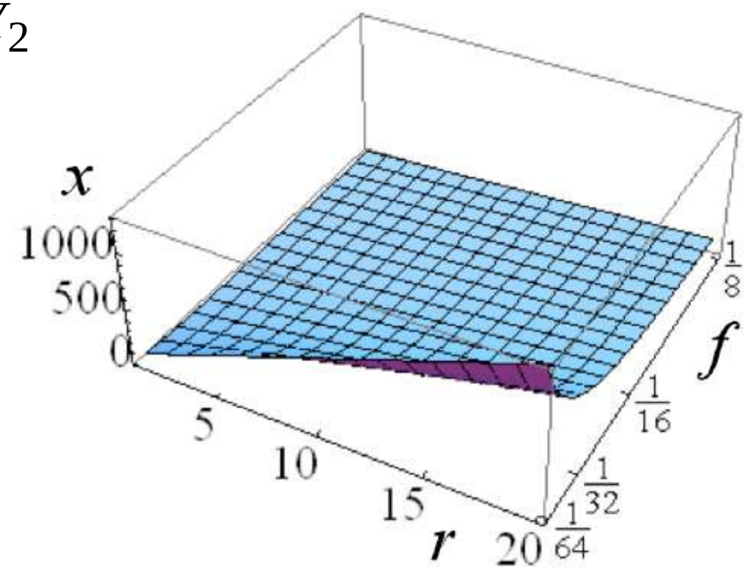
$$Y_2 \xrightarrow{\gamma} Z$$

$$\frac{dY_1}{dt} = \alpha X Y_1 - \beta Y_1 Y_2$$

$$\frac{dY_2}{dt} = \beta Y_1 Y_2 - \gamma Y_2$$

Lotka-Volterra System





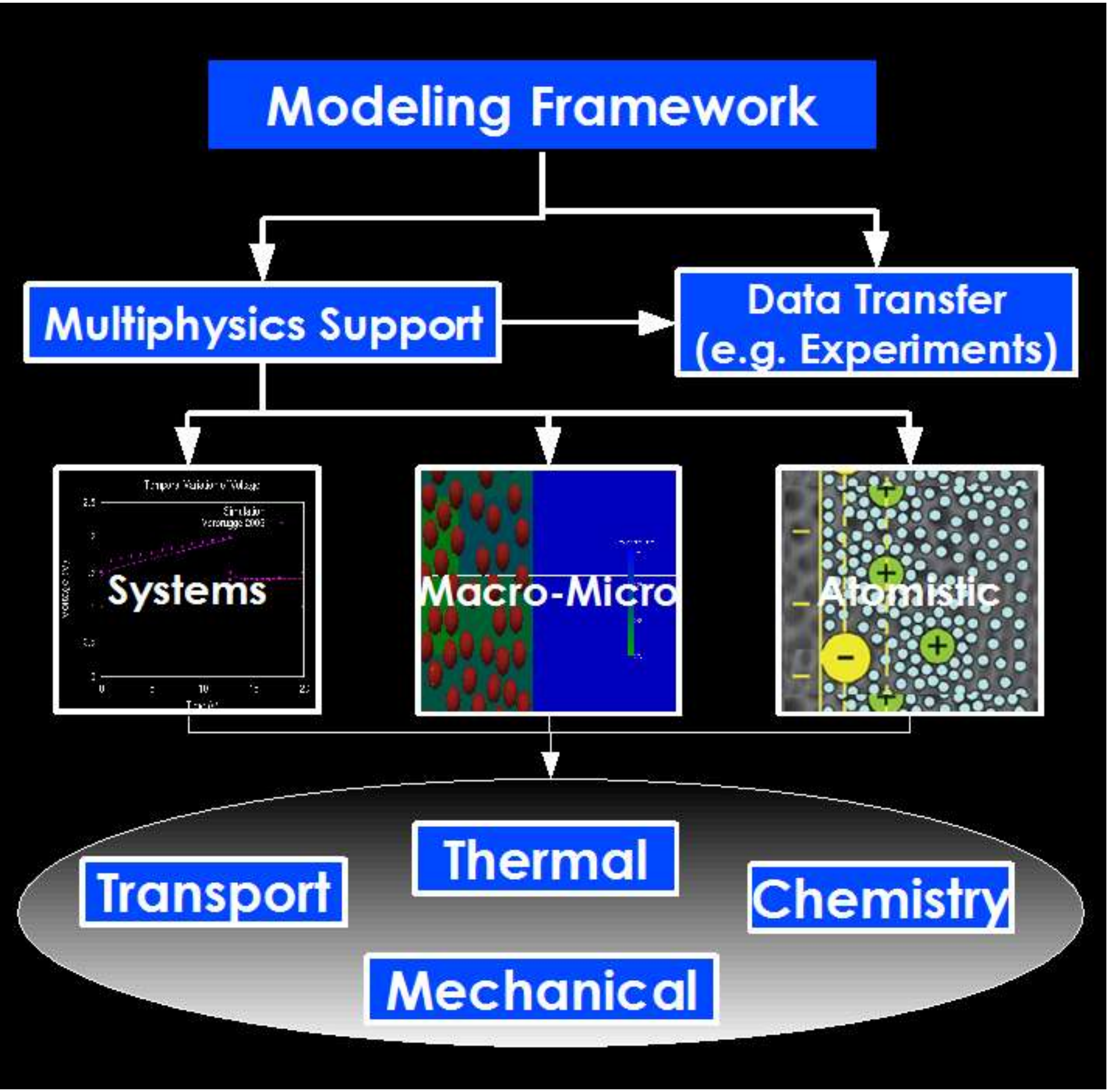
Factor of computational savings, X as a function of the ratio r (number of processors/number of iterations) and the fraction f (fraction of KMC time used in each assigned time interval).

Three orders of magnitude savings can be achieved by r in the range of 20 and f in the order of 1/64.

SP with Frantziskonis et al., Journal of Computational Physics, 2009.

OPPORTUNITIES AND CHALLENGES

General Simulation Framework



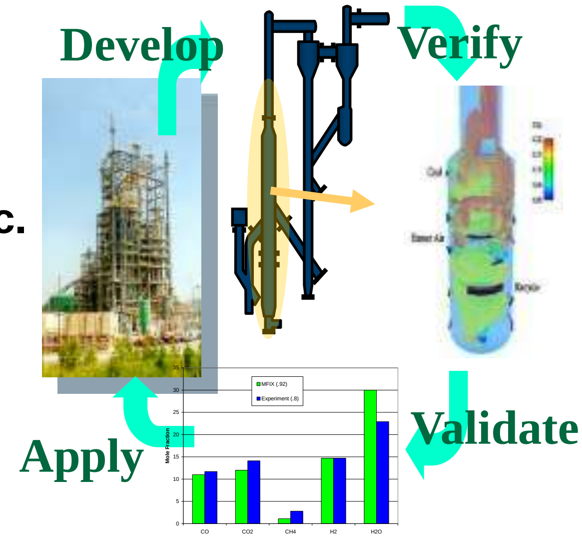
- Flexible and adaptive to handle various multi-physics codes operating at various scales in an hierarchical fashion
- Scalable from desktop to HPC platforms
- Automatic optimization based on the architecture
- Automatically chose optimal physical models and numerical methods to give the required accuracy with given resources
- Propagation of quantified uncertainties through models and across scales

Opportunities

- **Revolutionize the way simulation tools are used in the design process**
  - **Move away from the current edisonian approach**
  - **Design new industrial scale devices at a very short turn-around**
    - **Today depending on the system it can take 10-30 years from concept to lab-scale to pilot-scale to industrial-scale**
- **Develop new designs exploiting the efficient paths at the molecular scales**
  - **All reactions and processes happen at the atomic and molecular scales**
  - **Today the design process is totally decoupled – data is handed over from a group working at one scale to the other group at another scale in a sequential iterative process**
  - **Some designs are 5-6 decades old**
- **Develop feedback control systems to run devices in most optimal fashion**

Computational Science Challenges

- Bringing a broad set of researchers working on materials related processes together to get their buy-in
  - Different disciplines (applied math, CS, domain scientists)
  - Academia, Research labs, Industry
  - Agree on common codes, interfaces, data standards etc.
- The future architectures (with millions of cores and 100s of cores to a processor) are more conducive to locally coupled simulations
  - Many physical processes are globally coupled
  - Running multiple codes would need large and fast data movements across the processors/cores
    - Need to have smart algorithms to overlap communications and computations
  - The new twist is GPGPUs
- Validation and verification
  - Most validation is at steady state or subset of time-/space-trajectories
    - Very difficult to get all the data required to verify all the components of the simulations
    - Considerable investments need to be made in non-intrusive experimental techniques to obtain enough data
    - March towards the integration of “Theory, Experiment and Simulation”



Coal Gasification

Courtesy: Chris Guenther, NETL

Summary

- **Energy crisis is real and we need tomorrow's technology today**
- **Integrated experiments and simulations at scale can revolutionize the design of energy materials and devices**
  - **Include all relevant scales so that molecular scale interactions are included when designing device scale**
  - **Cut down the current 10-30 year design cycle**
  - **Break cultural barriers**
- **Develop computations based feedback control systems to run devices in most optimal fashion**
  - **Adjust for feedstock etc. online rather than offline adjustments with huge safety margins**
- **Simulation science can and *has to* play a catalytic and important role in bringing innovation to the energy market place**
  - **Reinvigorate the economic machine**

FORMULATION/SOLUTION FOR MULTIPHASE REACTING FLOWS

Objective of this section

- **Provide an introduction to multiphase flow modeling of gas-solids fluidized beds**
  - **Background information on fluidization**
  - **Overview of multiphase CFD: theory and numerics**
  - **Introduction to MFIX code**
    - **Code walk-through so that you can get familiar with the source – advantage of open-source code**
  - **Model validation**
  - **Fluidized bed reactors**
  - **Industrial application of multiphase CFD**

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- Introduction to Fluidization
  - Phenomena and Terminology
- Multiphase CFD
  - Introduction
  - Hydrodynamic Equations
  - Interphase Forces
  - Granular Stress
  - Gas-solids turbulence
  - Energy balance
  - Species balance
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Fluidization Phenomena

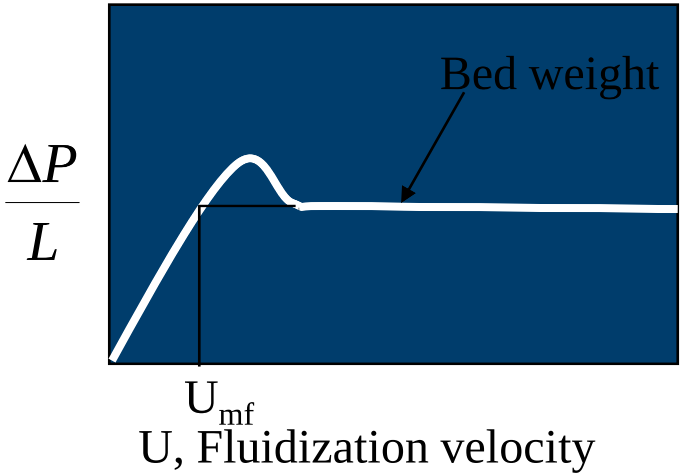
- **The pressure drop in a fluid flowing upward through a bed of solids supports the weight of the bed**

U_{mf} - minimum fluidization velocity

- **For $U > U_{mf}$ the bed behaves like a fluid:**
  - **lighter objects float,**
  - **solids material readily mix and circulate,**
  - **levels are equalized,**
  - **good gas-solids contacting**
  - **uniform temperature distribution**

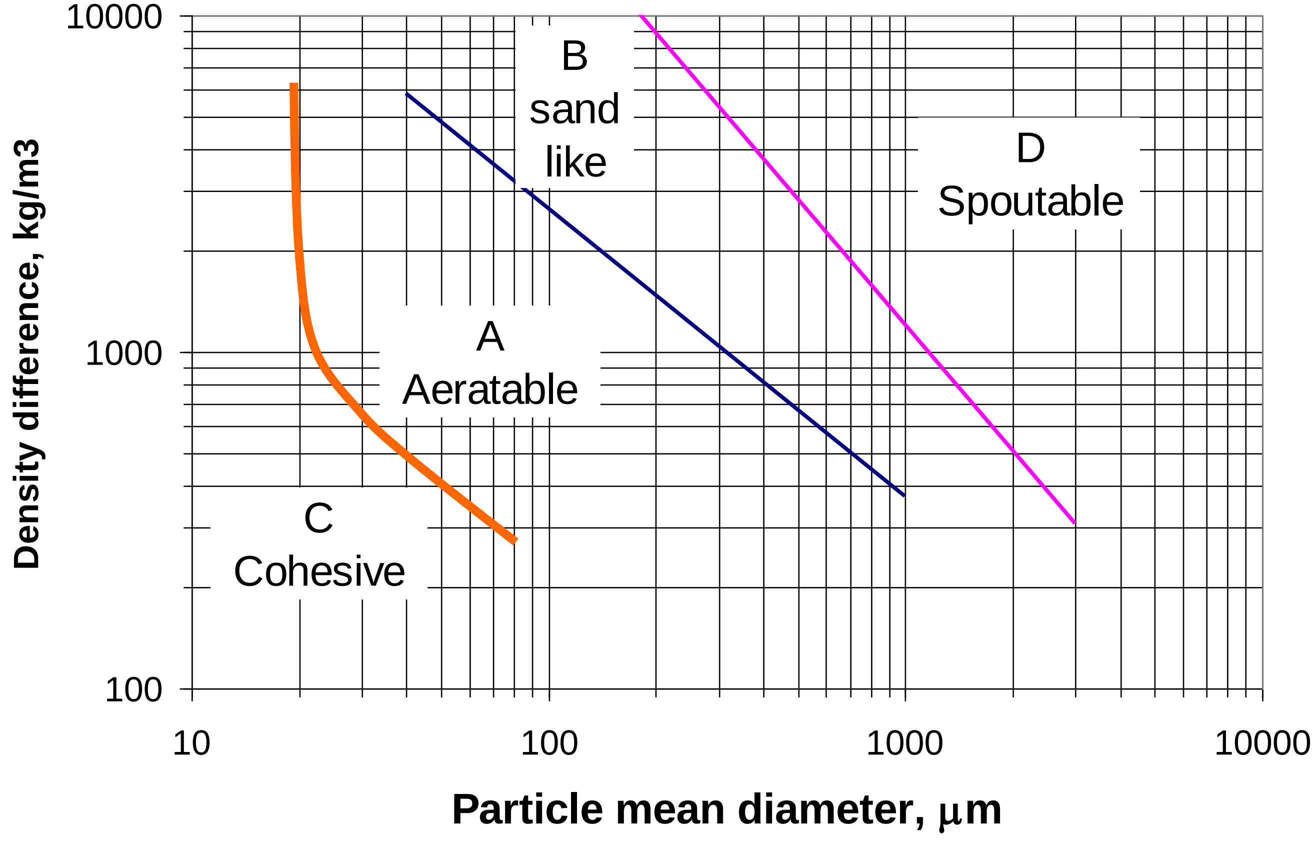
(Ideally suited for many gas-solids unit operations)

- **For $U < U_{mf}$ the bed is fixed (moving)**



Rhodes (2001)

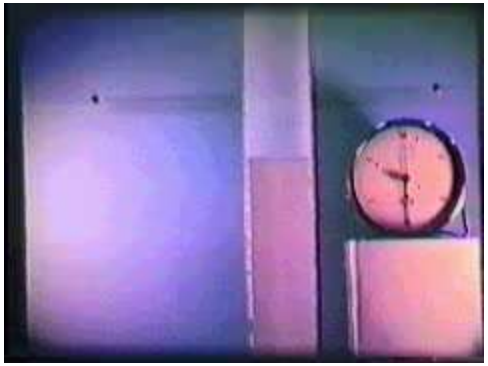
Geldart Particle Type Classification based on Fluidization Characteristics



Geldart (1986)

Group A (Aeratable)

- **Significant interparticle forces**
  van der Waals,
- **Bubble-free expansion $U_{mf} < U < U_{mb}$**
- **Bubbles when $U > U_{mb}$; attains maximum bubble size**
- **Slow deaeration upon defluidization**
- **High solids mixing, High gas backmixing**
- **FCC catalyst**
- **Limited success with CFD models**



Non-bubbling expansion powder as the gas velocity is gradually increased.

Collapse of a fluidized bed of Group A powder when the air supply is stopped: rapid drop in bed height as bubbles escape followed by a slow aeration.

Geldart (1986), Rhodes (2001)

Group A

- **“Slow” bubbles**

Bubble rise velocity < interstitial gas velocity

- **Through splitting and coalescence, bubbles achieve a maximum stable size, effectively independent of the gas velocity or vessel size.**

Rhodes (2001)

Group B (Sand-like)

- **Interparticle forces are negligible**
- **Bubbles when $U > U_{mf}$**

  $U_{mf} = U_{mb}$
- **Bubble size continues to grow as they rise … bubble size is limited only by the bed height**
- **Bubble rise velocity is usually greater than U and increases with height in bed (bubble size)**
- **Fast bed deaeration upon defluidization**
- **Moderate solids mixing and gas back mixing**

- **Glass beads, sand, table salt**
- **Good success with CFD models**

The bubble size continues to increase with distance from the distributor and with increasing gas velocity.

Geldart (1986), Rhodes (2001)

Group C (Cohesive)

- Large interparticle forces
  - cohesion
- No bubbles; channels and cracks
- Very low solids mixing and gas back mixing
- Powders: flour, cement, …

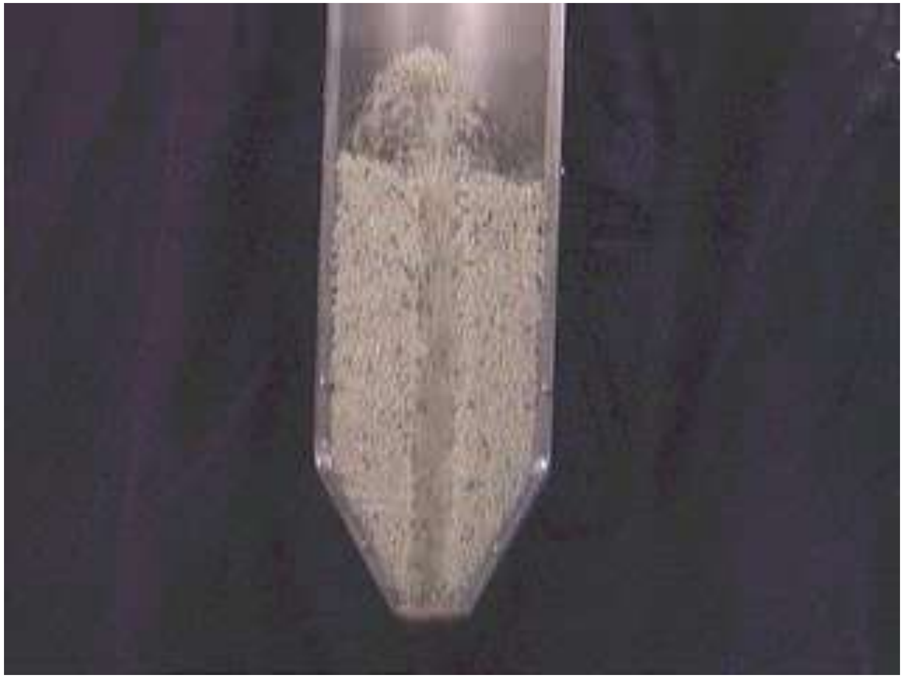
- No success with CFD models

An attempt to fluidize a Group C powder produces channels or a discrete plug

Geldart (1986), Rhodes (2001)

Group D (Spouting)

- Negligible interparticle forces
- Bubbles (spouts) when $U > U_{mf}$
- Bubble rise velocity less than U
- Able to produce deep spouting beds
- Fast bed deaeration upon defluidization
- Low solids mixing and gas back mixing
- Annular region is a moving bed
- Crushed limestone, grains, coffee beans, gravel
- Well describe by CFD simulations, for the limited studies done.



Spouted bed of rice

Geldart (1986), Rhodes (2001)

Fluidization Regimes

- **Bubbling:** Bubbles form in a bed with a distinct bed surface
- **Slugging:** Bubble diameter is equal to bed diameter
- **Spouted:** Bed with a central spout and a fountain of solids above
- **Turbulent:** Two different coexisting regions – a bottom dense, bubbling region below a dilute, dispersed flow region
- **Fast fluidization:** A relatively dense suspension flow with no distinct upper surface

- **Circulating: Upward gas-solids flow**
  - **Solids are circulated back through a cyclone and standpipe arrangement**
  - **low density: <5% solids fraction, low solids flux (< 200 $kg/m^2 \cdot s$**
  - **high density: 10-20% solids fraction, high solids flux ~400 $kg/m^2 \cdot s$**
- **Pneumatic conveying**
  - **Similar regimes as above**
  - **Solids are not recycled**

Fluidization terminology

- **Attrition**: breakdown of particles
- **Choking**: collapse of a dilute-phase suspension into a dense-phase flow as the gas velocity is reduced at constant solids flow
- **Distributor or Grid**: support plate at bottom which introduces the gas to the bottom of the bed and supports the weight of the bed when gas flow is shut down
- **Elutriation**: tendency for fine particles to be preferentially entrained from the reactor
- **Entrainment**: Removal of solids from bed by fluidizing gas
- **Freeboard**: region extending from top of bed surface to top of reactor vessel
- **Fines**: generally particles smaller than 37 µm in diameter (smallest regular sieve size)
- **Jetsam/Flotsam**: Solids that sink/float
- **Minimum fluidization velocity**: Superficial velocity at which bed weight equals pressure drop
- **Mixing**: Mixing of particles of different size and/or density
- **Saltation velocity**: minimum velocity for horizontal gas-solids flow
- **Segregation**: tendency for particles to gather in different zones according to their size and/or density
- **Transport disengagement zone**: region in freeboard beginning at bed surface in which particle flux decreases with height and above which the entrainment is independent of height

Fluidization Devices/Applications

- **Bin/Hopper - solids storage**
- **Chutes - solids transfer**
- **Cyclones - solids separation**
- **Downer (column where particles fall under gravity, assisted by co-current gas flow)**
- **Nonmechanical valves (L-, N-, ..) - solids transfer (*e.g.*, from a standpipe to the riser)**
- **Risers – solids are carried upwards by the gas, with no distinct bed surface**
- **Stand-pipes – moving beds for returning solids down-flow while matching the pressure drop in the riser**

Industrial Applications – 1

- **Solid-Catalysed Gas-Phase Reactions:**
  - **Fluid catalytic cracking, reforming**
  - **Phthalic and maleic anhydride**
  - **Acrylonitrile and aniline**
  - **Chlorination and bromination of hydrocarbons**
  - **Polyethylene and polypropylene**
  - **Oxidation of SO_2 to SO_3**
- **Gas-Solid Reactions:**
  - **Gasification of coal, biomass**
  - **CO_2 Absorbers**
  - **Transport desulfurizer**
  - **Chemical looping process**
  - **Combustion/incineration**
  - **Roasting of ores, *e.g.,* ZnS, Cu_2S, nickel sulphides**
  - **Pyrolysis/carbonization**
  - **Calcination *e.g.,* limestone, phosphates, $Al(OH)_3$**
  - **Uranium oxide fluorination**
  - **Fluid coking**
  - **Reduction of iron oxide**
  - **Catalyst regeneration**

Kunii and Levenspiel (1977)

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Industrial Applications – 2

- Gas-Phase Non-Catalytic Reactions:
  - Natural gas combustion
- Gas-Liquid-Solid:
  - Fischer-Tropsch synthesis
  - Hydrotreating, hydroprocessing
  - Biochemical processes
- Physical Processes:
  - Drying of particles
  - Coating of surfaces
  - Granulation (growing particles)
  - Heat treatment (e.g. annealing, quenching)
  - Medical beds
  - Filtration
  - Back-purging of filters
  - Blending
  - Classification

Kunii and Levenspiel (1977)

Advantages of Fluidized Beds

- **The smooth, liquid-like flow of particles allows continuous automatically controlled operations with ease of handling.**
- **The rapid mixing of solids leads to nearly isothermal conditions throughout the reactor, hence the operation can be controlled simply and reliably.**
- **Suited to large-scale operations.**
- **The circulation of solids between two fluidized beds makes it possible to transport the vast quantities of heat produced or needed in large reactors.**
- **Heat and mass transfer rates between gas and particles are high when compared with other modes of contacting.**
- **The rate of heat transfer between a fluidized bed and an immersed object is high, hence heat exchangers within fluidized beds require relatively small surface areas.**

Kunii and Levenspiel (1977)

Disadvantages of Fluidized Beds

- **Rapid mixing of solids leads to nonuniform solids residence times.**
- **Friable solids are pulverized and entrained by the gas.**
- **Erosion of pipes and vessels from abrasion by particles.**
- **Agglomeration and sintering of fine particles.**
- **Difficult-to-describe flow of gas and solids.**
- **Difficult to scale up[6,7]. For example,**
  - **Fischer–Tropsch: Pilot-scale reactors (12, 25, 50 and 195 mm diameter) gave conversions > 95%. The conversion dropped to 40–50% in a 5 m diameter industrial reactor[2].**
  - **The Shell Chlorination Process: To get 90% yield 50-mm-diameter reactor required 1.5-m-depth, 300-mm-diameter, 2.8 m depth and 3-m-diameter, 10 m depth[3,4,5].**

1. Kunii and Levenspiel (1977), 2. Geldart (1967), 3. de Vries et al., 1972), 4. Werther (1980) 5. Wen (1984), 6. Constantineau et al. (2007), 7. Knowlton et al. (2005)

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Modeling Approaches – 1

- Phenomenological models
  - Empirical correlations
  - Two-phase (bubble/emulsion), (e.g., Davidson Model, Kunii-Levenspiel) Model
  - Applicable only over a limited parameter range
  - Do not give new process insights
- Discrete phase model (DPM)
  - Particle motion is tracked in a Lagrangian frame of reference
  - Model heat and mass transfer
  - Calculate steady state from a large number of trajectories
  - Disregards volume occupied by the particles
  - Disregards particle interactions
  - Applicable only to low solids volume fraction (<1%) and low solids to gas mass flow ratio (<1)

Modeling Approaches – 2

- Discrete Element Model (DEM) – 1
  - Track <u>interacting</u> particle motion by solving Newton's laws of motion (linear and angular momentum conservation) for all particles, simultaneously.
  - Considers all forces on the particles
    - Gas-solids drag; friction between particles in contact; inelastic collisions; gravity; cohesion between particles; adhesion to wall; liquid bridging; electrostatic attraction or repulsion, van der Waals force
  - Considers the volume occupied by the particles
  - Soft-sphere method: time-step driven, allows particle over-lap, requires modeling of inter-particle forces, allows multiple particle contacts, one method available in MFIX
  - Hard-sphere method: event-driven, only binary collisions

Modeling Approaches – 3

- Discrete Element Model (DEM) – 2
  - Advantages
    - Constitutive laws for particle interaction are known
    - "Gold standard": simulation results can be used validate continuum models
    - Gives information beyond the reach of experiments, *e.g.*, force networks formed in a granular media
    - No numerical diffusion
  - Disadvantages
    - Computational effort for industrial reactors is too large
      - e.g., Paul Cleary predicted that by 2017 DEM will be able to handle 1 billion particles with realistic 3D geometry[1]. Compare that with ~100 billion, 100 μm particles in 1 m^3 reactor at 5% solids volume fraction.
    - Modeling of non-spherical particles not yet well developed
    - Fluid-solids interphase forces need to be modeled

1. Tuzun and Cleary (2006)

Modeling Approaches – 4

- **Lattice-Boltzmann Method (LBM) -** discrete computational method based upon the Boltzmann equation
  - **Fluid-particle distributions "live" on lattice nodes**
  - **At each time step the fluid-particles "move" according ot rules and can they "collide" with each other**
  - **The collision rules are designed such that the time-averaged motion of the LB fluid-particles is consistent with the Navier-Stokes equation.**
  - **Suitable for implementing complex boundary conditions**
  - **Easy to parallelize computations**
  - **Has been used for gas-solids drag calculations[1,2]**

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1. Hill et al. (2001), 2. Van der Hoef et al. (2005)

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Modeling Approaches – 5

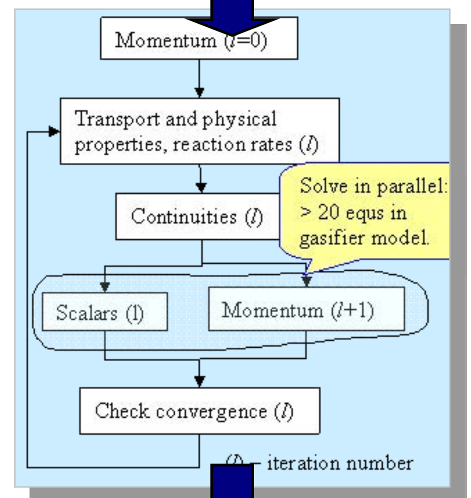
- **Multiphase Particle-in-Cell (MP-PIC)[1]**
  - **Continuum fluid phase and discrete particles**
  - **Difficulties with interparticle interactions eliminated by mapping particle properties to an Eulerian grid and then mapping back computed stress tensors to particle positions**
  - **Allows for distributions of types, sizes, and density of particles**
  - **No numerical diffusion from the Lagrangian particle calculations.**
- **Interpenetrating Continuum, Two-fluid, or Eulerian-Eulerian Model**
  - **Rest of this presentation**

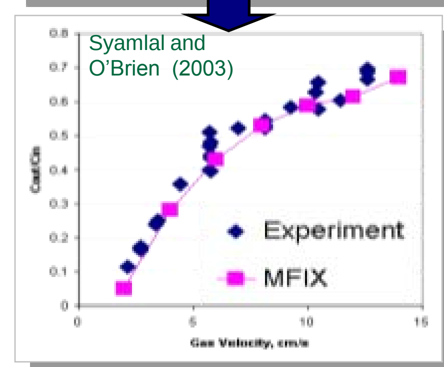
1. Snider (2001)

Steps in multiphase continuum model development

- **Theory development**: drag relations, granular stress, chemistry models …
- **Numerics development**: solvers, HR schemes, hybrid DECM, explicit schemes, parallelization, …
- **Computational Software development**
- **Validation studies**: bubbling, circulating, and spouted beds, gas-solids jets, …
- **Applications**: Coal gasification and combustion, SiH_4 Pyrolysis, polyethylene, volcanology, nuclear fuel particle coating, …
- **Reduced Order Model:** Fast models based on high fidelity models
- **Advanced Process Simulation:** APECS - integration of high fidelity models into a common framework.

$$\frac{\partial}{\partial t}(\varepsilon_m \rho_m) + \nabla \cdot (\varepsilon_m \rho_m \vec{v}_m) = \sum_{n=1}^{N_m} R_{mn}$$





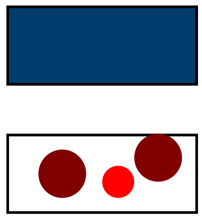
From physics formulation, to solution algorithm development, to validation.

Continuum Modeling of Gas-solids Flows

- **Two Phases**

Fluid

Solids

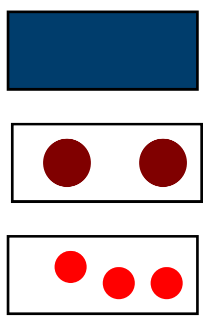


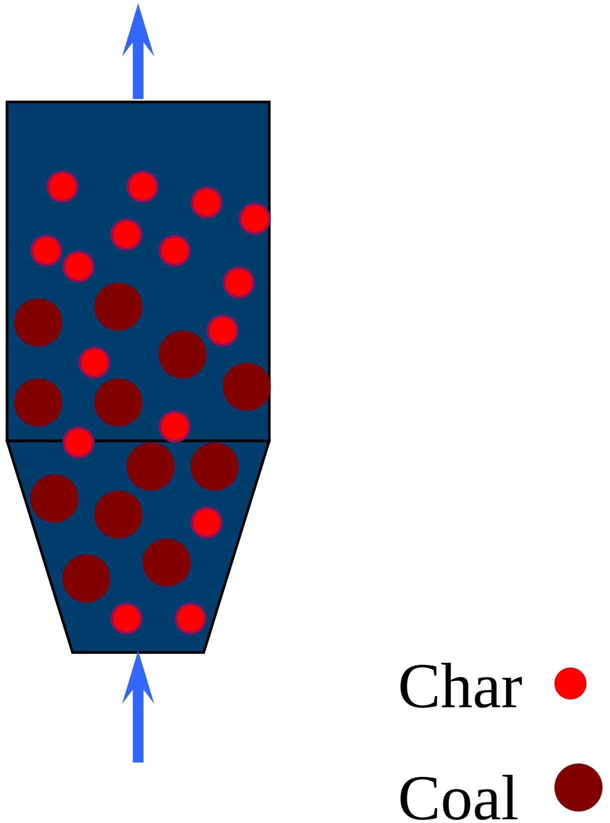
- **Three phases**

Fluid

Solids - 1

Solids - 2





Formulation of Continuum Equations

- Average out details of flow field around particles and individual particle collisions
- "Derive" balance equations by averaging local, instantaneous behavior:
  - Space, time, or ensemble averaging[1,2,3,4,5]
  - Mixture theory[6]
- Account for the information lost due to averaging through constitutive relations, which specify how the phases behave and interact with each other

1. Drew and Lahey (1993); 2. Anderson and Jackson (1967), 3. Drew and Segel (1971), 4. Ishii (1975), 5. Joseph and Lundgren (1990), 6. Bowen (1976)

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Nomenclature

$\varepsilon_m(x,t)$	Volume fraction of phase m: gas, solid, liquid, ….
ρ_m	Density of species of phase m
$\vec{V}_m$	Velocity of phase m
R_{ml}	Reaction rate of species ℓ of phase m
$\bar{\bar{S}}_m$	Stress tensor of phase m
$\vec{I}_{ml}$	Interaction between phase m and phase ℓ

Continuity Equation

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

$$\sum_{m=1}^{N} \varepsilon_m = 1$$

index.html

solve_continuity_8f.html

Momentum Equation

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

Interaction within the phase → stresses

–collisions, sliding or rolling friction

–electrostatic, van der Waals, capillary

solve_vel_star_8f.html

Momentum Equation

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

Interaction between phases → interphase forces

Momentum Equation

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

Interactions with rest of the universe → body forces

Constitutive Relations

Obtained from …

- **Microscopic description of the material behavior of interest**
  - **e.g., kinetic theory[1,2] → granular stresses**
- **Experimental information**
  - **e.g., Ergun equation [2] → fluid-particle drag**
- **Analogy**
  - **e.g., k-ε equation for granular phase turbulence[3]**
- **All of the above**

1. Sinclair and Jackson (1989); 2. Gidaspow (1994 p. 35); 3. Dasgupta et al. (1994)

Restrictions on the Allowable Forms of Constitutive Relations – 1

- **Coordinate invariance**: equations must be written in tensor form
- **Objectivity or material-frame-indifference**: Material behavior must not dependent upon the frame of reference or observer
- **Well-posedness**: solution exists and depends continuously on initial and boundary conditions
- **Second-law:** Places restrictions on the values of the coefficients
  - **e.g., drag coefficient, as it appears in MFIX manual, must have positive values**

Truesdell and Toupin (1960), Bowen (1976), Johnson et al. (1990), Drew and Lahey (1993)

Restrictions on the Allowable Forms of Constitutive Relations – 2

- **Correct low concentration limits:**

  e.g., the mixture behaves like the fluid and the granular phase behaves like isolated particles when $(1-\varepsilon) \rightarrow 0$

- **Self consistency of multiphase equations**: When a solids phase is arbitrarily described as multiple phases the relations for multiple phases must add up to the single phase relation.[1,2]
  - **thus, in a multiparticle system the gas-solids drag must be a <u>linear</u> function of ε_m**

1. Syamlal (1985), 2. Syamlal and O'Brien (1988), 3. Drew and Lahey (1993)

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- Industrial application of multiphase CFD

Dimensionless Numbers

- **Froude number:** inertial/gravitational

$$Fr = \frac{V_g}{\sqrt{g d_p}}$$

- **Particle Reynolds number:** inertial/viscous

$$Re = \frac{d_p \; V_g \; \rho_g}{\mu_g}$$

- **Archimedes number:** (Galileo number) gravitational/viscous

$$Ar = \frac{d_p^3 \, \rho_g \, (\rho_s - \rho_g) \, g}{\mu_g^2}$$

- **Stokes number:** particle relaxation/ flow time scales

$$St = \frac{d_p \; V_g \; \rho_s}{\mu_g}$$

- **Bagnold number:** grain inertia/viscous

$$Ba = \frac{\rho_g d_p^2 \sqrt{\lambda} \; \gamma}{\mu_g}, \; \lambda = \frac{1}{1 - \left(\frac{\varepsilon_s}{\varepsilon_{s\max}} \right)^{1/3}}$$

Interphase Forces – 1

- **Action – Reaction: sum of interphase momentum transfer terms vanish**

$$\sum_{m}^{M}\sum_{l}^{M}\vec{I}_{ml}=0$$

- e.g., in two-phase flow

$$\vec{I}_{fp}=-\vec{I}_{pf}$$

Interphase Forces – 2

- **Based on forces in single particle motion, corrected for effects such as**
  - **Nearness of other particles in a cloud**
  - **Particle size distribution**
  - **Fine particle clustering**
  - **Particle shape, finite-size effects, wakes, and turning couples on long bodies[1]**
  - **Heat and mass transfer effects**

1. Joseph (1993)

Interphase Forces – 3

- **Fluid-particle forces: caused by relative motion between fluid and particles**
  - Drag
  - Buoyancy
  - Virtual mass force
  - Lift force
  - Magnus force
  - Basset force
  - Faxen force
- **Particle-particle drag: caused by relative motion between two particulate phases**

Drag

- Single particle:

$$\vec{I}_{fp} = \frac{3}{4}\frac{\mu_f}{d_p^2} C_d \operatorname{Re}\left(\left|\vec{u}_f - \vec{u}_p\right|\right)$$

- Granular phase:

$$\vec{I}_{fp} = \varepsilon_f \varepsilon_p \frac{3}{4}\frac{\mu_f}{d_p^2} C_d \operatorname{Re}\left(\left|\vec{u}_f - \vec{u}_p\right|\right)$$

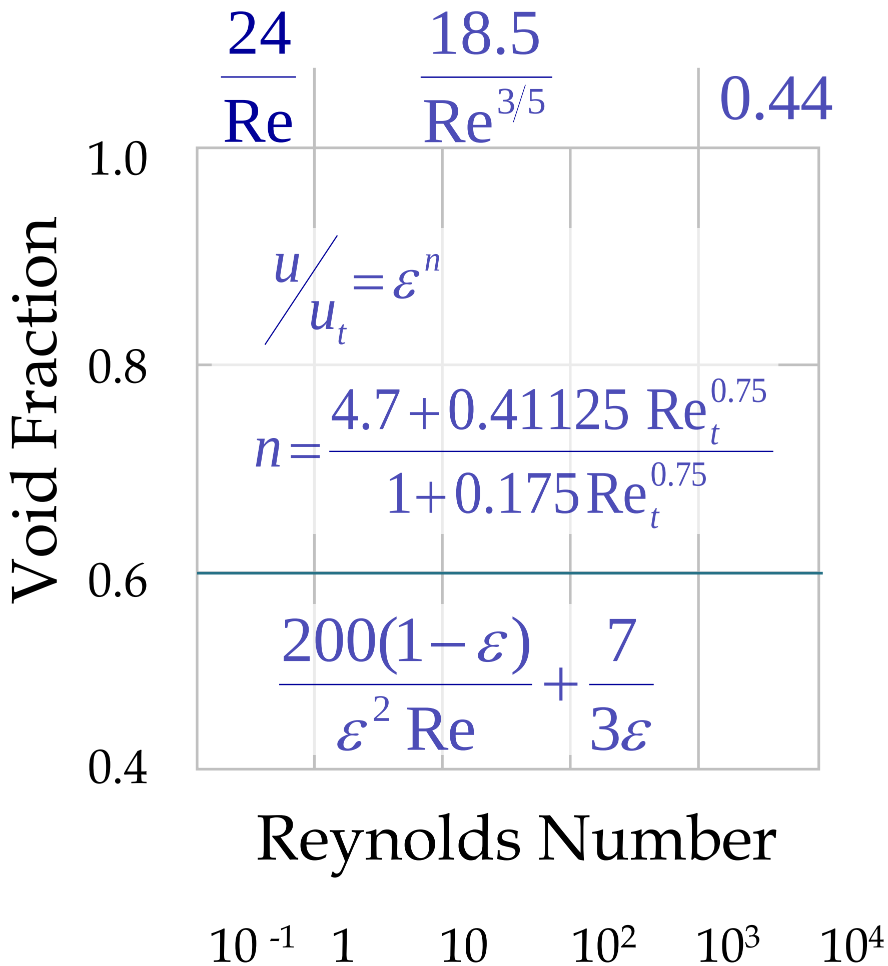
The most important force term in gas-solids flow!

Drew and Lahey (1993)

Single particle drag

- **Chart and formulas for sphere**
- **Changes with respect to sphericity**
- **Particle size distribution**
  - **Different distributions**
  - **Effect of different means**

Drag: Data Available



Single sphere drag[1]

$$C_{ds} = \left(0.63 + \frac{4.8}{\sqrt{Re}}\right)^2$$

Particle settling data : Richardson-Zaki eq[2,3]

Packed bed pressure drop -- Ergun eq[4]

1. Dalla Valle (1948); 2. Richardson & Zaki (1954); 3. Rowe (1987); 4. Ergun (1952)

Drag: Gidaspow

- **For ε < 0.8 use Ergun eq**

$$C_d = \frac{200(1-\varepsilon)}{\varepsilon^2 \mathrm{Re}} + \frac{7}{3\varepsilon}$$

$$Re = \frac{d_p \left| V_g - V_s \right| \rho_g}{\mu_g}$$

- **To get correct dependence on Re as ε → 1 switch to Wen and Yu eq. for ε > 0.8**

$$C_d = \begin{cases} \frac{24}{\varepsilon \mathrm{Re}} \left(1 + 0.15(\varepsilon \mathrm{Re})^{0.687}\right) \varepsilon^{-2.65} & (\varepsilon \mathrm{Re}) < 1000 \\ 0.44 \varepsilon^{-2.65} & (\varepsilon \mathrm{Re}) \geq 1000 \end{cases}$$

calc_drag_8f.html

drag_gs_8f.html

Wen and Yu (1966), Gidaspow (1994, p.35)

Drag: Syamlal-O'Brien

- C_d from a Richardson and Zaki correlation

$$C_d = \left(\frac{0.63}{V_r} + \frac{4.8}{\sqrt{V_r \mathrm{Re}}} \right)^2$$

$$V_r = 0.5\left(A - 0.06\mathrm{Re} + \sqrt{0.0036\mathrm{Re}^2 + 0.12\mathrm{Re}(2B - A) + A^2} \right)$$

$$A = \varepsilon^{4.14}$$

$$B = \begin{cases} 0.8\varepsilon^{1.28} & \varepsilon \le 0.85 \\ \varepsilon^{2.65} & \varepsilon > 0.85 \end{cases}$$

Syamlal, Rogers, O'Brien (1993), p.10

Drag: Others

- **Foscolo et al. (1983) -- based on Ergun eq.**

$$C_d = \left(\frac{23.07}{\varepsilon \mathrm{Re}} + 0.448 \right) \varepsilon^{-2.8}$$

- **Gibilaro et al. (1985) -- based on Richardson-Zaki eq.**

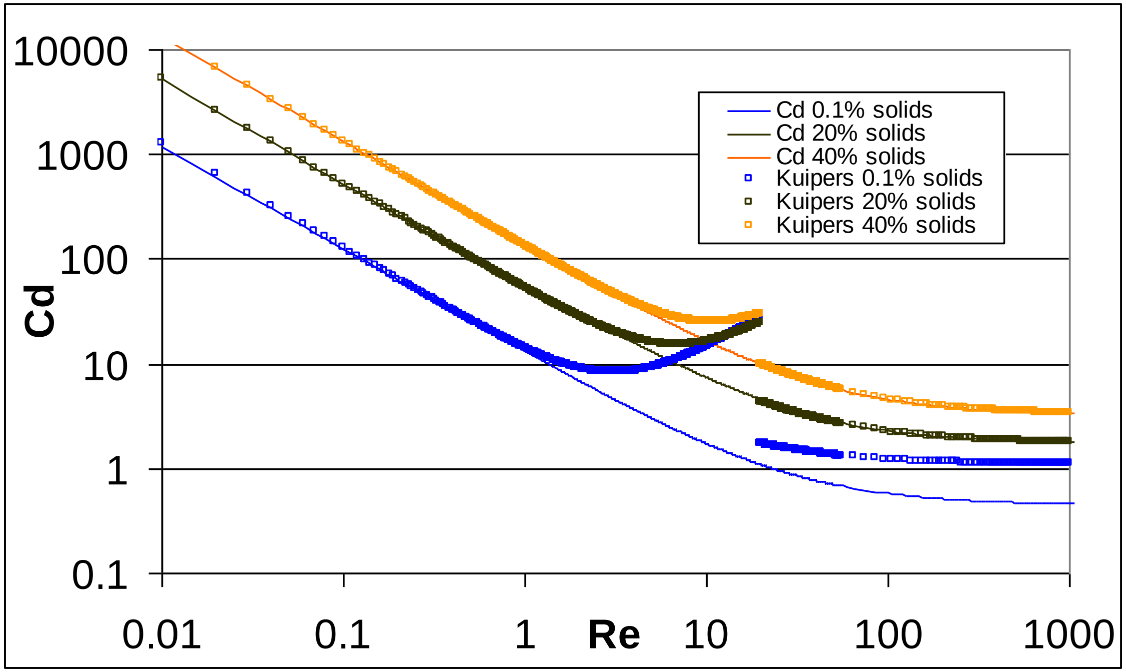
$$C_d = C_{ds}(\mathrm{Re}_t) \left(\frac{\varepsilon \, | u_f - u_p |}{U_t} \right)^{\frac{4.8-2n}{n}} \varepsilon^{-3.8}$$

Drag: From LBM Simulations

- **Extension of Hill et al. (2001) drag correlation**
  - **Range of validity:**
    - **Solids volume fraction: 0.1 to packing (needs fitting at several solids volume fractions because of switches in formulas)**
    - **Re > 20 and Re << 1**
  - **Fitting the different formulas in all regions of the Re-ε space**
  - **Extended these drag formulas to known limits at high and low Re number**
  - **Corrected a common misrepresentation of this drag law[2]**
  - **Published these findings in Powder Tech[3]**

1. Hill, Koch and Ladd (2001), 2. Bokkers et al. (2004), 3. Benyahia et al. (2006)

Extension of Koch and Hill drag correlations based on LBM data



Comparison of our modified Koch and Hill correlation with that previously published[2] in the literature

Benyahia, Syamlal, and O'Brien, (2006)

Drag: Mean particle diameter

- d_p – diameter of a sphere with the same surface area to volume ratio
- d_v – diameter of a sphere having the same volume; measured with Coulter counter (< 75 μm)
- $d_{sieve\text{-}size}$ – measured by sieving (>75 μm)
- For spherical particles

$$d_p = d_v = d_{sieve\text{-}size}$$

- For non-spherical particles

$$d_p \approx 0.87\, d_{sieve\text{-}size}$$

$$d_p \approx 0.773\, d_v$$

Geldart (1986)

Drag: Mean particle diameter

- **Sphericity (d_p/d_v) is used to account for the effect of particle shape**

	Sphericity
Round sand	.8 - .9
Salt	.84
Crushed coal	.75
Crushed glass	.65
Mica flakes	.28

Geldart (1986)

Accounting for Size distribution

- **Inertia dominated regime, Re > 2000 (CD ~ constant): Sauter mean diameter (D_{32})**

$$\left(D_{ij}\right)^{i-j} = \frac{\int_0^\infty f(D) D^i dD}{\int_0^\infty f(D) D^j dD}$$

- **Creeping flow regime, Re << 1 (CD ~ 1/Re): Volume-width mean diameter (D_{31})**

- **At intermediate Re: (D_{3j}), where j is given by an empirical formula (Loth et al. 2004)**

$$D_{32} = \frac{1}{\sum x_i / d_{pi}}$$

Loth et al. (2004)

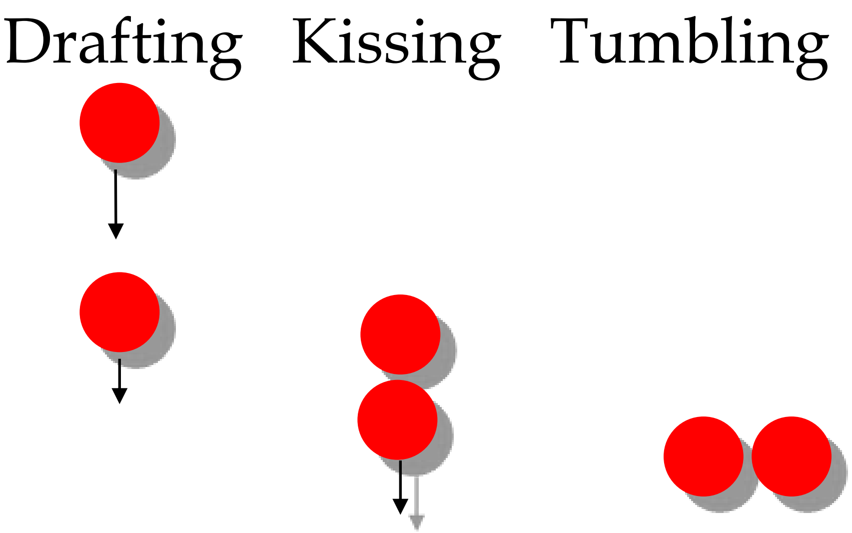
Effective Particle Size in the Bed

- **In a CFB the average size may depend upon other factors:**
  - **the average size in the riser will be larger than the average size based on the feed because of powder classification**
  - **in fine particle fluidization (Geldart A) the effective particle size is larger because of particle clustering[1]**

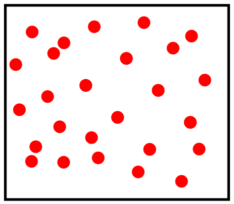
1. O'Brien and Syamlal (1993)

Particle Clustering

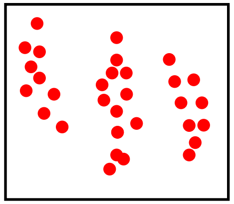
– **wake effects[1] and interparticle forces cause aggregation and modify drag**



Idealized



Actual ?



1. Joseph (1993); also see O'Brien and Syamlal (1993)

Which drag formula to use?

- For a comparison of drag correlations see, for example, Enwald et al. (1996)
- Any of standard drag correlation will suffice, but ...
  - Ensure that the U_{mf} is correctly predicted
  - Ensure that the terminal velocity is correctly predicted
  - May need to adjust ε_{mf} and d_p
  - May use the calibration method of Syamlal and O'Brien (2003)

Buoyancy

- **Force exerted on particles by the ‘undistorted’ fluid pressure field**
- **In steady rectilinear flows this reduces to Archimedean buoyancy**
- **Modeled as a pressure drop (Model A) or as a modified body force (Model B).**

$$\vec{F} = \int \vec{f}\, dS = \int (p\vec{n} + \vec{t})\, dS$$

$$p = p_h + p_r$$

$$\vec{F} = \int p_h \vec{n}\, dS \quad buoyancy$$

$$+ \int p_r \vec{n}\, dS \quad form drag$$

$$+ \int \vec{t}\, dS \quad skin drag$$

Astarita (1993), Drew and Lahey (1993)

Buoyancy

Model A:

$$\varepsilon_f \rho_f \vec{u}_f \frac{d\vec{u}_f}{dt_f} = -\varepsilon_f \nabla p_f + F_{fp}(\vec{u}_p - \vec{u}_f) + \varepsilon_f \rho_f \vec{g}$$

$$\varepsilon_p \rho_p \vec{u}_p \frac{d\vec{u}_p}{dt_p} = -\varepsilon_p \nabla p_f + F_{fp}(\vec{u}_f - \vec{u}_p) + \varepsilon_p \rho_p \vec{g}$$

Gidaspow (1994, p. 37)

Buoyancy

Model A:

$$\varepsilon_f \rho_f \vec{u}_f \frac{d\vec{u}_f}{dt_f} = -\varepsilon_f \nabla p_f + F_{fp}(\vec{u}_p - \vec{u}_f) + \varepsilon_f \rho_f \vec{g}$$

$$\varepsilon_p \rho_p \vec{u}_p \frac{d\vec{u}_p}{dt_p} = -\varepsilon_p \nabla p_f + F_{fp}(\vec{u}_f - \vec{u}_p) + \varepsilon_p \rho_p \vec{g}$$

Model B:

$$\varepsilon_f \rho_f \vec{u}_f \frac{d\vec{u}_f}{dt_f} = -\nabla p_f + \frac{F_{fp}}{\varepsilon_f}(\vec{u}_p - \vec{u}_f) + \varepsilon_f \rho_f \vec{g}$$

$$\varepsilon_p \rho_p \vec{u}_p \frac{d\vec{u}_s}{dt_p} = \frac{F_{fp}}{\varepsilon_f}(\vec{u}_f - \vec{u}_p) + \varepsilon_p (\rho_p - \rho_f)\vec{g}$$

Gidaspow (1994, p. 37)

Buoyancy

- **Model A**
  - full description of buoyancy
  - 1-D model has imaginary characteristics; leads to ill-posed initial value problem[1]
- **Model B**
  - describes only Archimedean buoyancy; e.g., doesn't describe buoyancy in rotating flow
  - 1-D model leads to well-posed problem[2]

1. Gidaspow (1994 p. 191); 2. p.134; Also see Enwald et al. (1996)

Virtual Mass

- **Caused by relative acceleration between phases**

- Single particle:

$$\frac{1}{2}\rho_f \frac{d\vec{u}_p}{dt}$$

- Granular phase:

$$\vec{I}_{fp} = C_{vm}\varepsilon_p \rho_f \left[\left(\frac{\partial \vec{u}_f}{\partial t} + \vec{u}_f \cdot \nabla \vec{u}_f \right) - \left(\frac{\partial \vec{u}_p}{\partial t} + \vec{u}_p \cdot \nabla \vec{u}_p \right) \right]$$

Johnson et al. (1990), Drew and Lahey (1993)

Lift Force

- **transverse force on a particle moving through shearing fluid**

- Single sphere $$\frac{3.08}{d_p}\sqrt{\mu_f \rho_f \left|\frac{du_f}{dy}\right|}(u_p - u_f)$$

- Granular phase

$$\vec{I}_{fp} = -C_L \varepsilon_p \rho_f (\vec{u}_f - \vec{u}_p) \times \left(\nabla \times \vec{u}_f\right)$$

- Objectivity requires that $C_{vm} = C_L$

Drew and Lahey (1993)

Other Interphase Forces

- **Magnus force: caused by particle spin**

$$\frac{3}{4}\rho_f \vec{\Omega}_p \times \vec{u}_f$$

$$\vec{\Omega}_p \approx \frac{1}{2}\nabla \times \vec{u}_p$$

- **Basset Force: history of particle motion**

$$\frac{-9\rho_f}{d_p}\sqrt{\frac{\mu_f}{\pi\rho_f}}\int_{t_0}^{t}\frac{1}{\sqrt{(t-t')}}\frac{d}{dt'}(u_p - u_f)dt'$$

Johnson et al. (1990)

Other Interphase Forces

- **Faxen force: correction to virtual mass and Basset forces due to fluid velocity gradients**
- **Forces caused by temperature and density gradients**

Particle-Particle Drag

- Drag function derived from kinetic theory[1]

$$\vec{I}_{ml}=\frac{3(1+e_{ml})(\pi/2+C_{fml}\pi^2/8)\varepsilon_m\rho_m\varepsilon_l\rho_l}{2\pi(\rho_m d_{pm}^3+\rho_l d_{pl}^3)}(d_{pm}+d_{pl})^2 g_{0ml}|u_l-u_m|(\vec{u}_l-\vec{u}_m)$$

$$g_{0ml}=\frac{1}{\varepsilon_f}+\frac{3d_{pm}d_{pl}}{\varepsilon_f^2(d_{pl}+d_{pm})}\sum_i\frac{\varepsilon_i}{d_{pi}}$$

- Gera et al. (2004) added a “hindrance effect” term, f(P*), to model enduring contact between particles

drag_ss_8.html

1. Syamlal (1987), 2. Gera et al. (2004)

Outline of Presentation

- Introduction to Fluidization
  - Phenomena and Terminology
- Multiphase CFD
  - Introduction
  - Hydrodynamic Equations
  - Interphase Forces
  - Granular Stress
  - Gas-solids turbulence
  - Energy balance
  - Species balance
  - Numerical techniques
- MFIX Code
- Validation of hydrodynamics
  - Bubbling Fluidized Bed
  - Circulating Fluidized Bed
  - Spouted bed
- Fluidized bed reactors
- Industrial application of multiphase CFD

Granular Flow Regimes

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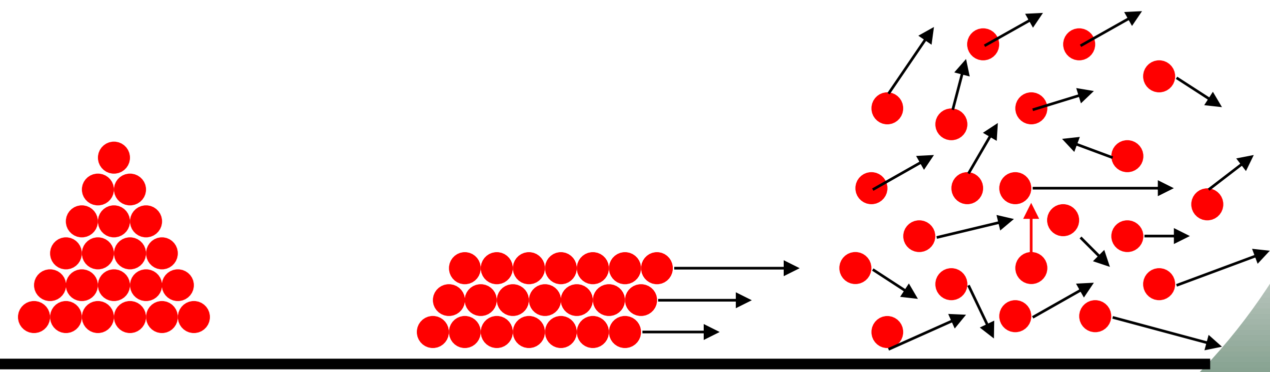
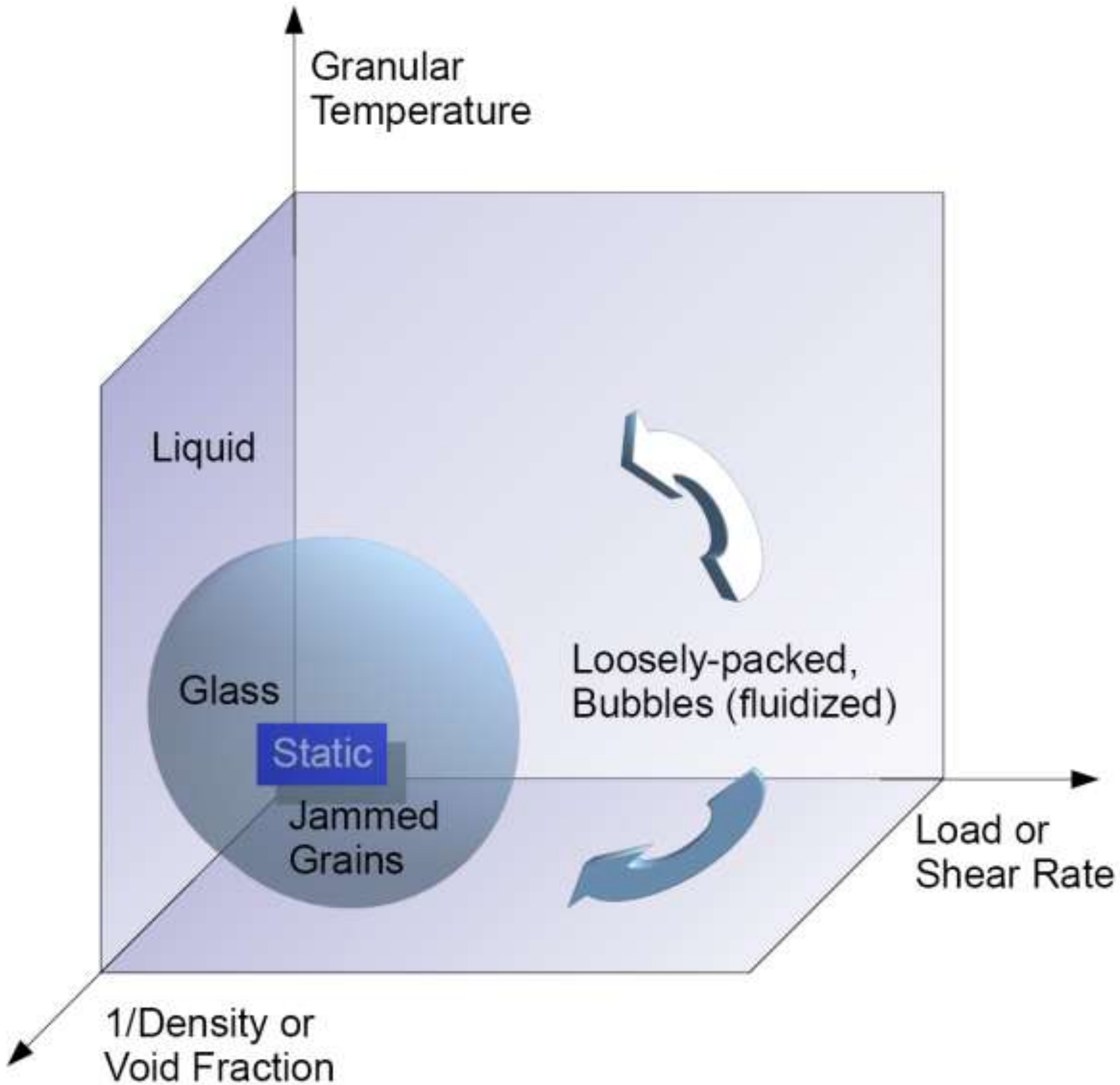
	Regime		
	Elastic	Frictional	Viscous
Type of flow	Stagnant	Slow flow	Rapid flow
Stress depends upon	Strain	Strain rate direction	Strain rate
Particle contact	Permanent	Enduring	Fleeting/binary
Type of theory	Elasticity	Plasticity, Soil mechanics	Kinetic theory



Another way to look at this....



Maintaining maximum packing constraint – 1

- **In the limit of maximum packing a granular pressure is needed to prevent further compaction**
  - **Incompressible granular medium**

$$\varepsilon_p \rho_p \vec{u}_p \frac{d\vec{u}_p}{dt_p} = -\varepsilon_p \nabla p_f + F_{fp}(\vec{u}_f - \vec{u}_p) + \varepsilon_p \rho_p \vec{g} - \nabla p_p$$

$$p_p = 0 \ if \ \varepsilon_f > \varepsilon_{cp}$$

  - **Otherwise calculate solids pressure such that**

$$\varepsilon_f = \varepsilon_{cp}$$

Syamlal and O'Brien (1988)

Maintaining maximum packing constraint – 2

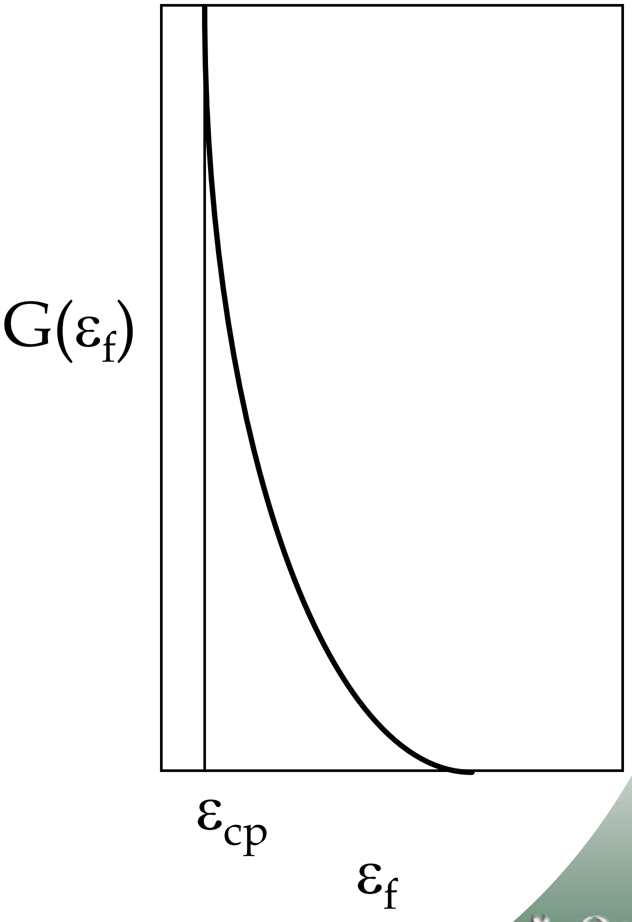
- Slightly compressible granular medium

$$\varepsilon_p \rho_p \vec{u}_p \frac{d\vec{u}_p}{dt_p} = -\varepsilon_p \nabla p_f$$

$$+ F_{fp}(\vec{u}_f - \vec{u}_p)$$

$$+ \varepsilon_p \rho_p \vec{g}$$

$$+ G(\varepsilon_f)\nabla \varepsilon_f$$



Gidaspow (1994) Sec. 4.4

Maintaining maximum packing constraint – 3

- **Usually $\varepsilon_{cp} < \varepsilon_{mf}$**
- **The models at present cannot describe the variation from ε_{cp} to ε_{mf} very well**
- **A good approximation is to set $\varepsilon_{cp} = \varepsilon_{mf}$**
- **Solids pressure models in MFIX**

Frictional Flow – 1

- **Particles are in enduring contact and momentum transfer is through friction**
- **We will illustrate the development of constitutive equations with 2D equations**
- **The Stress can be represented in 2D as**

$$S_p = \sigma \begin{vmatrix} 1 & 0 \\ 0 & 1 \end{vmatrix} + \tau \begin{vmatrix} \cos(2\psi) & \sin(2\psi) \\ \sin(2\psi) & -\cos(2\psi) \end{vmatrix}$$

where

$$\sigma = (\sigma_1 + \sigma_2)/2$$

$$\tau = (\sigma_1 - \sigma_2)/2$$

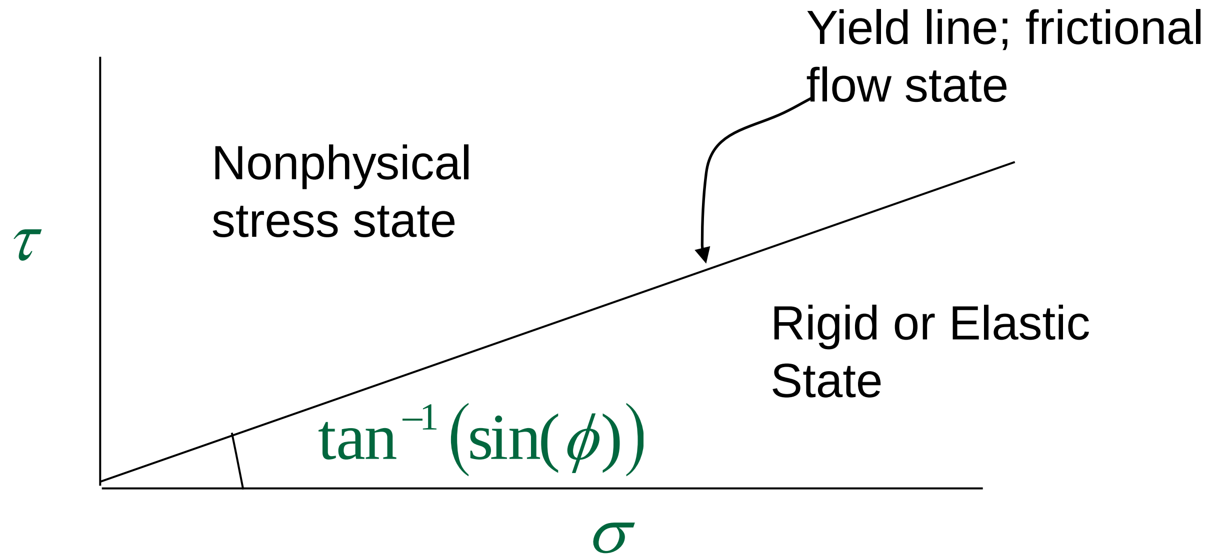
$$\psi = \text{Angle between principal direction and X-axis}$$

Jackson (1983)

Frictional Flow – 2

- **Yield function: a relation between components of stress tensor for a material about to yield. For example, Coulomb's yield condition gives**

$$\tau = \sigma \sin(\phi)$$



Jackson (1983)

Frictional Flow – 3

- **Flow rule: relations between components of stress and rate of strain tensors**
  - **Co-axiality or alignment condition – principal axes of rate of deformation are aligned with that of stress**
  - **Normality condition – ratio of the principal rates of deformation is equal to the ratio of the components of the inward normal to the yield surface**
- **In 2D the three equations (yield condition, coaxiality, normality) give the three unknowns to fully define the stress tensor:** τ, σ, ψ

Jackson (1983)

Frictional Flow – 4

- **Schaeffer's[1] formula**

$$\overline{\overline{S}} = 2\mu_p \overline{\overline{D}}_p$$

$$\mu_p = \frac{p_p \sin\phi}{2\sqrt{I_{2D}}}$$

$$I_{2D} = \frac{1}{6}\left[(D_{11} - D_{22})^2 + (D_{22} - D_{33})^2 + (D_{33} - D_{11})^2\right]$$

$$+ D_{12}^2 + D_{23}^2 + D_{31}^2$$

1. Schaeffer (1987); also see Johnson and Jackson and (1987), Tardos(1997)

Kinetic Theory – 1

solve_granular_energy_8f.html

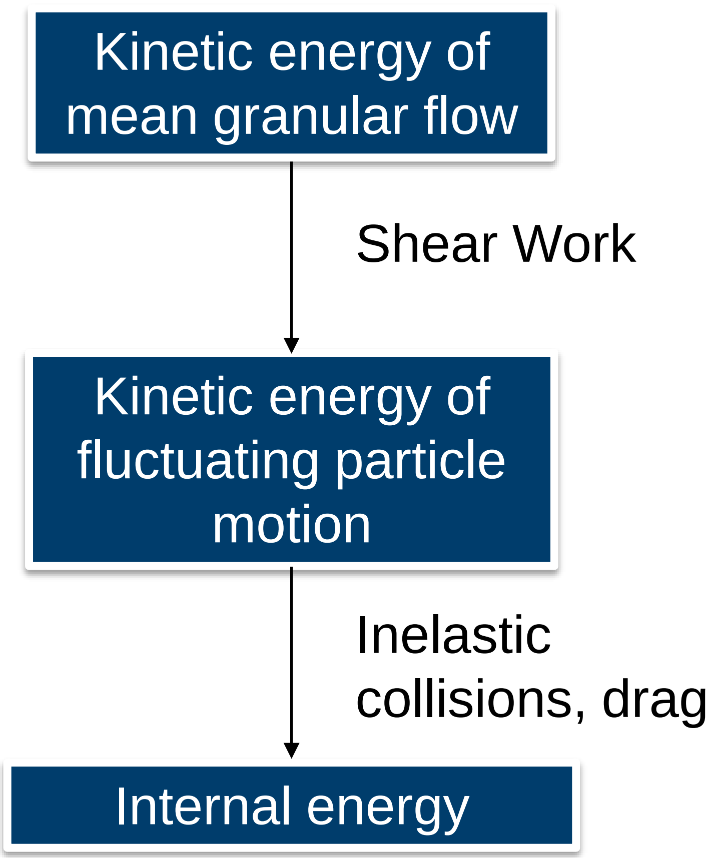
- **Macroscopic properties of granular media can be calculated from the velocity-distribution function *f*, where**

$$f\,(c,r,t)\,dc\,dr$$

is the number of particles at time *t*, in the volume (*r*, *dr*) having velocities in the range *c*, *c+dc*

- ***f* satisfies the Boltzmann equation**

$$\frac{\partial f}{\partial t}+c_i\frac{\partial f}{\partial x_i}+F_i\frac{\partial f}{\partial c_i}=\left(\frac{\partial f}{\partial t}\right)_c$$



Chapman and Cowling (1970), Lun et al. (1984), Ding and Gidaspow (1990), Gidaspow (1994)

Kinetic Theory – 2

- **which gives Maxwell's transport equation for an ensemble average**

$$\frac{\partial n\langle\psi\rangle}{\partial t}+\frac{\partial n\langle\psi c_i\rangle}{\partial x_i}-n\left[\left\langle\frac{\partial\psi}{\partial t}\right\rangle+\left\langle c_i\frac{\partial\psi}{\partial x_i}\right\rangle+\left\langle F_i\frac{\partial\psi}{\partial c_i}\right\rangle\right]=\int\psi\left(\frac{\partial f}{\partial t}\right)_{coll}dc$$

where $\langle\psi\rangle=\frac{1}{n}\int\psi\ fdc$ **and the number density** $n=\int fdc$

- **The equation in terms of peculiar velocity C = c - v**

$$\frac{Dn\langle\psi\rangle}{Dt}+n\langle\psi\rangle\frac{\partial v_i}{\partial x_i}+\frac{\partial n\langle\psi C_i\rangle}{\partial x_i}-n\left[F_i-\frac{Dv_i}{Dt}\right]\left\langle\frac{\partial\psi}{\partial C_i}\right\rangle+n\left\langle\frac{\partial\psi}{\partial C_i}C_j\right\rangle\frac{\partial v_j}{\partial x_i}=\int\psi\left(\frac{\partial f}{\partial t}\right)_{coll}dc$$

- **Substituting *m*, *mC*, ½ *mC*^{2} in the above equation conservation equation for mass, momentum, and granular energy are derived.**

Chapman and Cowling (1970), Lun et al. (1984), Ding and Gidaspow (1990), Gidaspow (1994)

Kinetic Theory – 3

- **Determine the collisional rate of change of mean value by assuming binary collisions of rigid particles**

$$\int \psi \left(\frac{\partial f}{\partial t} \right)_{coll} dc = -\frac{\partial \theta_i}{\partial x_i} + \chi$$

$$\theta = -\frac{1}{2} d_p^3 \int_{c_{12}\cdot k>0} (\psi_1' - \psi_1) c_{12} \cdot kk\, f^{(2)}(r - \frac{1}{2} d_p k, c_1, r + \frac{1}{2} d_p k, c_2)\, dk\, dc_1\, dc_2$$

$$\chi = -\frac{1}{2} d_p^2 \int_{c_{12}\cdot k>0} (\psi_2' + \psi_1' - \psi_2 - \psi_1) c_{12} \cdot k\, f^{(2)}(r - d_p k, c_1, r + d_p k, c_2)\, dk\, dc_1\, dc_2$$

- **From the above get Jenkins-Savage transport theorem**

$$\frac{Dn\langle \psi \rangle}{Dt} + n\langle \psi \rangle \frac{\partial v_i}{\partial x_i} + \frac{\partial n(\langle \psi C_i \rangle + \theta_i)}{\partial x_i} - n\left[F_i - \frac{Dv_i}{Dt} \right] \left\langle \frac{\partial \psi}{\partial C_i} \right\rangle + n \left\langle \frac{\partial \psi}{\partial C_i} C_j \right\rangle \frac{\partial v_j}{\partial x_i} = n\chi$$

Chapman and Cowling (1970), Lun et al. (1984), Ding and Gidaspow (1990), Gidaspow (1994)

Kinetic Theory – 4

- Assuming that the pair distribution function is a product of the single particle distribution functions multiplied by the radial distribution function and using a Taylor series expansion at *r*

$$f^{(2)}(r-\frac{1}{2}d_p k, c_1, r+\frac{1}{2}d_p k, c_2) = g_0\left[f_1 f_2 + \frac{1}{2} d_p f_1 f_2 \nabla \ln \frac{f_2}{f_1} \right]$$

- Closed-form constitutive relations can be obtained by assuming a velocity distribution such as Maxwellian

$$f = \frac{n}{(2\pi\Theta)^{3/2}} \exp\left[-\frac{(c-v)^2}{2\Theta} \right]$$

Chapman and Cowling (1970), Lun et al. (1984), Ding and Gidaspow (1990), Gidaspow (1994)

Granular Energy Equation

$$\frac{3}{2}\varepsilon_m \rho_m \left[\frac{\partial \Theta_m}{\partial t} + U_{mj} \frac{\partial \Theta_m}{\partial x_j} \right] = \frac{\partial}{\partial x_i}\left(\kappa_m \frac{\partial \Theta_m}{\partial x_i} \right) + \tau_{mij} \frac{\partial U_{mi}}{\partial x_j} + \prod_m - \varepsilon_m \rho_m J_m$$

$$\Theta = \frac{1}{3}\left\langle C^2 \right\rangle$$

Granular energy dissipation mechanisms

- Collisional dissipation

$$J_m = \frac{48}{\sqrt{\pi}}\eta(1-\eta)\frac{\varepsilon_m g_0}{d_{pm}}\Theta_m^{3/2}$$

- Drag dissipation

$$\Pi_m = -3\beta\Theta_m + \frac{81\varepsilon_s \mu_g^2 \left| U_g - U_m \right|^2}{g_0 d_{pm}^3 \rho_m \sqrt{\pi \Theta_m}}$$

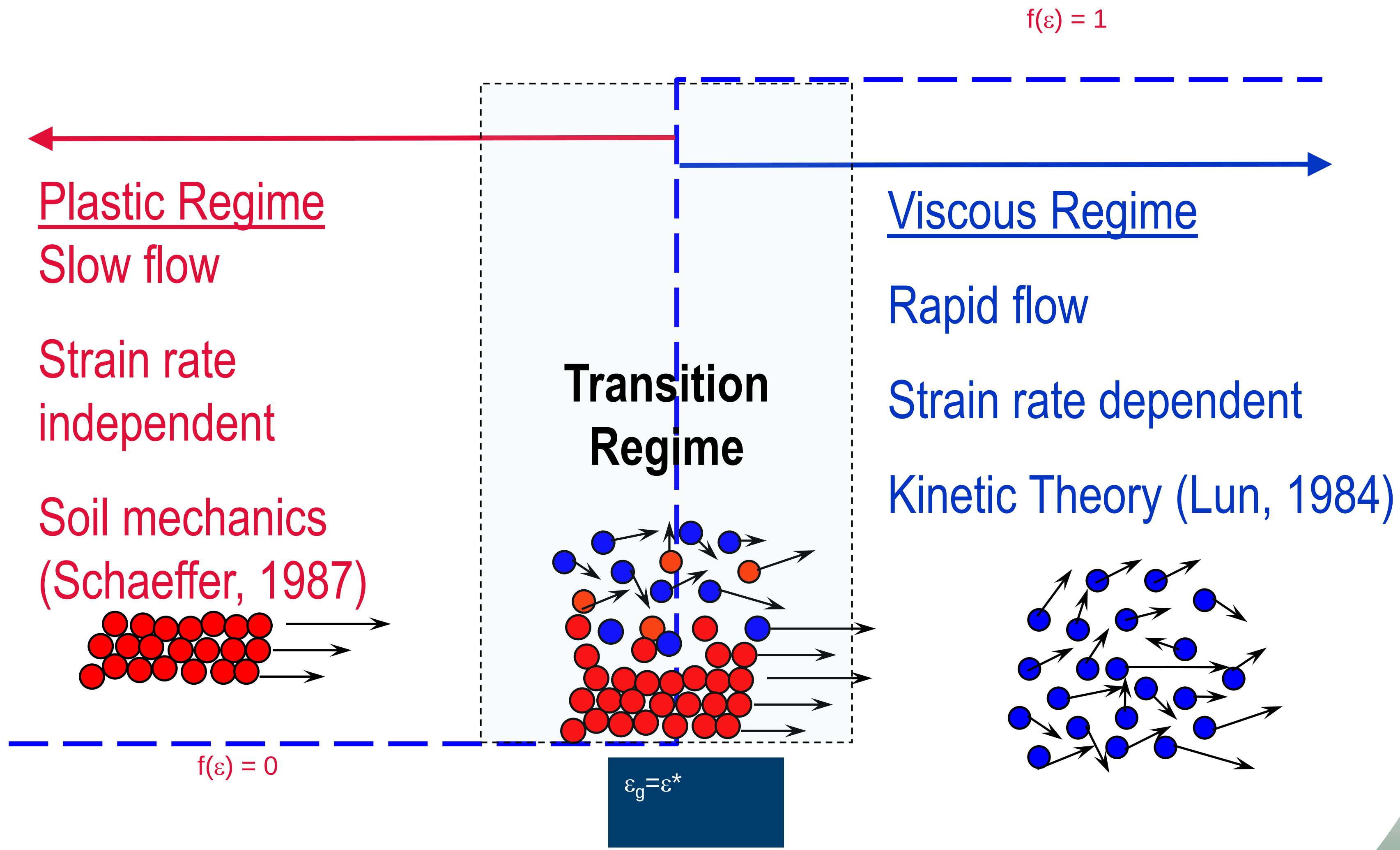
Granular Stress

$$\tau_{sij} = \left(-P_s + \eta\mu_b \frac{\partial U_{si}}{\partial x_i} \right)\delta_{ij} + 2\mu_s S_{sij}$$

$$P_s = \varepsilon_s \rho_s \Theta_s \left[1 + 4\eta\varepsilon_s g_0 \right]$$

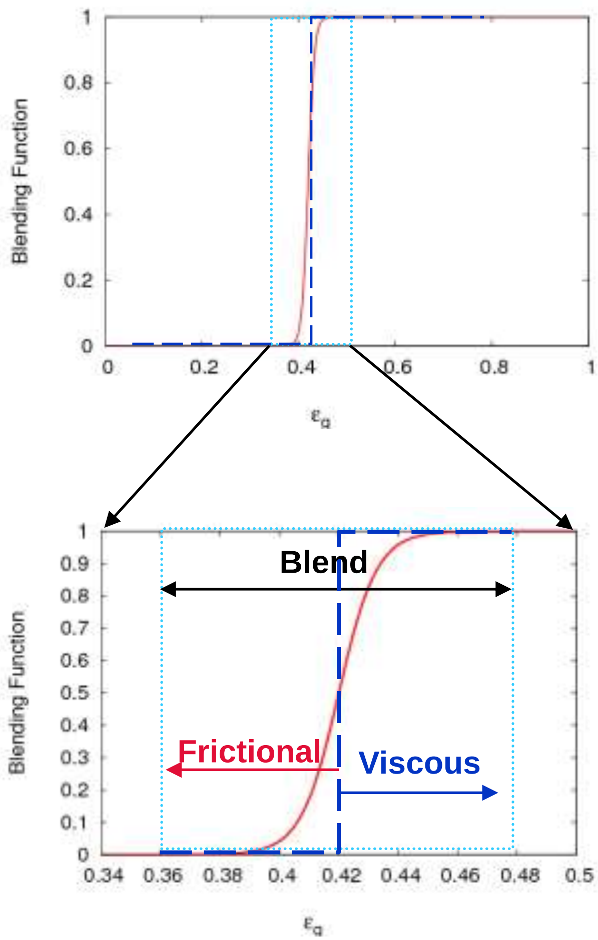
$$S_{sij} = \frac{1}{2}\left(\frac{\partial U_{si}}{\partial x_j} + \frac{\partial U_{sj}}{\partial x_i} \right) - \frac{1}{3}\frac{\partial U_{si}}{\partial x_i}$$

Blending Function (1): Motivation

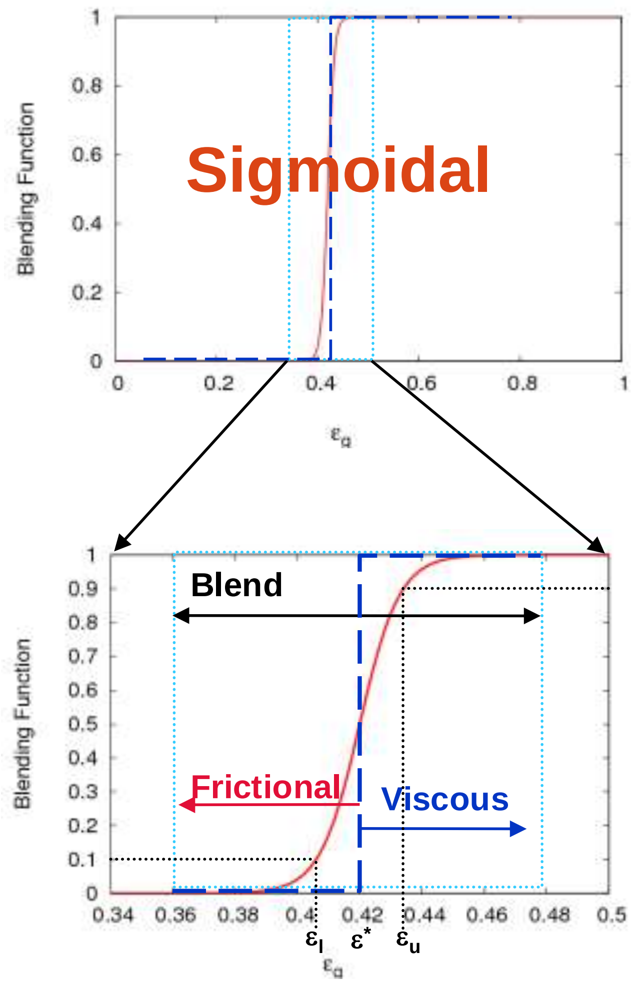


Blending Function – Details, Nomenclature (2)

- Blending function
  - Smoother transition
  - Still preserving the viscous/frictional stress formulation
  - Bridge to address the transition region
- We now introduce a blending function in the void-fraction space with the following properties:
  - Has smooth but rapid transitioning around critical packing void fraction (ε*).
    - Goes to near zero at ε*-δε
    - Goes to near one at ε*+δε
  - Some obvious choices for this function are:
    - Hyperbolic tangent (used in many grid-stretching programs, blending drag formulations etc.)
    - Sigmoidal function (used for rapid transitioning, e.g. for combustion efficiency dependency on equivalence ratio, as in Daw et al., 1996)

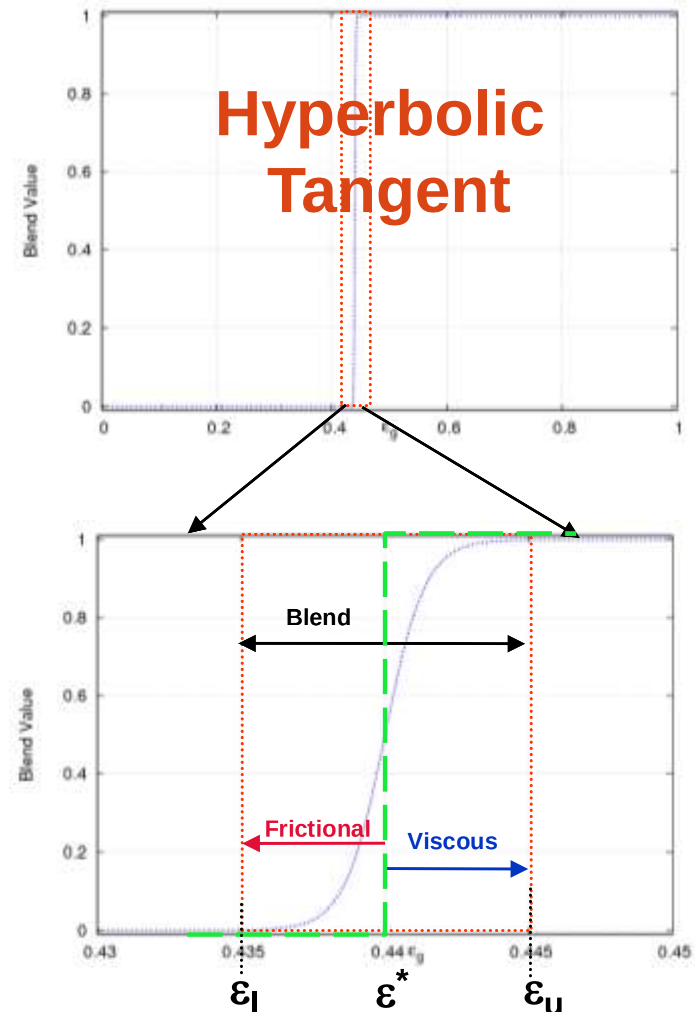


Blending Function – Details, Nomenclature (3)



$$\varphi(\varepsilon_g) = \left(1 + 100^{-\left(\frac{\varepsilon_g - \varepsilon^*}{\varepsilon_u - \varepsilon_l}\right)}\right)^{-1}$$

, where $\varphi(\varepsilon_u) = 0.9$ and $\varphi(\varepsilon_l) = 0.1$



$$\varphi(\varepsilon_g) = \left(\tanh\left(\frac{2\pi(\varepsilon - \varepsilon^*)}{\varepsilon_u - \varepsilon_l}\right) + 1\right) \Big/ 2,$$

where $\varphi(\varepsilon_u) = 1.0$ and $\varphi(\varepsilon_l) = 0.0$; $\varepsilon_u = 1.01\varepsilon^*$ and $\varepsilon_l = 0.99\varepsilon^*$;

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Turbulence equations for gas/solids flows

solve_k_epsilon_eq_8f.html

For Simonin model: $\Pi_{k1} = \beta\left(k_{12} - 2k_1\right)$

For Ahmadi model: $\Pi_{k1} = \beta\left(3\Theta_s - 2k_1\right)$

$$\alpha_1\rho_1\left[\frac{\partial k_1}{\partial t} + U_{1j}\frac{\partial k_1}{\partial x_j}\right] = \frac{\partial}{\partial x_i}\left(\alpha_1\frac{\mu_1^t}{\sigma_k}\frac{\partial k_1}{\partial x_i}\right) + \alpha_1\tau_{1ij}\frac{\partial U_i}{\partial x_j} + \Pi_{k1} - \alpha_1\rho_1\varepsilon_1$$

$$\alpha_1\rho_1\left[\frac{\partial \varepsilon_1}{\partial t} + U_{1j}\frac{\partial \varepsilon_1}{\partial x_j}\right] = \frac{\partial}{\partial x_i}\left(\alpha_1\frac{\mu_1^t}{\sigma_\varepsilon}\frac{\partial \varepsilon_1}{\partial x_i}\right) + \alpha_1\frac{\varepsilon_1}{k_1}\left(C_{1\varepsilon}\tau_{1ij}\frac{\partial U_i}{\partial x_j} - \rho_1 C_{2\varepsilon}\varepsilon_1\right) + \Pi_{\varepsilon 1}$$

For Simonin model: $\Pi_{\varepsilon 1} = C_{3\varepsilon}\left(\varepsilon_1 / k_1\right)\Pi_{k1}$

For Ahmadi model: $\Pi_{\varepsilon 1} = 0$

Benyahia et al. (2005)

1. Cao and Ahmadi (1995), 2. Balzer et al. (1996)

Turbulence modeling of the dispersed phase

$$\Theta = \frac{1}{3}\langle u_2 u_2 \rangle$$

$$\left.\begin{aligned}\lambda_2^{dilute} &= 0.1953\rho_2 d_p \sqrt{\pi\Theta} \\ \lambda_2^{dense} &= 2\alpha_2^2 \rho_2 d_p g_0 (1+e)\sqrt{\frac{\Theta}{\pi}}\end{aligned}\right\} \Rightarrow \lambda_2 / \mu_2 \approx 2.5 - 3.76$$

For Simonin model: $\Pi_{k2} = \beta(k_{12} - 3\Theta)$

For Ahmadi model: $\Pi_{k2} = \beta\left(\frac{2k_1}{1+\tau_{12}^x/\tau_1} - 3\Theta\right)$

$$\alpha_2\rho_2\left[\frac{\partial\Theta_s}{\partial t} + U_{2j}\frac{\partial\Theta}{\partial x_j}\right] = \frac{\partial}{\partial x_i}\left(\alpha_2\rho_2\lambda_2\frac{\partial\Theta}{\partial x_i}\right) + \alpha_2\rho_2\tau_{2ij}\frac{\partial U_{2i}}{\partial x_j} + \prod_{k2} - \alpha_2\rho_2\varepsilon_2$$

For all models: $\varepsilon_2 = 12(1-e^2)\alpha_2^2\rho_2 g_0 \frac{\Theta_s^{3/2}}{d_p}$

For Simonin model: $k_{12} = \langle u_1 u_2 \rangle$

$$k_{12} = \frac{\eta_t}{1+(1+X_{21})\eta_t}\left(2k_1 + 3X_{21}\Theta_s\right)$$

Benyahia et al. (2005)

NETL

Oak Ridge National Laboratory

Wall boundary conditions

bc__theta_8f.html

– **Jenkins and Louge**

$$\mu_2 \frac{\partial u_2}{\partial x}\bigg|_w = P_2 \tan(\phi_w)\frac{u_2}{|u_2|}$$

Generalization →

$$\begin{cases} -\dfrac{\partial u}{\partial x} - \left[\dfrac{P_2 \tan(\phi_w)}{\mu_2\sqrt{u^2+v^2}}\right]u = 0 \\ -\dfrac{\partial v}{\partial x} - \left[\dfrac{P_2 \tan(\phi_w)}{\mu_2\sqrt{u^2+v^2}}\right]v = 0 \end{cases}$$

$$\lambda_2 \frac{\partial \Theta_s}{\partial x}\bigg|_w = P_2\sqrt{3\Theta_s}\,\frac{3}{8}\left[\underbrace{\frac{7}{2}(1+e_w)\tan^2(\phi_w)}_{\text{Production due to friction}} - \underbrace{(1-e_w)}_{\text{Dissipation due to inelastic collisions}}\right]$$

$$if\ \frac{7}{2}(1+e_w)\tan^2(\phi_w) > (1-e_w) \quad \Rightarrow \text{Turbulence generation at walls}$$

Benyahia et al. (2005), Jenkins and Louge (1997)

Wall boundary conditions

bc__theta_8f.html

– **Johnson and Jackson**

Specularity coefficient: keep it small (less than 0.01)

$$\mu_2 \frac{\partial V_s}{\partial x}\bigg|_w + \frac{\phi \pi \rho_2 V_s g_0 \sqrt{\Theta}}{2\sqrt{3}\,\alpha_2^{\max}} = 0$$

Particle-wall restitution coefficient: lower values yield higher solids concentration at walls

$$\lambda_2 \frac{\partial \Theta}{\partial x}\bigg|_w - \underbrace{\frac{\phi \pi \rho_2 V_s^2 g_0 \sqrt{\Theta}}{2\sqrt{3}\,\alpha_2^{\max}}}_{\text{Production due to slip}} + \underbrace{\frac{\sqrt{3}\pi\, \rho_2 g_0 \left(1 - e_w^2\right) \Theta^{3/2}}{4\,\alpha_2^{\max}}}_{\text{Dissipation due to inelastic collisions}} = 0$$

Production due to slip

Dissipation due to inelastic collisions

Benyahia et al. (2005), Johnson and Jackson (1987)

Wall boundary conditions

– **D. Eskin** ***(not recommended)***

$$\mu_2 \frac{\partial V_s}{\partial x}\bigg|_w + \rho_2 V_s (1 - e_t)\sqrt{\frac{\Theta}{2\pi}} = 0$$

$$\lambda_2 \frac{\partial \Theta}{\partial x}\bigg|_w - \underbrace{\frac{1}{2}\rho_2 \alpha_2 V_2^2 (1 - e_t)^2 \sqrt{\frac{\Theta}{2\pi}}}_{\text{Only production due to slip}} = 0$$

Only production due to slip

Eskin (2005)

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Energy Balance

solve_energy_eq.f.html

originates from a work term for ε changes

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

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

Energy Balance

Viscous dissipation

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

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

Energy Balance

Energy sources; e.g..,
radiation

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

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

Energy Balance

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

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

heat conduction

Energy Balance

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

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

Interphase heat transfer

Energy Balance

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

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

Energy transfer with mass transfer

Energy Balance – In Terms of Temperature

Energy balance equations for solids phases m = 1, M

$$\varepsilon_m \rho_m C_{pm}\left[\frac{\partial T_m}{\partial t} + U_{mj}\frac{\partial T_m}{\partial x_j}\right] = -\frac{\partial q_{mi}}{\partial x_i} - \gamma_{gm}\left(T_m - T_g\right) - \Delta H_m + \gamma_{Rm}\left(T_{Rm}^4 - T_m^4\right)$$

Energy balance equation for gas phase g:

$$\varepsilon_g \rho_g C_{pg}\left[\frac{\partial T_g}{\partial t} + U_{gj}\frac{\partial T_g}{\partial x_j}\right] = -\frac{\partial q_{gi}}{\partial x_i} + \sum_{m=1}^{M}\gamma_{gm}\left(T_m - T_g\right) - \Delta H_g + \gamma_{Rg}\left(T_{Rg}^4 - T_g^4\right)$$

Heats of Reaction

$$-\Delta H_m = \sum_n \left[\left(H_{m,ref} \right)_n + \int_{T_{ref}}^{T_s} C_{pmn}(T)\,dT \right] \varepsilon_g \rho_g \left(\frac{\partial X_{gn}}{\partial t} + U_{gi} \frac{\partial X_{gn}}{\partial x_i} \right)$$

$$\approx \sum_n \left[\left(H_{m,ref} \right)_n + \int_{T_{ref}}^{T_s} C_{pmn}(T)\,dT \right] \left(R_{mn} - \sum_{n=1}^{N_m} R_{mn} X_{mn} \right)$$

$$-\Delta H_g \approx \sum_n \left[\left(H_{g,ref} \right)_n + \int_{T_{ref}}^{T_g} C_{pgn}(T)\,dT \right] \left(R_{gn} - \sum_{n=1}^{N_g} R_{gn} X_{gn} \right)$$

Fluid-Particle Heat Transfer

The interphase heat transfer coefficient

$$\gamma_{fm} = \frac{6\kappa_f \varepsilon_m Nu_m}{d_{pm}^2}$$

where the Nusselt number is calculated using Gunn (1978) correlation

$$Nu_m = (7 - 10\varepsilon_f + 5\varepsilon_f^2)(1 + 0.7 \,\mathrm{Re}_m^{0.2} \,\mathrm{Pr}^{1/3})$$
$$+ (1.33 - 2.4\varepsilon_f + 1.2\varepsilon_f^2)\,\mathrm{Re}_m^{0.7}\,\mathrm{Pr}^{1/3}$$

1. Gunn (1978)

Fluid-Particle Heat Transfer

- **To predict heat transfer to immersed tubes (with coarse numerical grid), the model will need a wall heat transfer coefficient[1]**

1. Syamlal and Gidaspow (1985), Kuipers et al. (1992), Witt and Perry (1996)

Heat Conduction

- **Fourier's law form assumed**

$$\vec{q}_m = -\varepsilon_m k_m \nabla T_m$$

- **k_m is obtained from packed bed conductivity formula[1]**

- **In packed bed combustion, k_m also accounts for interparticle radiation; *e.g.*[2],** $k_p = 2\sigma d_p T_p^3$

1. MFIX manual, p.20; 2. Gort(1993)

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Species Mass Balance

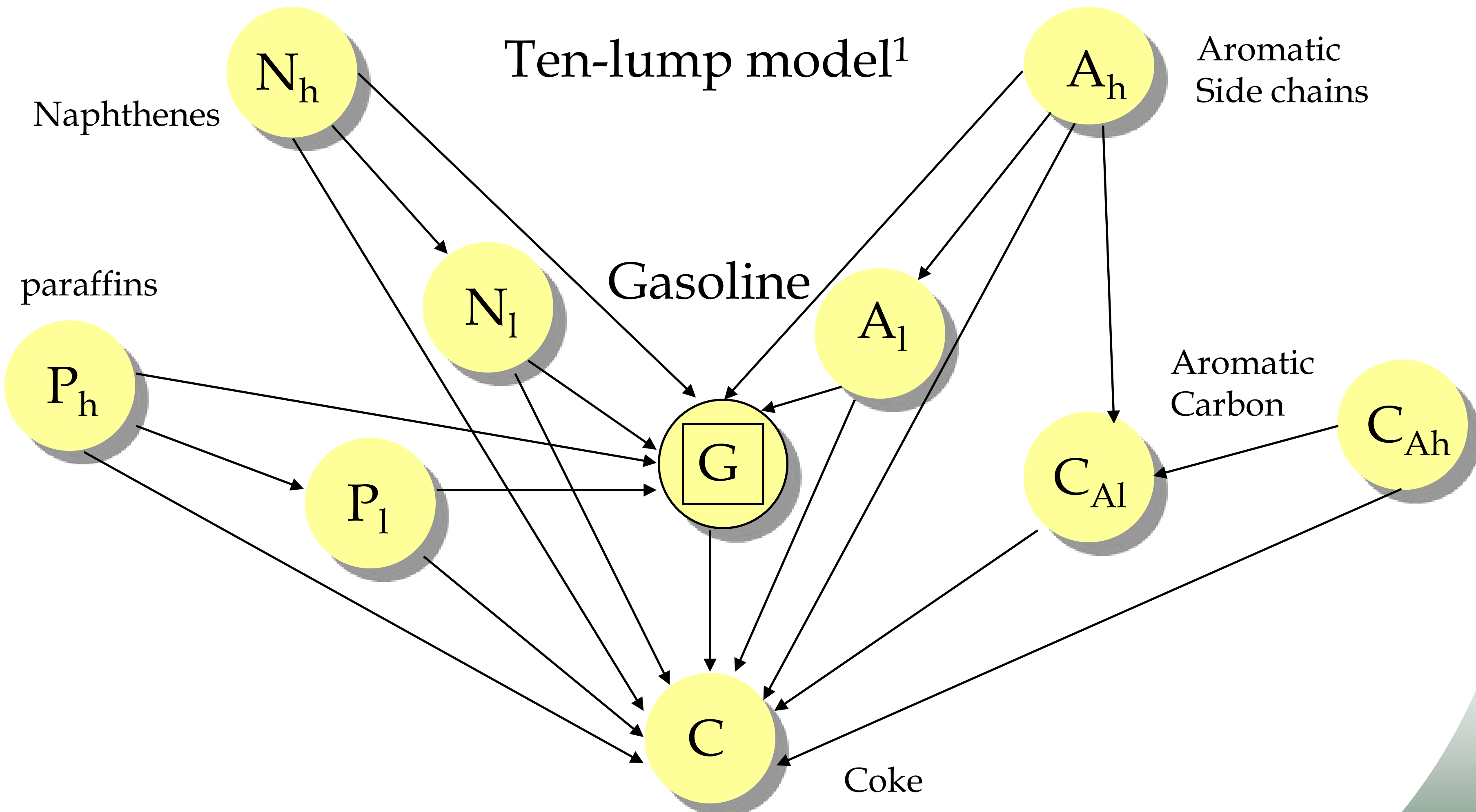
- **Multiphase chemical reactions are described by tracking chemical species in each of the phases**

$$\frac{\partial}{\partial t}(\varepsilon_m \rho_m X_{mn}) + \nabla \cdot (\varepsilon_m \rho_m X_{mn} \vec{u}_m) = \nabla \cdot (\varepsilon_m \rho_m D_{mn} \nabla X_{mn}) + R_{mn}$$

solve_species_eq_8f.html

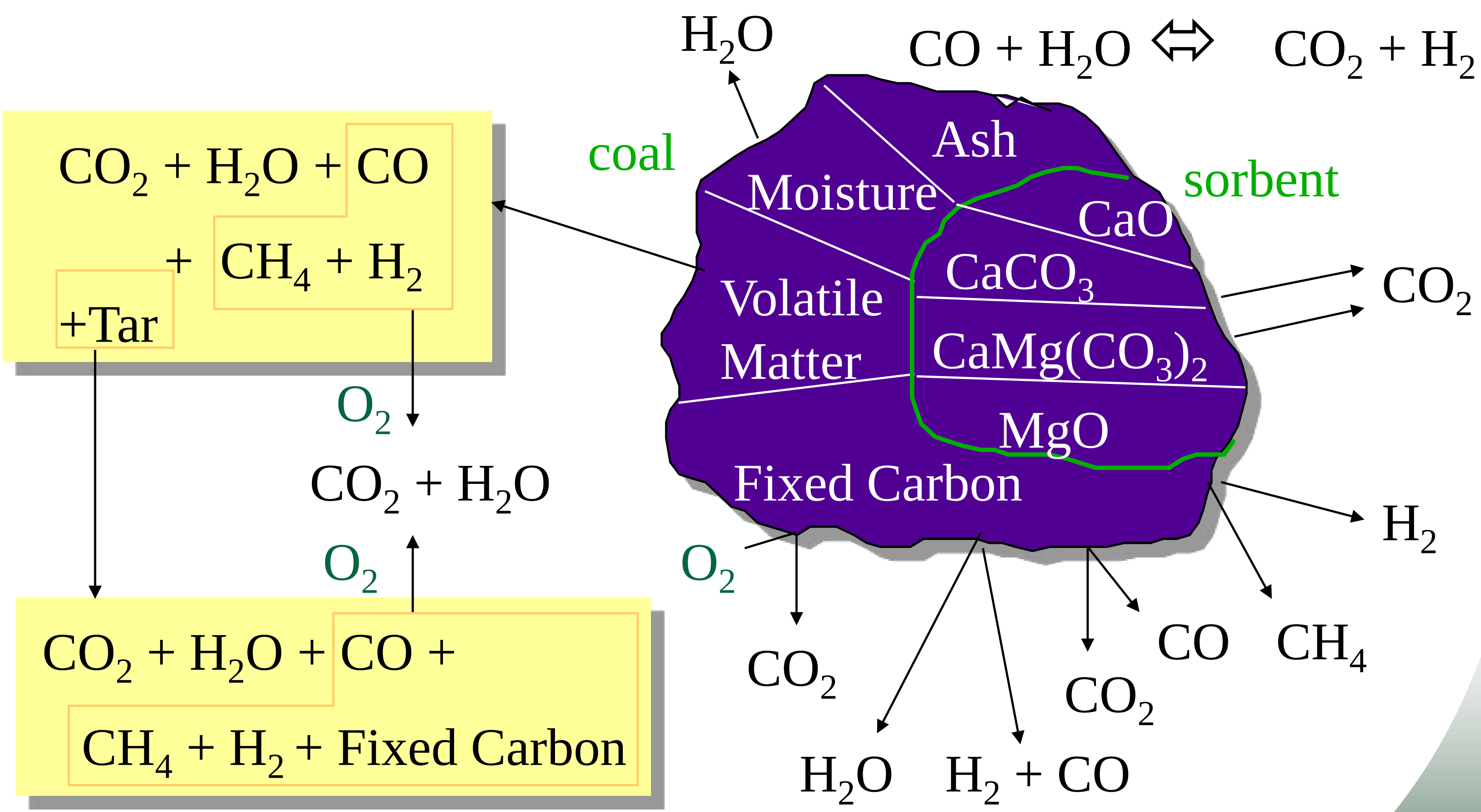
rates_8f.html

Reaction Model: Fluid Catalytic Cracking



1. Mobil/Sundaresan

Reaction Model: Coal Gasification



Homogeneous Reaction

- **Kinetics equation[1] for $CO + {}_2O_2 \rightarrow CO_2$**

$$r_a = 3.98 \cdot 10^{14} \exp\left(\frac{-40{,}000}{1.987 T_f}\right)\left(\frac{\rho_f X_{fO2}}{32}\right)^{0.25}\left(\frac{\rho_f X_{fCO}}{28}\right)$$

$$\left(\frac{\rho_f X_{fH2O}}{18}\right)^{0.5} \varepsilon_f \; (g - mole / cm^3 \cdot s)$$

- **In multiphase formulation the rate expression is multiplied by ε_f**

1. Westbrook and Dryer (1981)

Heterogeneous Reaction

- Kinetics eq[1] for C + CO_2 ←→ 2CO

$$r_b = 930 \exp\left(\frac{-45{,}000}{1.987 T_{fp}}\right)\left(\frac{\varepsilon_p \rho_p X_{pFC}}{12}\right)\left(p_{CO2} - p_{CO}^2 / K\right)$$

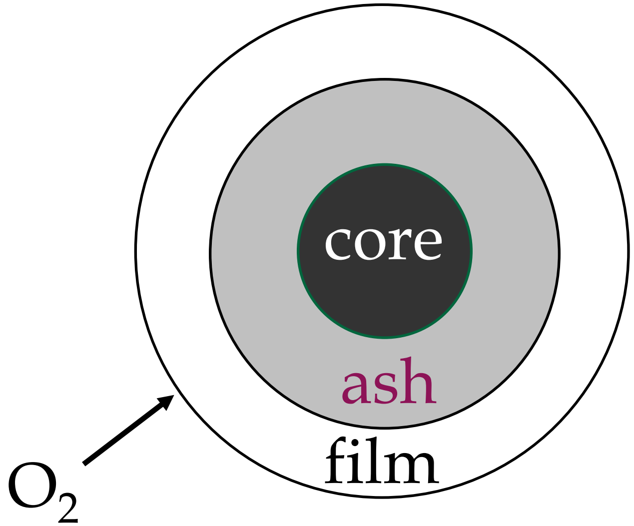
- Need a reaction temperature; e.g., $T_{fp} = (T_f + T_p)/2$
- Need a volume fraction, which depends upon the volumetric basis of the original rate expression

1. Syamlal and Bissett (1992), Wen et al. (1982)

Heterogeneous Reaction

- **Kinetics equation[1] for $2C + O_2 \rightarrow 2CO$**

$$r_c = \frac{3\varepsilon_m p_{O2}}{16 d_{pm}\left(\frac{1}{k_{fm}} + \frac{1}{k_{am}} + \frac{1}{k_{rm}}\right)}$$



- **Mass transfer coefficient from Gunn equation[2]**

1. MFIX manual p.22

Heat of Reaction

- In heterogeneous rxns ΔH for each phase could change depending upon the representation of reactions
  - Averaging erases info on reaction front
  - e.g., in coal combustion the flame may reside at the core surface, in the ash layer, or in surrounding film[1]
  - e.g., ΔH for coal combustion[2]:
    - $C + 2O_2 \rightarrow CO$ (solids); $CO + 2O_2 \rightarrow CO_2$(gas)

1. Arri and Amundson (1978); 2. Syamlal and Bissett (1992)

Species Mass Production

- **Based on above three rates the species mass production and mass transfer are**

$$R_{fCO} = 28(2r_b + 2r_c - r_a)$$

$$R_{fO_2} = -32\left(\frac{r_a}{2} + r_c\right)$$

$$R_{fCO_2} = 44(r_a - r_b)$$

$$R_{pFC} = -12(r_b + 2r_c)$$

$$R_{pf} = 12(r_b + 2r_c)$$

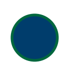
Effects of Mass Transfer

- **On heat transfer**
  - **transfer coefficient needs to be modified[1]**
  - **add an extra heat transfer term**

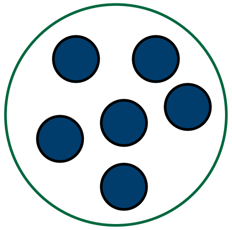
$$R_{ml} h_{ml}$$

- **Group combustion[2]**

single particle combustion



group combustion



1. MFIX manual p.18, 2. Annamalai et al. (1993, 1994)

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Iteration Method

time_march_8f.html

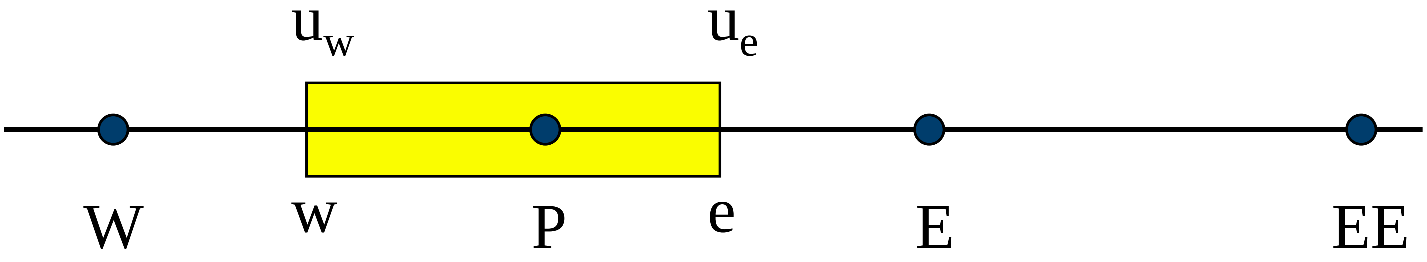
- Calculate physical and transport properties and exchange coefficients
- Solve starred-velocity
- Calculate reaction rates
- Solve solids volume fraction correction equations
- Correct solids volume fractions and velocities
- Calculate gas volume fractions
- Calculate the face values of densities
- Solve pressure correction equation
- Correct pressure, velocities, and density
- Calculate the face values of mass fluxes
- Solve energy equations, granular energy equation, species equations, and turbulence equations
- Check for convergence

Syamlal (1998)

Discretization Scheme

- **Integrating the convection term over a control volume gives**

$$\int_w^e \rho u \frac{\partial \phi}{\partial x} dx = \left(\rho u_e \phi_e - \rho u_w \phi_w\right)$$



Calculation of ϕ_e

- **Determine face values using downwind factor method[1]. First, get normalized ϕ:**

$$\phi_C = \begin{cases} (\phi_P - \phi_W)/(\phi_E - \phi_W) & u_e \geq 0 \\ (\phi_E - \phi_{EE})/(\phi_P - \phi_{EE}) & u_e < 0 \end{cases}$$

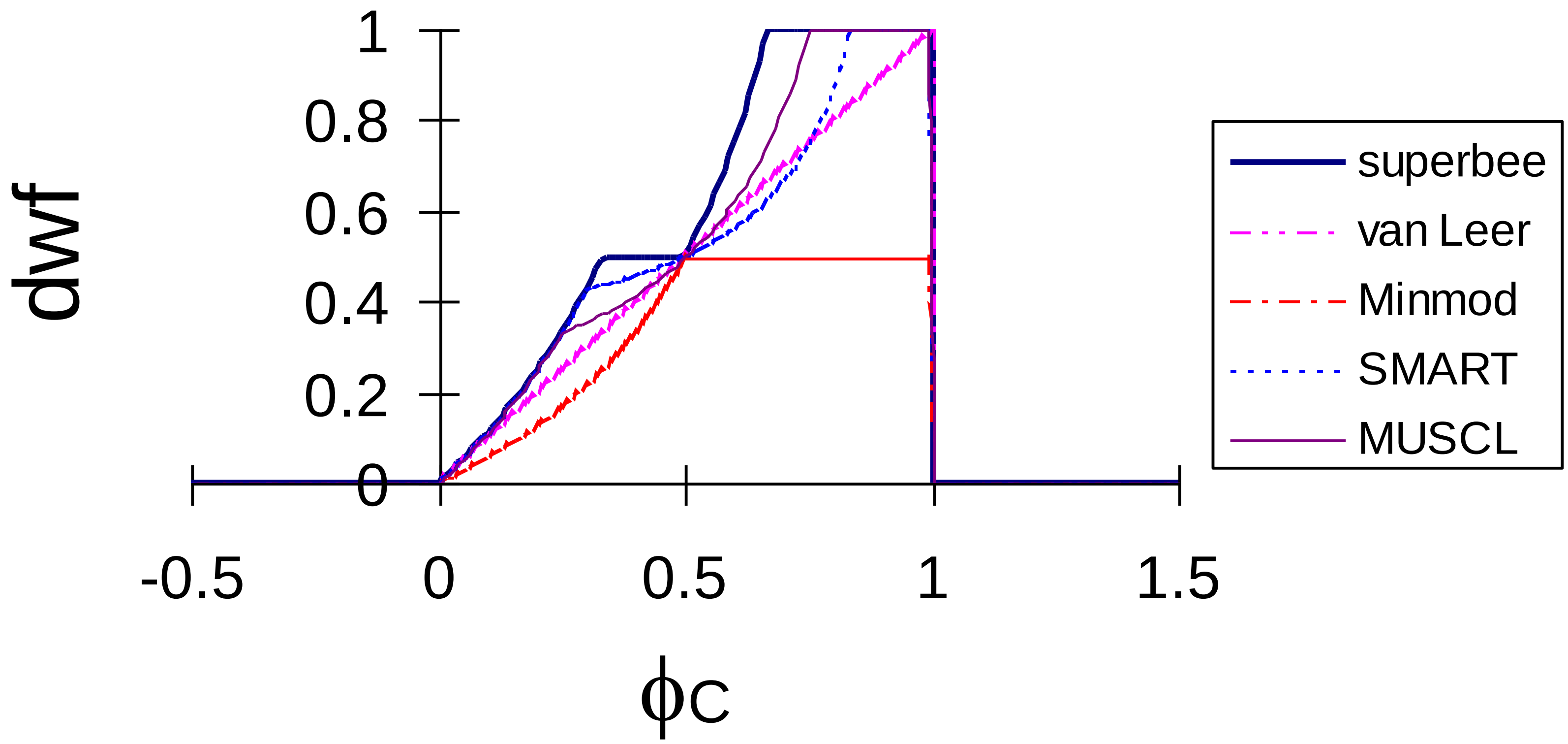
$$\theta = \frac{\phi_C}{1 - \phi_C}$$

1 Leonard and Mokhtari (1990)

Downwind Factors

Scheme	dwf
First Order Upwind	0
Sec. Order Upwind	$\theta/2$
Central Diff.	$1/2$
TVD	$0 \text{ if } \phi_C < 0 \text{ or } \phi_C > 1 \text{ else}$
van Leer	ϕ_C
min mod	$\max[0, \min(1, \theta)] / 2$
MUSCL	$\max[0, \min(2\theta, 0.5(1+\theta), 2)] / 2$
SMART	$\max[0, \min(4\theta, (3+\theta)/4, 2)] / 2$
Superbee	$\max[0, \min(1, 2\theta), \min(2, \theta)] / 2$

Downwind Factors



Calculation of ϕ_e

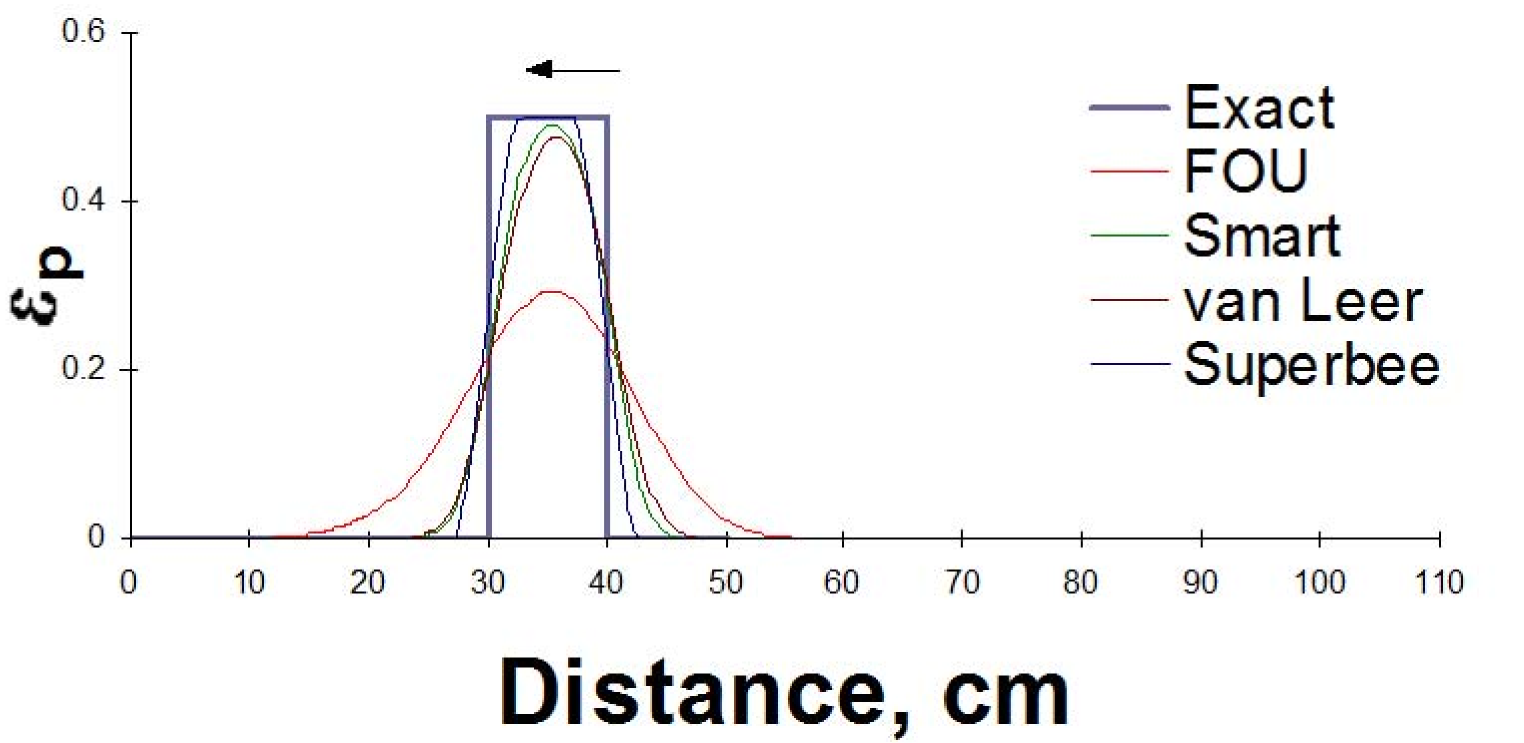
- **Determine the downwind factor using a formula from the table and calculate ξ_e:**

$$\xi_e = \begin{cases} dwf_e & u_e \geq 0 \\ 1 - dwf_e & u_e < 0 \end{cases}$$

- **Then the east-face value of ϕ is given by**

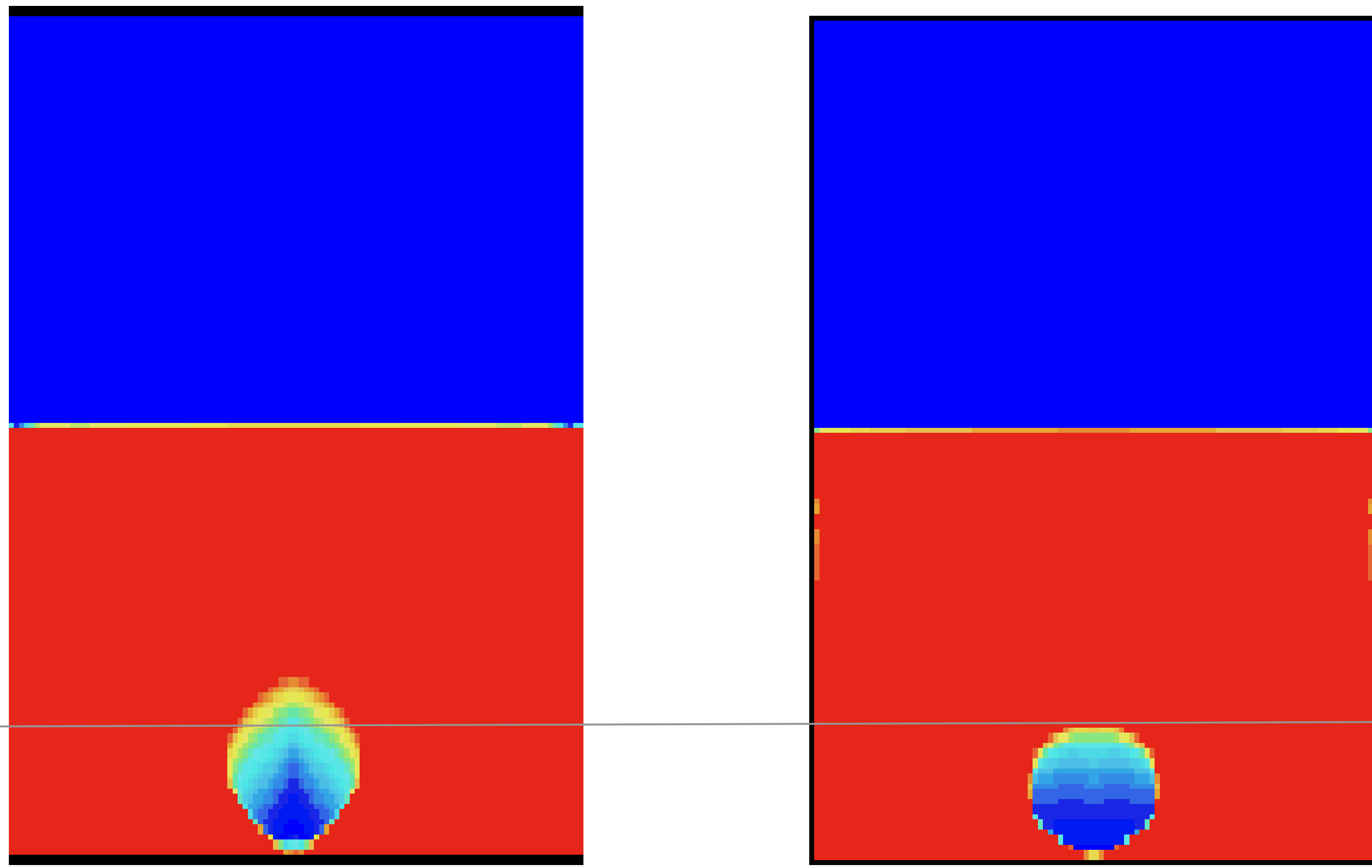
$$\phi_e = \xi_e \phi_E + (1 - \xi_e)\phi_P$$

Plug Flow Simulation



Normalized	FOU	Smart	van Leer	Superbee
CPU time	1	4	5	81

Bubble shape
Upwind vs Superbee



Syamlal (1997)

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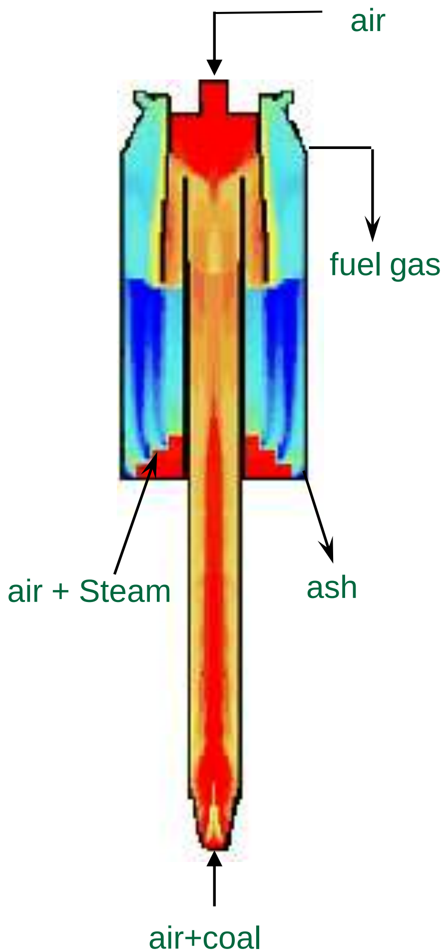
MFIX Background

- 3D, transient, multiphase flow model
- Cartesian and cylindrical coordinates
- Shared and distributed memory parallel
- Supported on various platforms
- *Test stand* for physics and numerical techniques development
- Development at NETL started in 1991
- Collaborations with ORNL, Fluent, Parsons, Aeolus Research, Princeton, Iowa State …
- Users/developers grew from an initial team of 3 in 1991 to over 70 in 2006
- Open source distribution started in 2001(http://mfix.netl.doe.gov)



The first application of MFIX was for PyGAS gasifier design, as shown in this CO mass fraction plot, Syamlal and Venkatesan 1993

MFIX OS Features – 1

- Source code and revision control
  - **120,000 lines of FORTRAN 90 code, organized into 508 files and 969 subprograms**
  - **Revision control using concurrent versioning system (CVS)**
  - **User contributions checked into CVS by *gatekeepers***
  - **Downloads: Stable, Development, CVS**
  - **A version referred to in a publication is *forever available* for public scrutiny**

set_constprop.f		1.13	*2 months*	sofiane	Set Yu_Standish and Fedors_Landel logical keywords + ep_star --> ep_star_array(i...
open_files.f		1.11	*2 months*	pannala	Keeping IFC 7.x compiler happy
location_check.f		1.4	*2 months*	msyaml	Removed the continuation of a string on two lines.
check_mass_balance.f		1.19	*2 months*	pannala	More changes from Luc Oger to make windows intel compiler happy
mfix_directory_path.inc		1.1	*2 months*	msyaml	The file is being checked in to help Windows users. Under Linux this file is au...

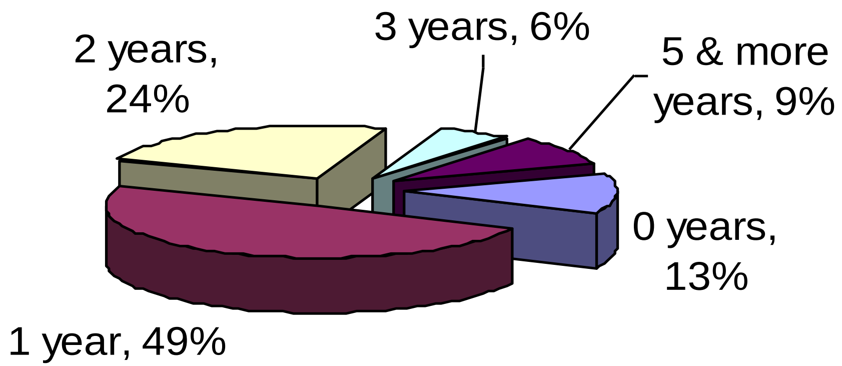
CVS web interface shows file names, version number, age of the version, developer name, and development notes

MFIX OS Features – 2

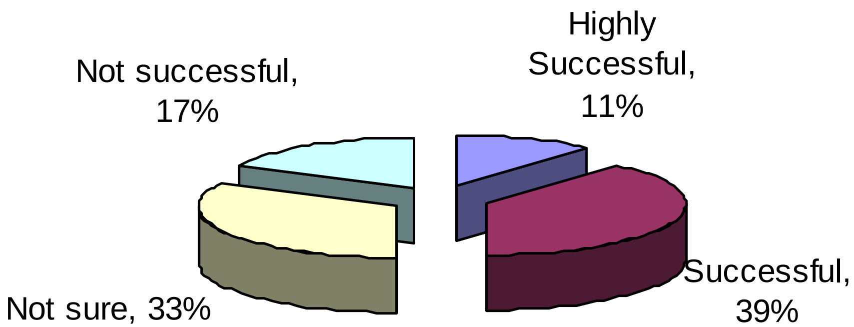
- Documentation
  - **Internal documentation, 62% comment lines**
  - **Constantly updated *readme* and *MFIX_equations* files**
  - **Legacy manuals, presentations and developer notes**
- Forty test cases and thirteen tutorial cases
- **Test harness** conducts nightly regression tests to assure software quality
- OS group communication through twenty mailing lists including mfix_help
- Open citations: list of papers relevant to computational gas-solids flow

Users' Experience with MFIX

- Survey conducted in 2005; 70 responses
- 40% had 2 or more years of experience



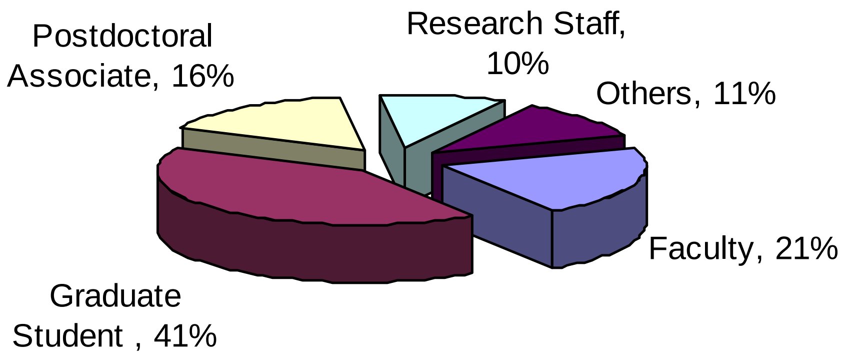
- 50% of users successful – seems reasonable, considering software complexity and minimal user support
- "Not successful" correlated well with less than a year of experience



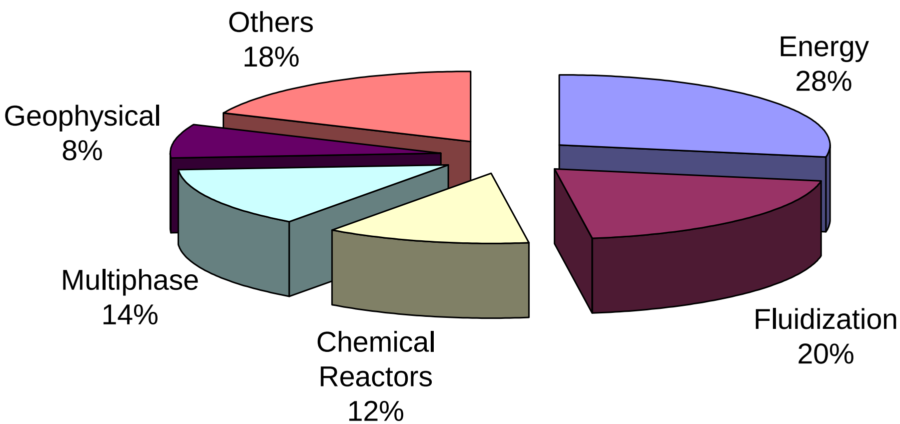
Gel et al. (2006)

User Profiles and Applications

- Nearly 80% of users are from universities



- Majority of the applications are in energy and fluidization categories, similar to MFIX's original applications
- Extension to other areas such as Geophysical



Gel et al. (2006)

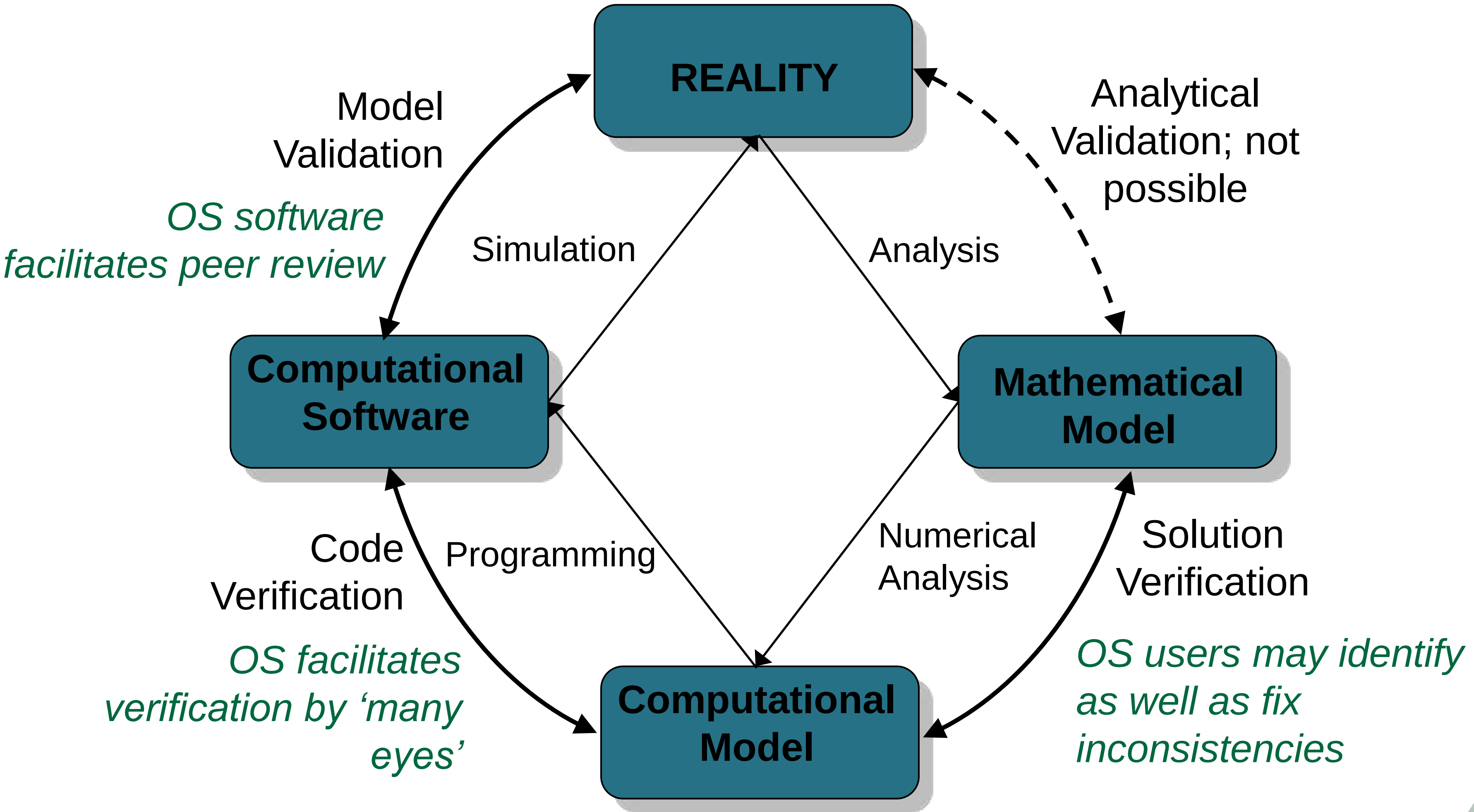
V&V – AIAA Definitions

- **Verification:** "The process of determining that a model implementation accurately represents the developer's conceptual description of the model and the solution to the model."

- **Validation:** "The process of determining the degree to which a model is an accurate representation of the real world from the perspective of the intended uses of the model."

Oberkampf and Trucano (2002)

Verification and Validation

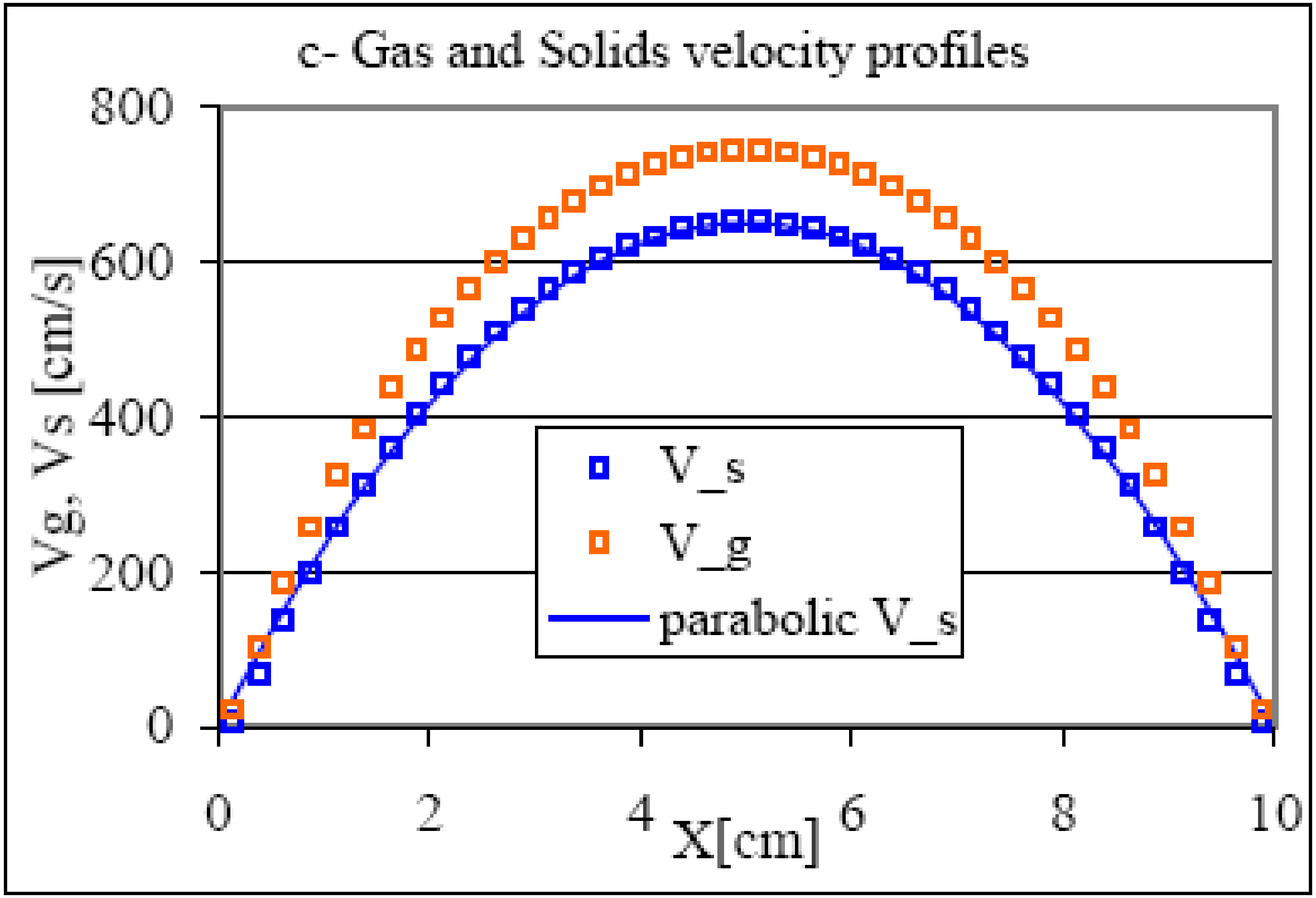


Adapted from Oberkampf and Trucano (2002)

Verification Problems

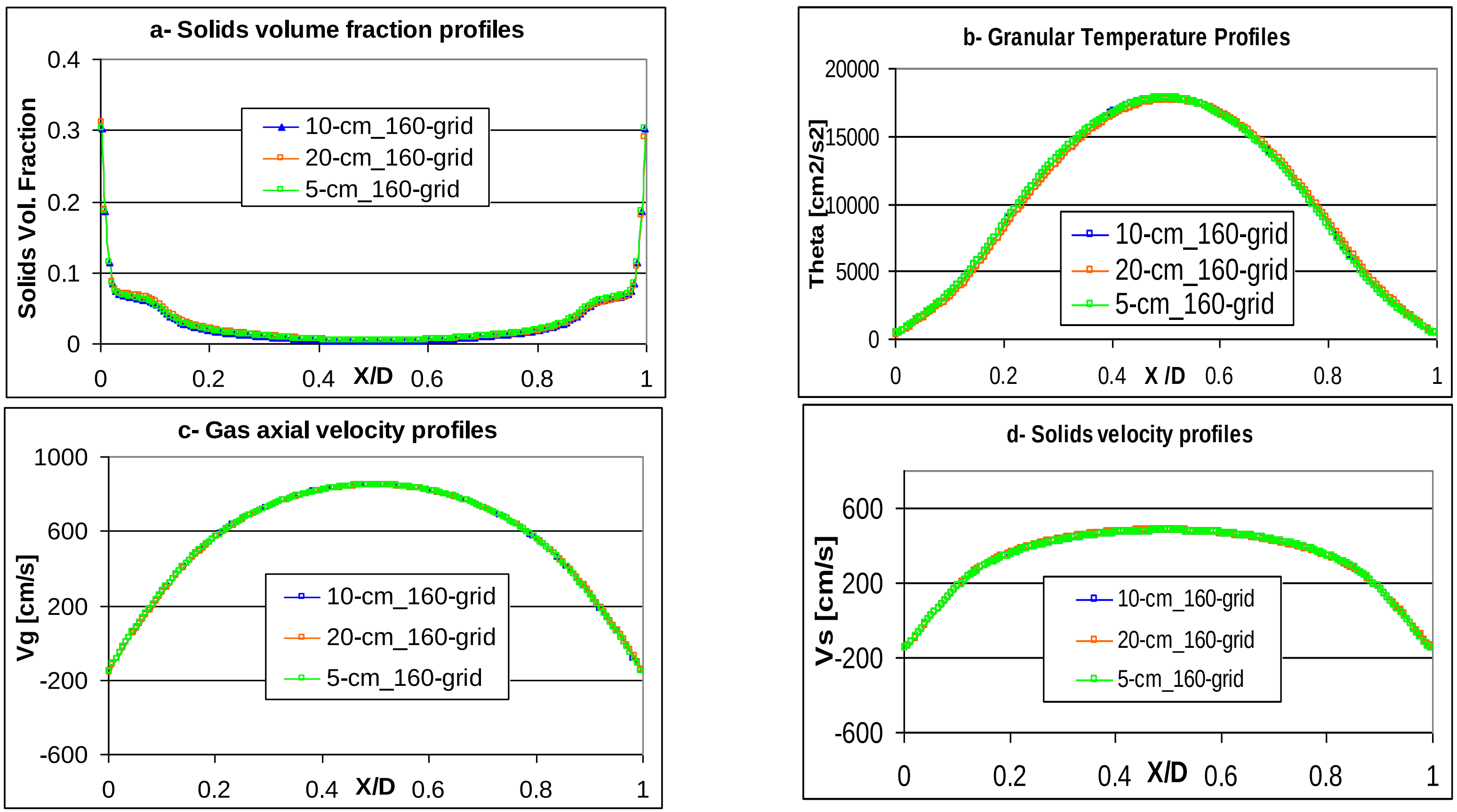
- Parabolic velocity profile
- Solids body rotation
- Heat conduction
- Minimum Fluidization
- Sod Problem (shock tube)
- MFIX-DEM
- …

Velocity profiles for a specified granular temperature profile



Benyahia et al. (2004)

Glicksman's Scaling Laws for Verification



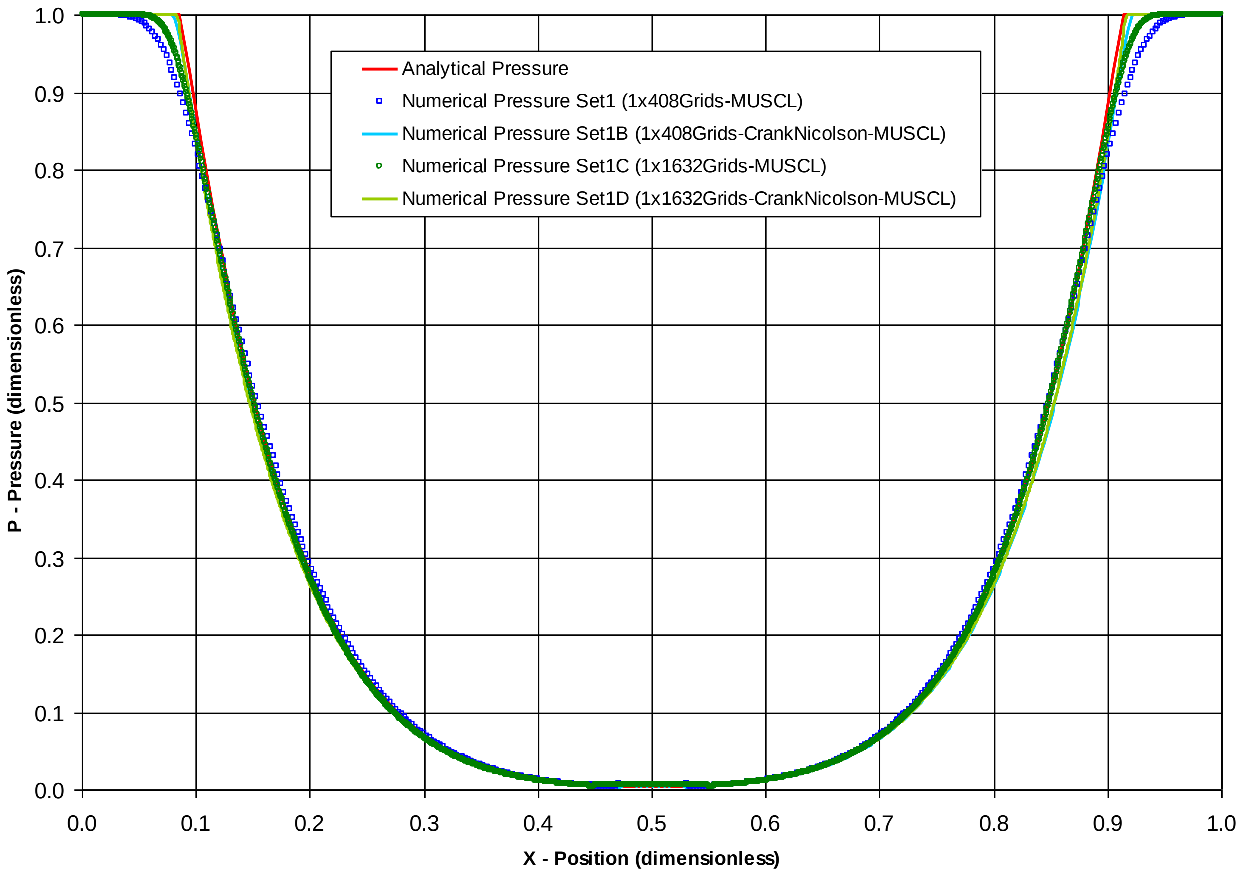
Pannala et al. (2005)

123 Problem

- Ideal gas in a tube is emptied from both ends of a tube with an initial velocity of ~2.7 times the speed of sound
- Initial p = 0.4 atm, T = 500 K, ρ = 0.2824 kg/m^3, v = +/- 1204.4 m/s
- Exact solution known from standard Riemann solver
  - Two rarefaction waves
  - a stationary contact discontinuity in the middle of the tube with p and ρ near zero
- Tests the capability of handling flows with very low p and ρ
- Tests the ability of the energy equation solver to handle the near 0/0 division (= p/ρ)

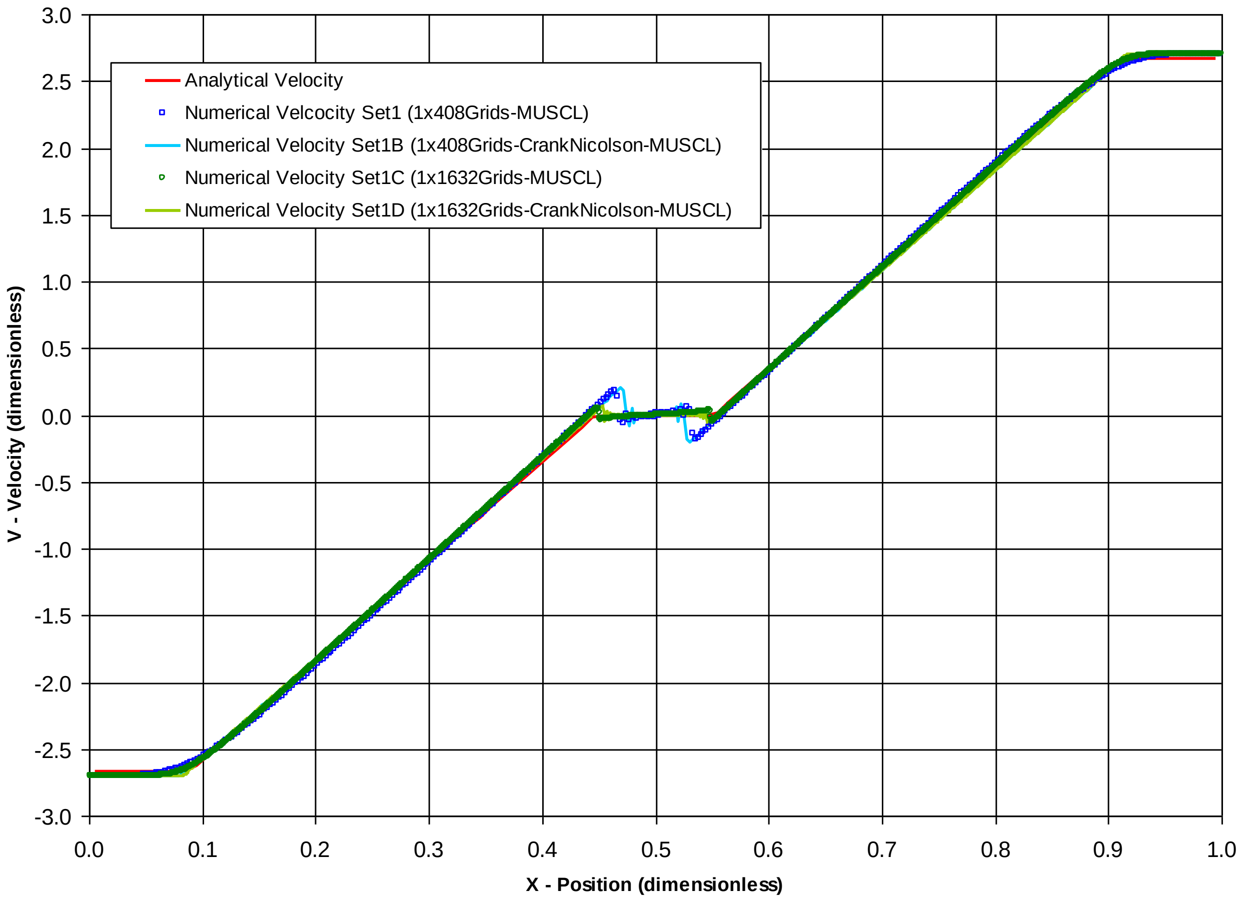
S. Dartevelle, Los Alamos, 2006

123 Problem – P



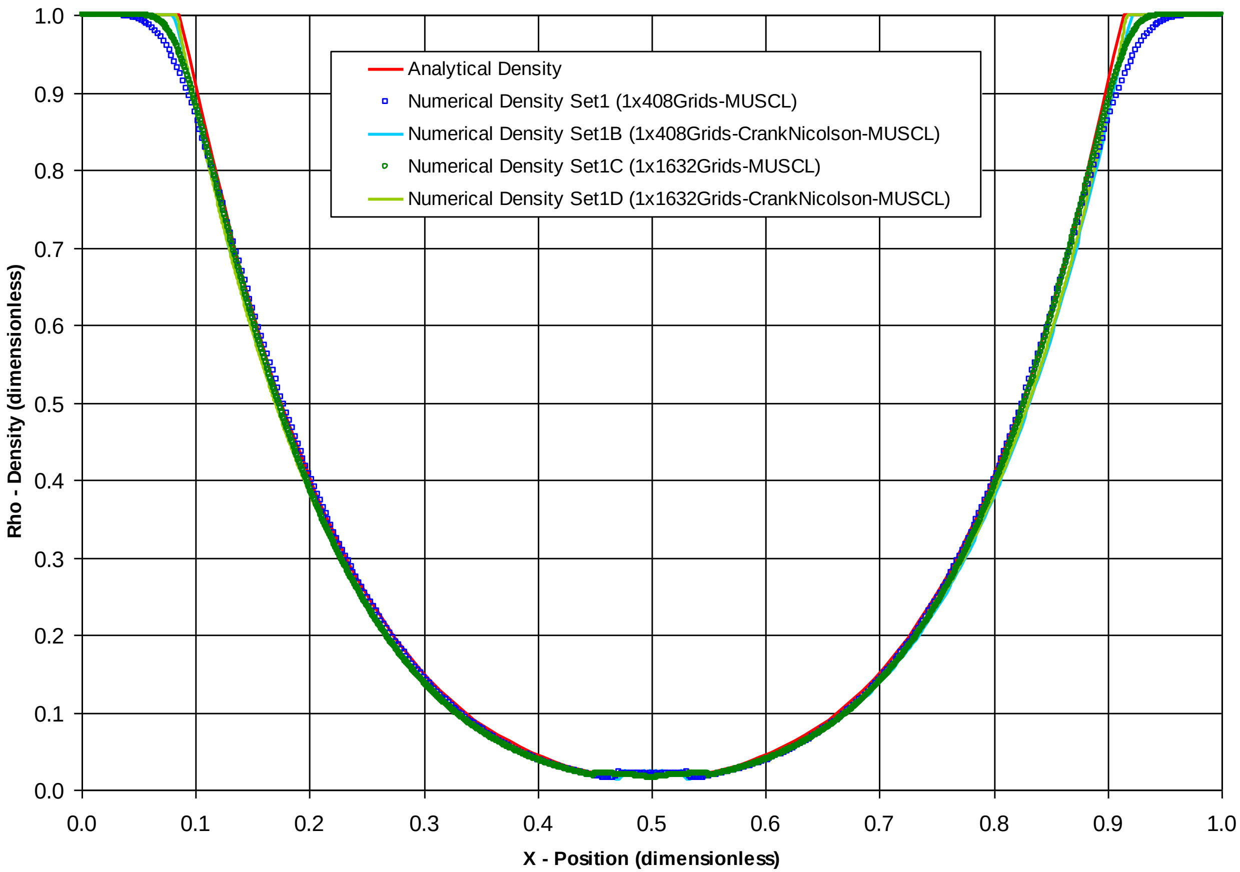
S. Dartevelle, Los Alamos, 2006

123 Problem - V



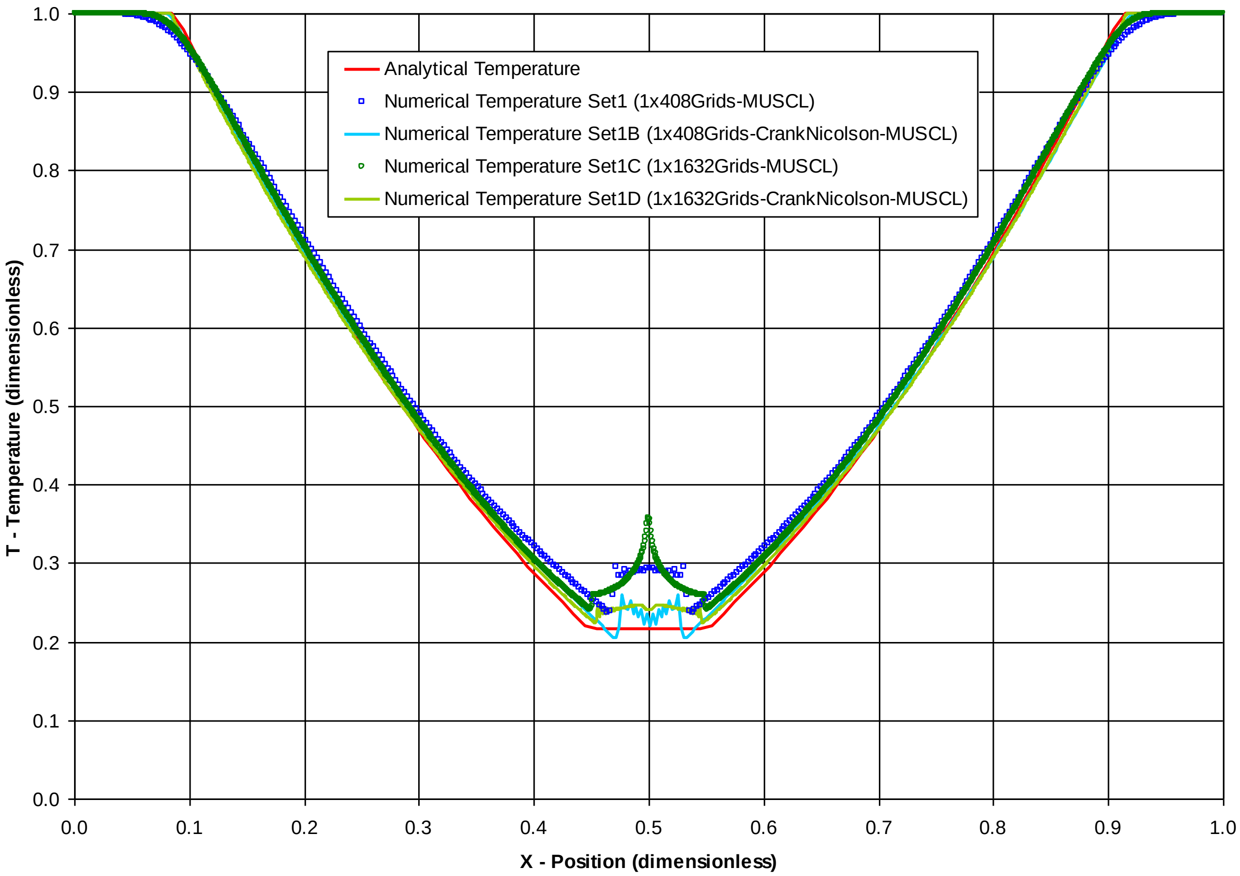
S. Dartevelle, Los Alamos, 2006

123 Problem - ρ



S. Dartevelle, Los Alamos, 2006

123 Problem - T



S. Dartevelle, Los Alamos, 2006

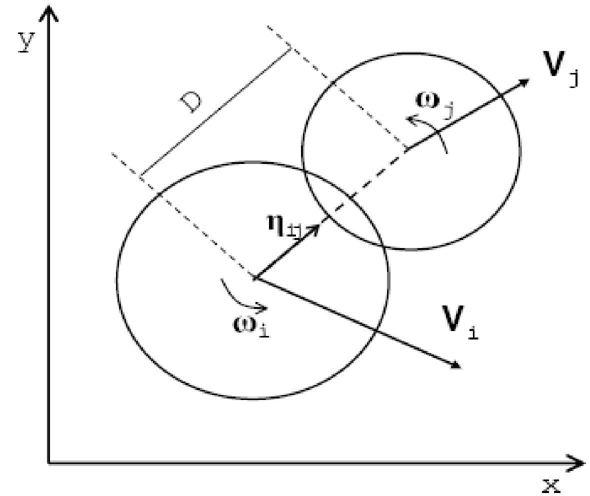
DEM Theory

Newton's Laws

$$\frac{d\mathbf{X}^{(i)}(t)}{dt} = \mathbf{V}^{(i)}(t),$$

$$m^{(i)}\frac{d\mathbf{V}^{(i)}(t)}{dt} = m^{(i)}\mathbf{g} + \mathbf{F}_{\mathrm{d}}^{(i\in k,m)}(t) + \mathbf{F}_{\mathrm{c}}^{(i)}(t),$$

$$I^{(i)}\frac{d\omega^{(i)}(t)}{dt} = \frac{1}{2}D^{(i)}\boldsymbol{\eta}\times\mathbf{F}_{\mathrm{c}}^{(i)}(t),$$

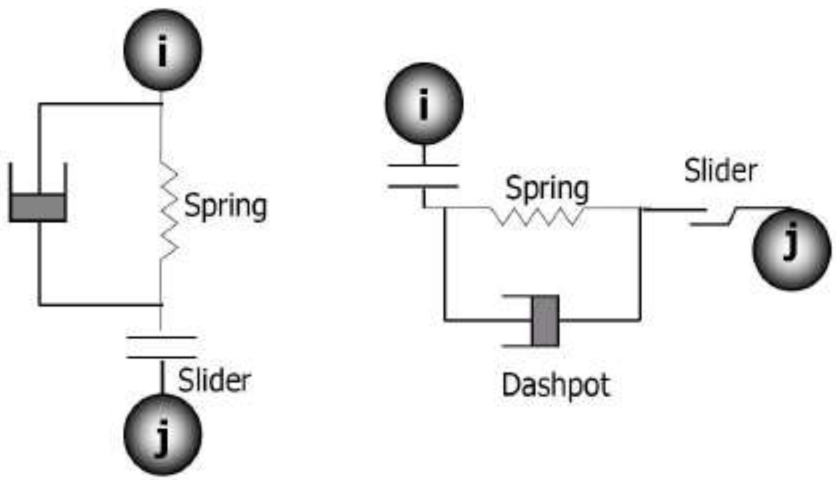


Soft-sphere model

$$\mathbf{F}_{\mathrm{c}}^{(i)}(t) = \sum_{\substack{j=1\\ j\neq i}}^{N}\left(\mathbf{F}_{ij}^{\mathrm{S}}(t) + \mathbf{F}_{ij}^{\mathrm{D}}(t)\right),$$

$$\mathbf{F}_{\mathrm{n}ij}(t) = \mathbf{F}_{\mathrm{n}ij}^{\mathrm{S}}(t) + \mathbf{F}_{\mathrm{n}ij}^{\mathrm{D}}(t),$$

$$\mathbf{F}_{\mathrm{t}ij}(t) = \mathbf{F}_{\mathrm{t}ij}^{\mathrm{S}}(t) + \mathbf{F}_{\mathrm{t}ij}^{\mathrm{D}}(t).$$



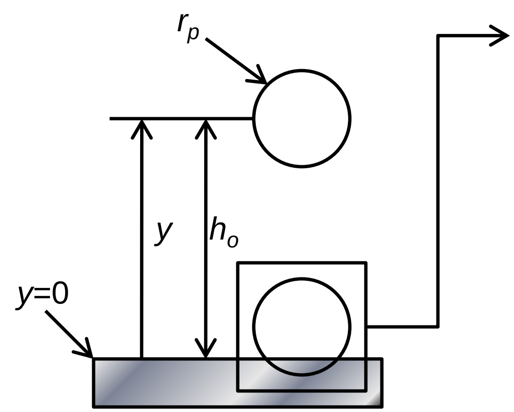
Linear-sprint dashpot (default model)

$$\eta_{\mathrm{n}m\ell} = \frac{2\sqrt{m_{\mathrm{eff}}k_{\mathrm{n}m\ell}}\,|\ln e_{\mathrm{n}m\ell}|}{\sqrt{\pi^2 + \ln^2 e_{\mathrm{n}m\ell}}}$$ normal dashpot

Case 1: Freely Falling Particle

r_p =10cm,
ρ_p =2.6g/cm^3
g =980cm/s^2
h_o =50cm

- **A smooth particle freely falling under gravity from its initial position bounces upon collision with a fixed wall**
- **Motion described in three stages: free fall, contact, rebound**



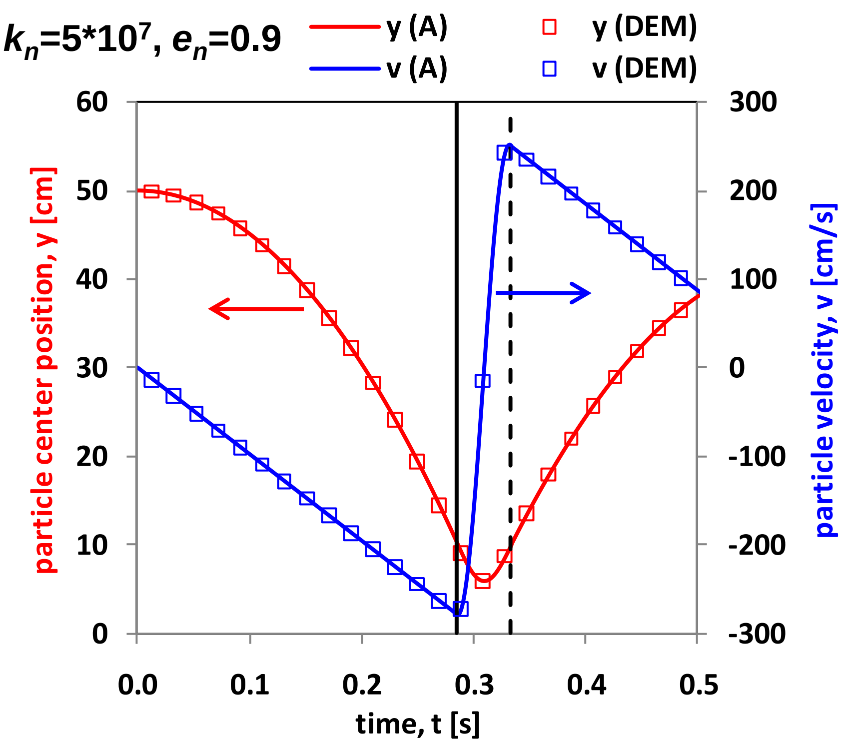
Contact Stage:

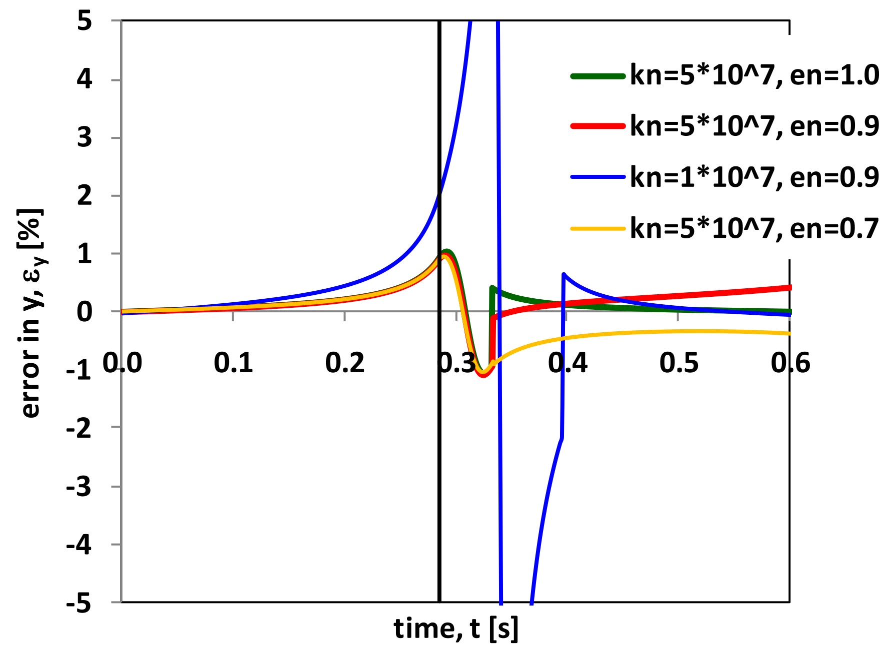
$$\ddot{y} = F_b + F_k + F_d$$

$$F_b = -g$$

$$F_k = -\frac{k}{m_p}\left(y - r_p\right)$$

$$F_d = -\frac{\eta_n}{m_p}\dot{y}$$

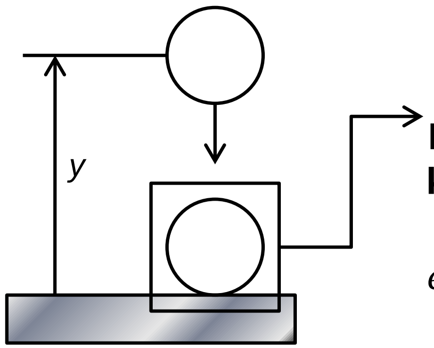




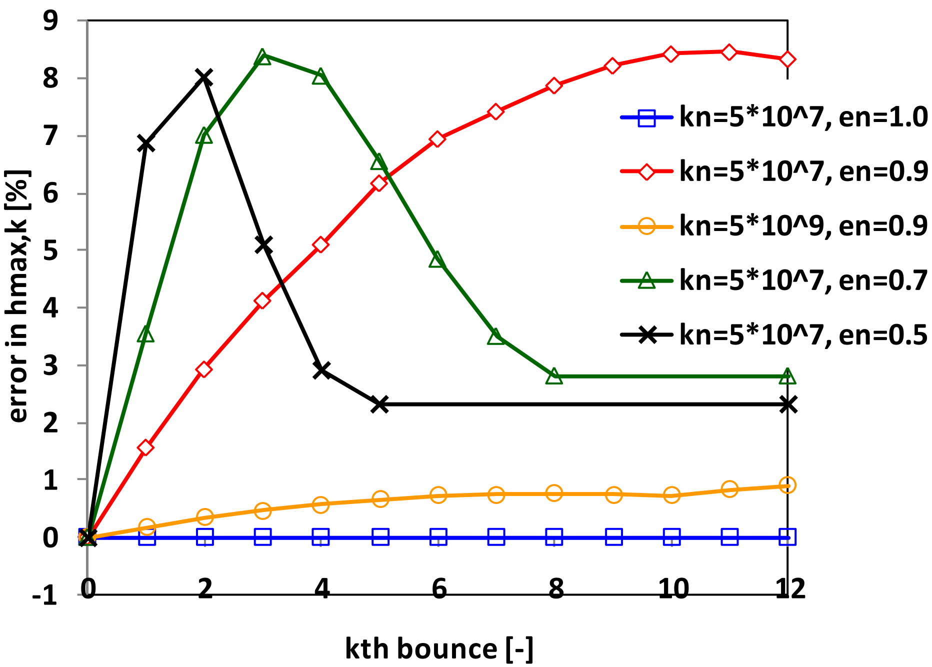
Following the work of Chen et al., Int. J. of Geomech., 2007

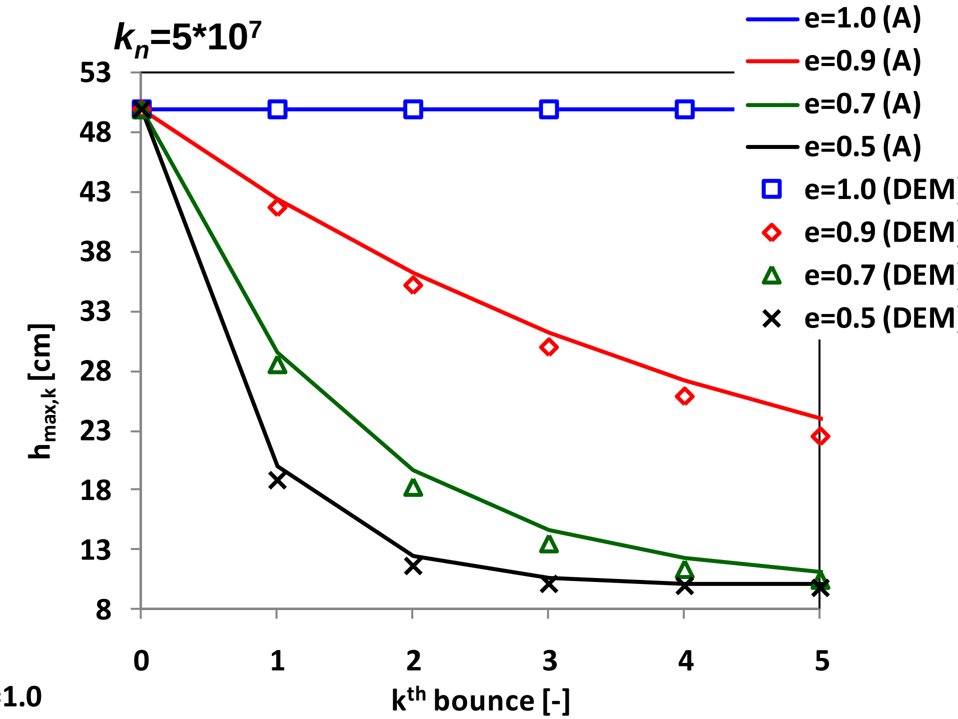
Case 1: Comparison with Hard-Sphere Model

- **No contact stage : instantaneous collision**



$$e = -\left(\frac{V_{post}}{V_{pre}}\right)$$



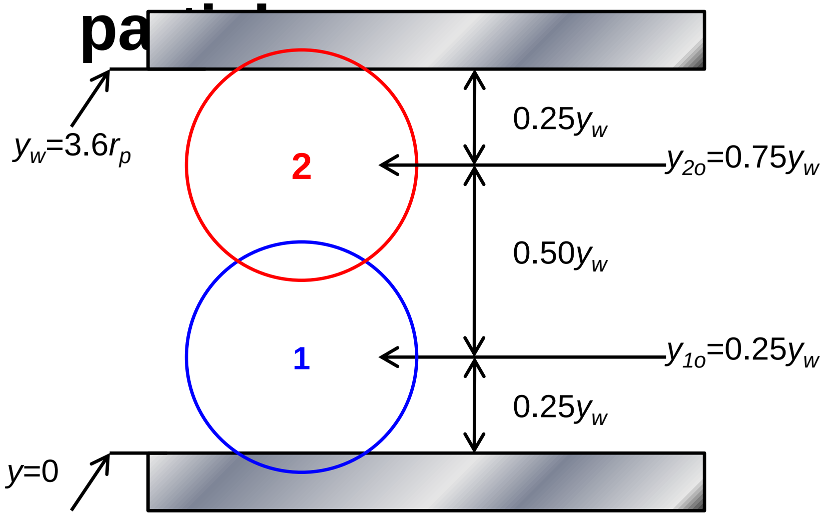


Error essentially reflects difference in hard-sphere vs. soft-sphere treatment

Case 2: Two Stacked Particles

r_p =0.05cm,
ρ_{p1} =20g/cm^3
ρ_{p2} =10g/cm^3
k_n =10^{6}dyne/c
g =980cm/s^2

- **A system of two stacked particles compressed between two fixed walls under gravity**
- **Equal size particles**
- **Top particle is twice as dense as upper pa**



Particle 1 force balance:

$$\ddot{y}_1 = F_{1b} + F_{1kw} + F_{12k} + F_{1dw} + F_{12d}$$

$$F_{1b} = -g \qquad F_{1kw} = -\frac{k_{nw}}{m_1}\left(y_1 - r_p\right)$$

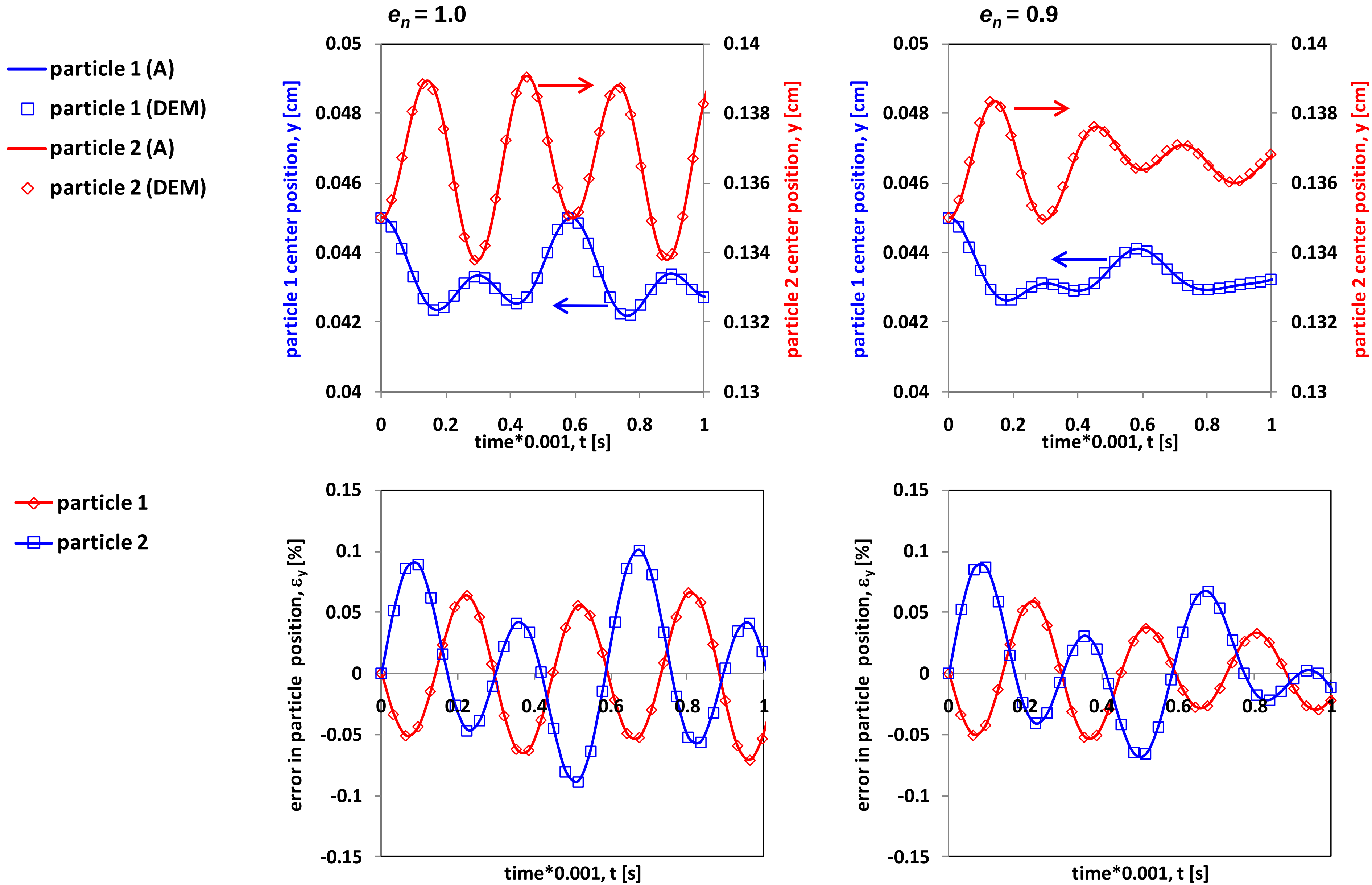
$$F_{12k} = -\frac{k_n}{m_1}\left(2r_p - \left(y_2 - y_1\right)\right)$$

$$F_{1dw} = -\frac{\eta_{n1w}}{m_1}\dot{y}_1$$

$$F_{12d} = -\frac{\eta_{n12}}{m_1}\left(\dot{y}_1 - \dot{y}_2\right)$$

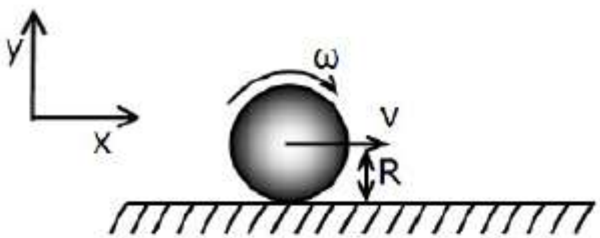
Following the work of Chen et al., Int. J. of Geomech., 2007

Case 2: Results



Case 3: Ball Slipping on a Rough Surface

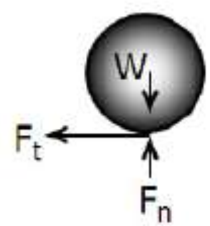
- **A ball is released on a rough surface with finite translational velocity (v_o) but zero angular velocity**
- **Sliding friction will create an angular velocity and reduce v_o until there is zero slip at point of contact ($v_x=\omega R$ at $t=t_s$)**

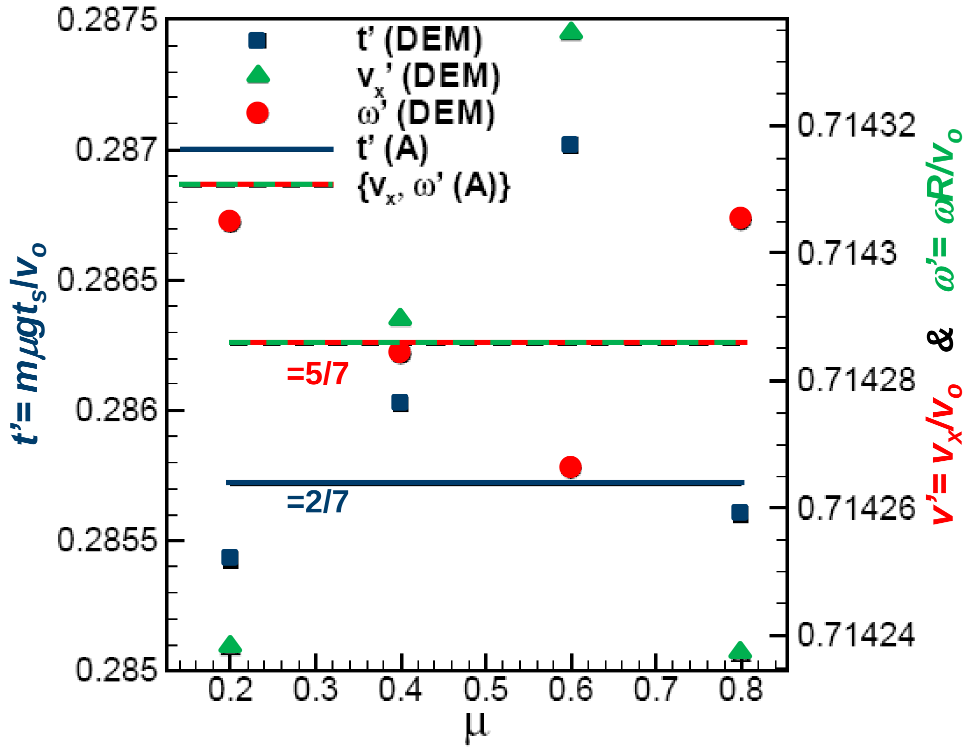


Particle motion:

$$\frac{dv_x}{dt} = \frac{-F_t}{m} - \mu g$$

$$\frac{d\omega}{dt} = \frac{\mu mgR}{I}$$





MFIX-CDEM Coupling

MFIX

- Drag on solids due to the gas (F_{gs})
- Drag on the gas due to solids ($-F_{gs}$)
- Gas velocity
- Pressure

CDEM

- **Multiple** Solid time steps:
  - CParticle-CParticle contact force
  - CParticle-Wall contact force
  - Drag force on each Cparticle
  - Pressure force on each Cparticle
  - Each Cparticle's position and velocity
- End of multiple solid time steps:
  - Volume fraction in each fluid cell
  - Volume averaged solid velocity in each cell

In every fluid time step

In every solid time step

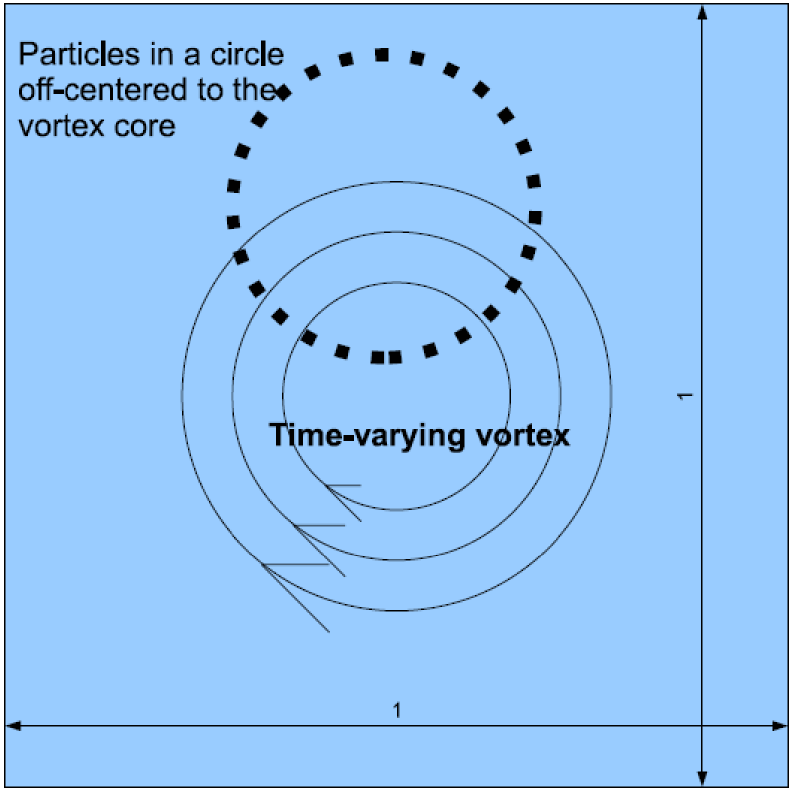
For next Fluid time step

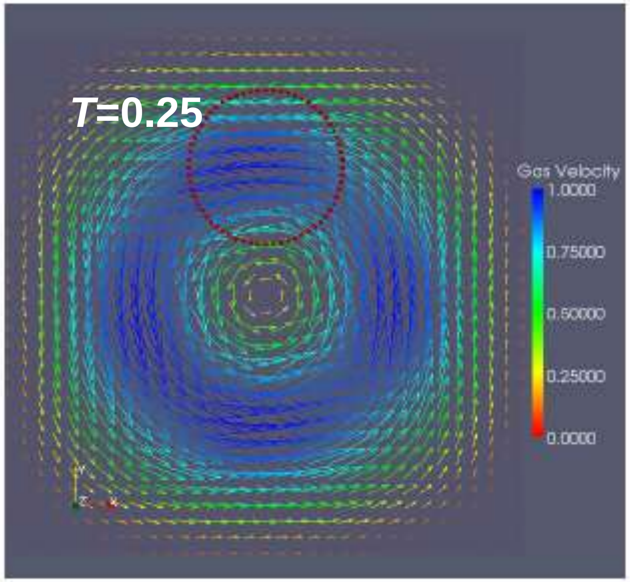
Case 4: Advection of a Circle in an Oscillating Vortex Field

- **Particles of zero mass are arranged in a circle (2D) or sphere (3D) and subject to an off-centered oscillating vortex field**

$$u = 2\sin^2(\pi x)\sin(2\pi y)\cos(\pi t/T),$$

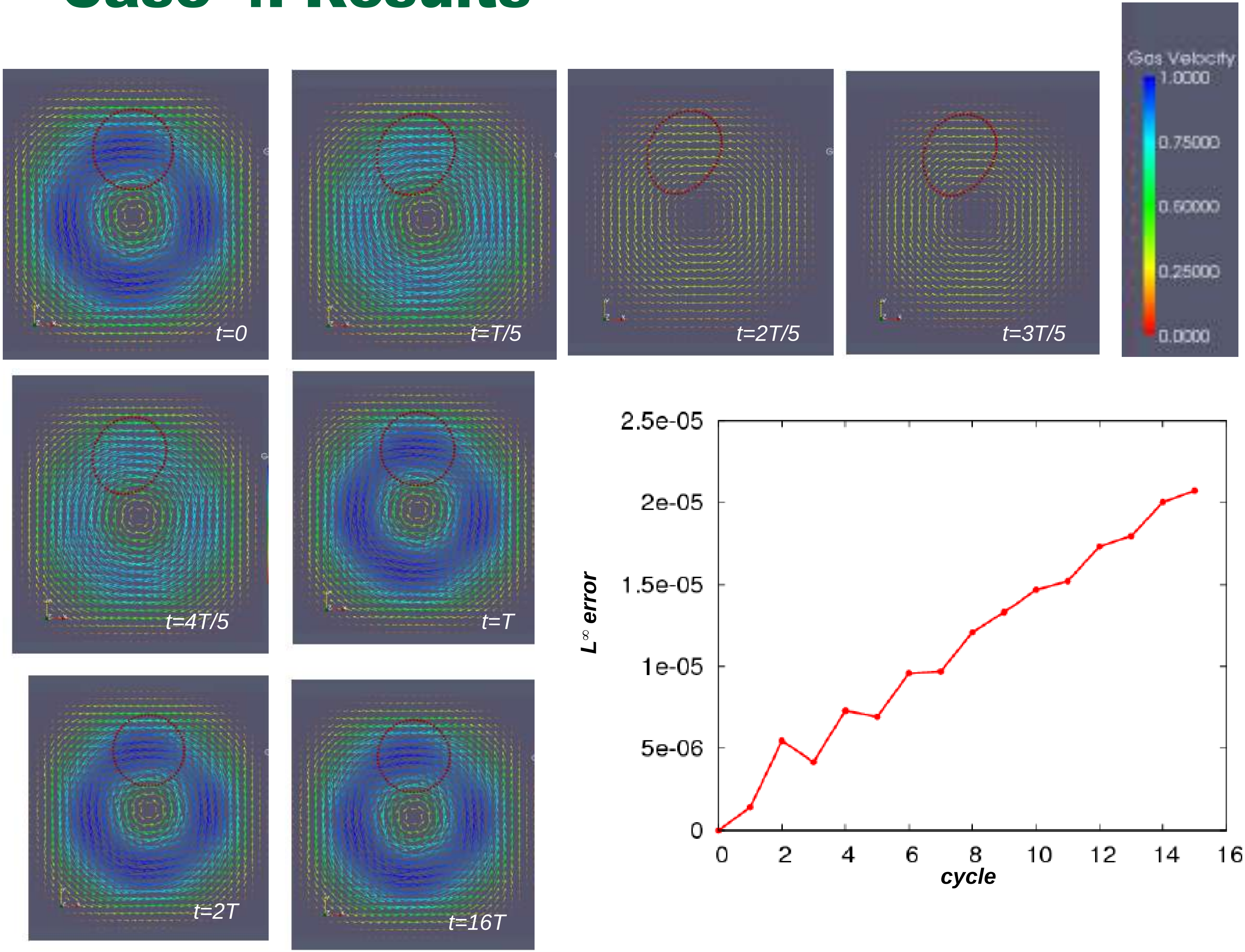
$$v = -\sin(2\pi x)\sin^2(\pi y)\cos(\pi t/T).$$





Setup has been by others used to test advection algorithms (Rider & Kothe, 1998; Liovic et al., 2006; Leveque, 1996)

Case 4: Results



Case 5: Particle Motion in Vortex

r_p =0.01cm,
ρ_p =1.8g/cm^3
v =0.05
μ_g =varied

- **Particles with finite mass are subject to a 2D vortex gas field**

$$u_{\mathrm{g}} = -\cos(k_x x)\sin(k_y y),$$

$$v_{\mathrm{g}} = \sin(k_x x)\cos(k_y y),$$

- The extent of gas-solids interaction is quantified by the particle Stokes number

$$\mathrm{St} = \frac{\tau_{\mathrm{p}}}{\tau_{\mathrm{g}}}$$

$$\tau_{\mathrm{p}} = \frac{\rho_{\mathrm{p}} {d_p}^2}{18\mu_{\mathrm{g}}}$$ particle response/ relaxation time

$$\tau_{\mathrm{g}} = \frac{L}{U}$$ fluid time-scale

St **<<** **1** ~ particles become flow tracers (drag dominates)

St **~** **O(1)** ~ particles follow local pathlines that circulate around large scale vortices

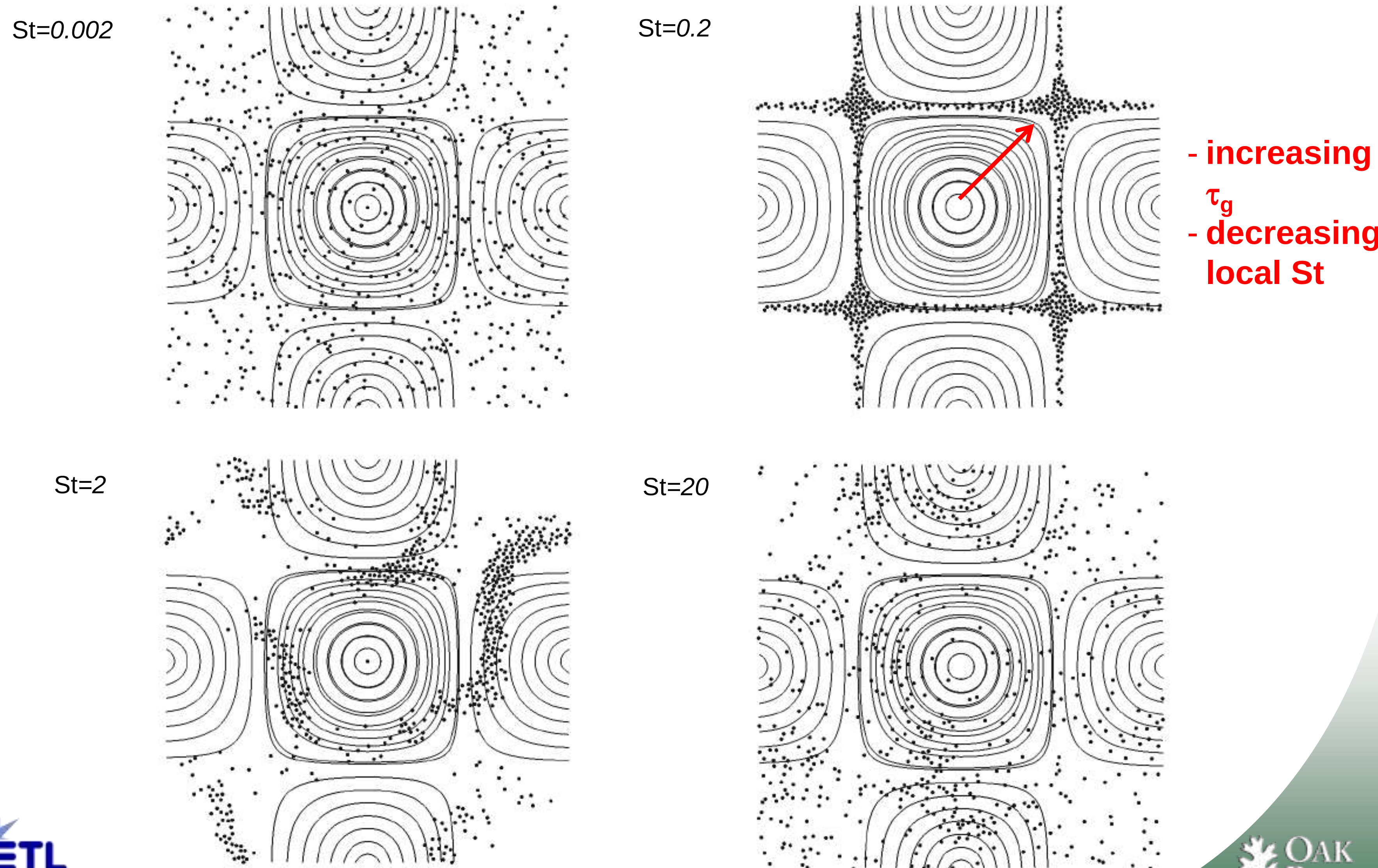
St **>>** **1** ~ particles move with their initial trajectories (inertia dominates)

NETL

Oak Ridge National Laboratory

Results

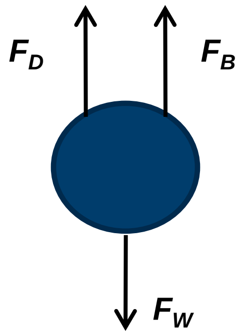
$$\mathrm{St} = \frac{\tau_p}{\tau_g}$$

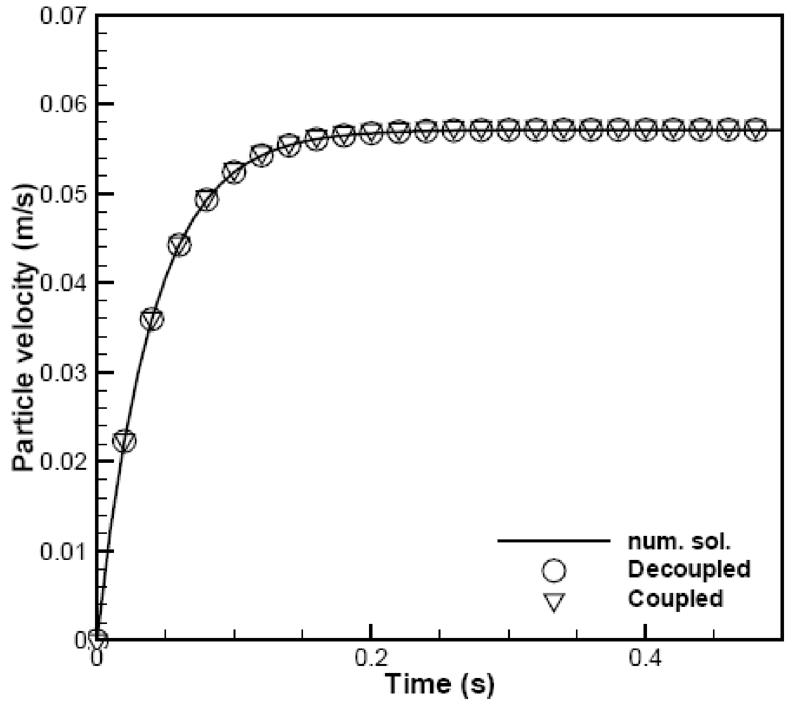


Case 6: Particle Terminal Velocity

r_p =0.01cm,
ρ_p =2.0g/cm^3
ρ_g =1.2x10^{-3}g/cm^3
μ_g =1.8x10^{-5} Pa.s
v_g =40cm/s

- **Terminal velocity of a single small particle freely falling under gravity through a gas phase**





Particle motion:

$$\frac{d\mathbf{v}_p}{dt} = \frac{\mathbf{g}(\rho_p - \rho_g)}{\rho_p} - \frac{3}{4}\frac{\rho_g\left|\mathbf{v}_p - \mathbf{v}_g\right|^2}{d_p\rho_p}C_d,$$

$$C_d = \frac{24}{\mathrm{Re}}(1 + 0.15\mathrm{Re}^{0.687})$$

Schiller & Naumann (1933)

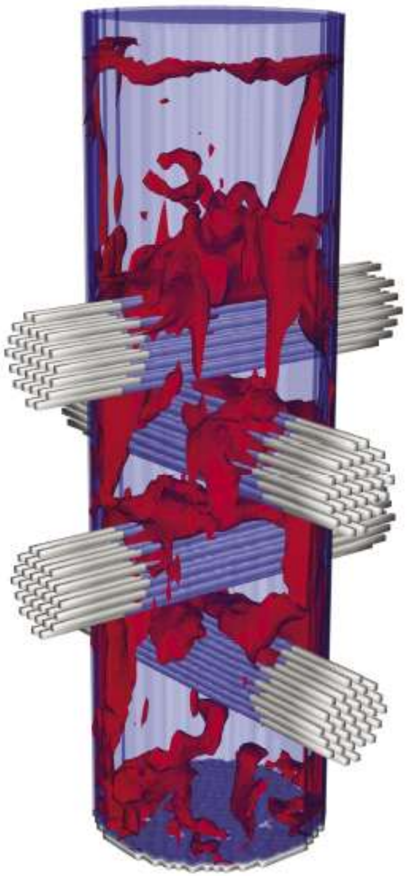
Summary of Verification Study

- Cases 1 and 2 involving a freely falling particle and two stacked particles targeted the implementation of the normal collision model and the time stepping algorithm
- Case 3 (ball slipping) targeted implementation of the tangential force model
- Cases 4 and 5 (advection & vortex flow) targeted the interpolation routines
- Case 6 (terminal velocity) served as a relatively simple test of the drag force
- All of these cases demonstrate fairly good agreement with the corresponding analytical solution (when available) or yielded the anticipated behavior

Garg, Galvin, Li and Pannala, Submitted to Powder Technology, 2010

MFIX Applications at NETL

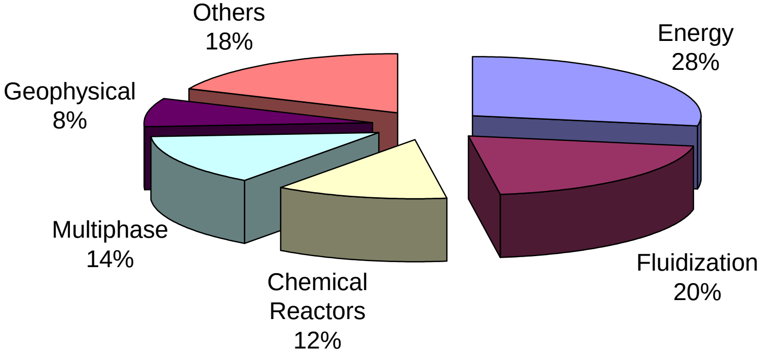
- Carbonizer, Foster Wheeler (1992-95)
- PyGAS™ gasifier, Jacobs Sirrine (1993-95)
- Ultra pure silicon production, MFDRC/Dow-Corning (1999-2003)
- Black liquor gasifier, Georgia Pacific (2003-04)
- Entrained flow gasifier, Boeing Rocketdyne (2005-)
- Chemical Looping (2005-)



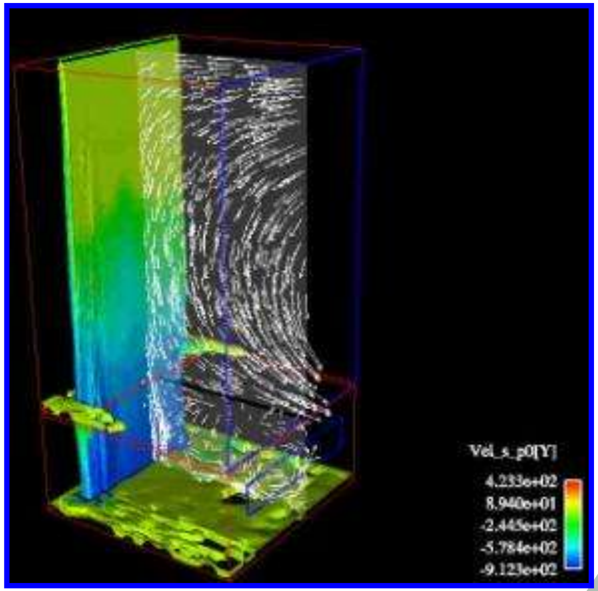
Simulation of a cold flow experiment conducted by University of Utah. Isosurfaces (red) for a void fraction value of 0.7 was used to determine gas by-passing behavior. C. Guenther (NETL)/G. Foss (PSC)

MFIX Applications at Labs

- **Yucca mountain nuclear repository (Los Alamos)**
- **Nuclear fuel particle coating (ORNL)**
- **Heterogeneous catalysis in micro-channel heat exchangers (Forschungszentrum Karlsruhe GmbH)**
- **Evaporating spray jet in a gas–solids suspension flow. (ANL)**
- **Solar collector (Sandia)**



Categories of MFIX applications



Solar collector model; C.Guenther, (NETL) and N. Siegel (Sandia)

MFIX Applications at Universities

Institution	Significant Research Outcome
Iowa State University	(a) Developed Direct Quadrature Method of Moments (DQMOM) to simulate particle aggregation and breakage; (b) Implemented the novel algorithm in situ adaptive tabulation (ISAT) to solve complex chemistry calculations.
University of Rennes and McGill University	Modelling study of air-gravity conveyors (airslides), in which the flow of the granular material is enhanced by the air that is forced through the bottom of the conveying trough.
Heriot-Watt University	Simulate bubbling fluidised beds (Group A/B and B particles) and compare predictions with Electrical Capacitance Tomography data.
Princeton University	Used the software (a) to construct closure relations for filtered two-fluid models (b) to develop a frictional stress model
UMR CNRS 5503, ENSIACET/ INPT	Modeling of chemical vapor deposition process for ultra pure silicon production.
University of Saskatchewan	Modeling dense phase fluidized beds containing fine catalyst powder (e.g. FCC stripper).
University of Colorado	(a) Implementation of cohesive forces into the discrete-particle framework (b) Studying segregation/mixing of dense binary mixtures (c) Polydispersity theory.
U. of Washington	Simulate a) high Reynolds number volcanic eruptions and associated multiphase gravity currents, and b) low Reynolds number chaotic convection in magma chambers.

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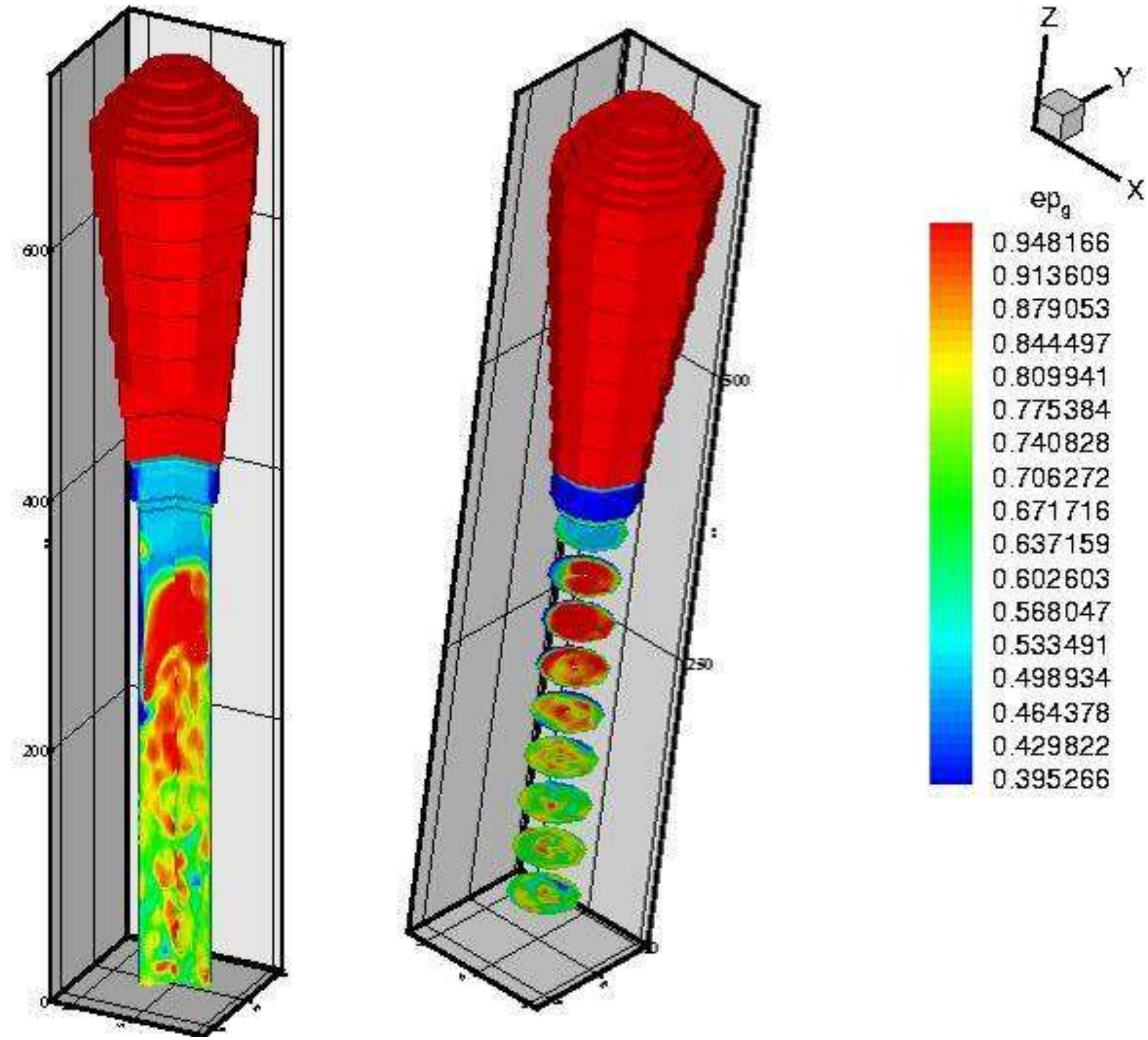
Polyethylene Reactor – Iowa State University/Univation

MFIX model of a polyethylene pilot-scale fluidized bed of Univation. validate the model and locate hot spots in the reactor. Ames/Iowa State/Univation. (Fan, Fox and Muhle 2005)

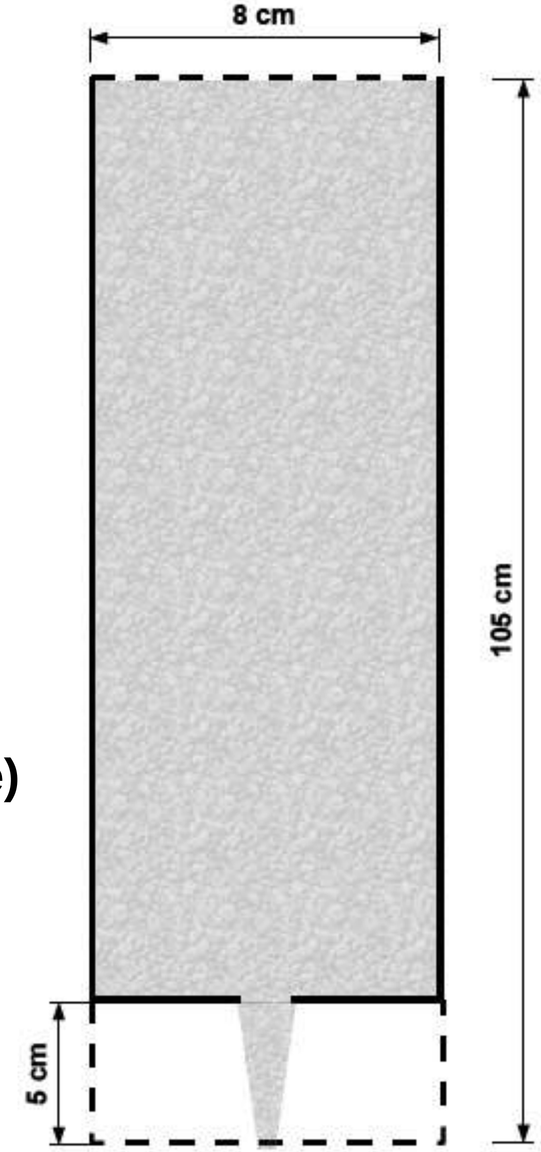


Outline of Presentation

- Introduction to Fluidization
  - Phenomena and Terminology
- Multiphase CFD
  - Introduction
  - Hydrodynamic Equations
  - Interphase Forces
  - Granular Stress
  - Gas-solids turbulence
  - Energy balance
  - Species balance
  - Numerical techniques
- MFIX Code
- Validation of hydrodynamics
  - Bubbling Fluidized Bed
  - Circulating Fluidized Bed
  - Spouted bed
- Fluidized bed reactors
- Industrial application of multiphase CFD

Bin Discharge Simulation - Setup

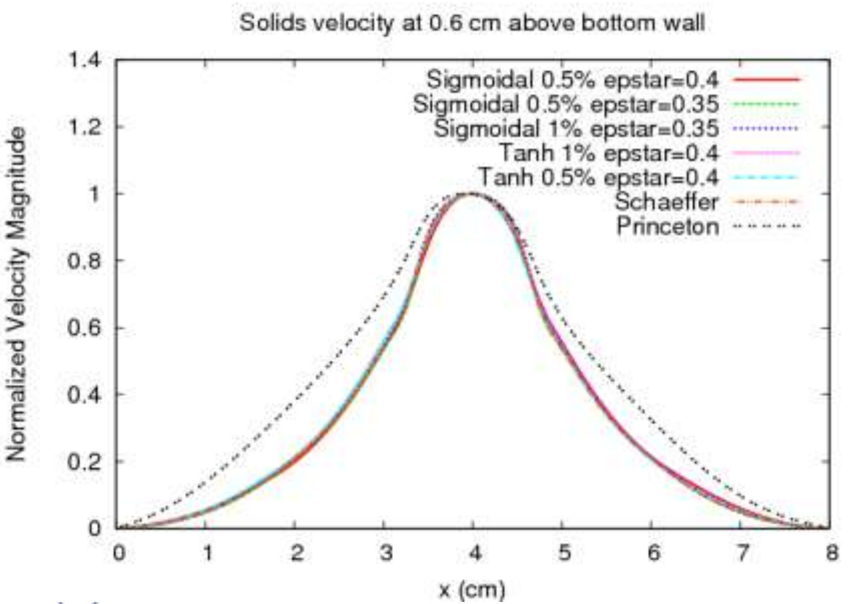
- Why bin discharge problem
  - A standard problem to test viscous/frictional stress formulation
  - Very simple correlation to compare
  - Easy to use in any laboratory to characterize particles
  - Simple to simulate
- Setup details
  - Solids Density = 2.9 gm/cm^3
  - Particle Diameter = 0.1 cm
  - Coefficient of restitution (particle-particle) = 0.91
  - Coefficient of restitution (particle-wall) = 0.91
  - Internal angle of friction = 28.5°
  - Void fraction at packing (ε*) = 0.35
  - Void fraction for Princeton model transition (ε_f_min) = 0.5

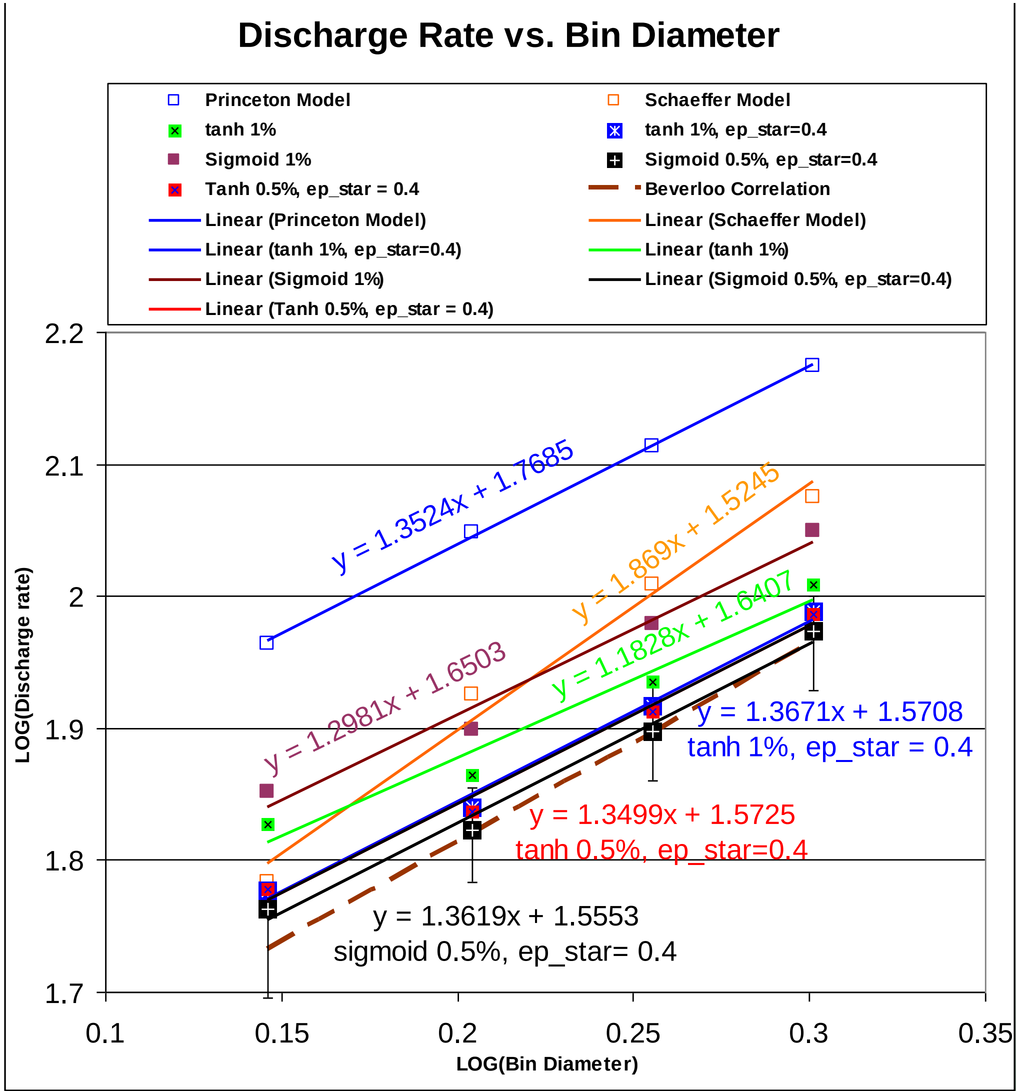


Pannala, Finney, Daw, Benyahia,
Syamlal and O'Brien, arXiv, 2008 (to be submitted)

Bin Discharge (with Max_mus)

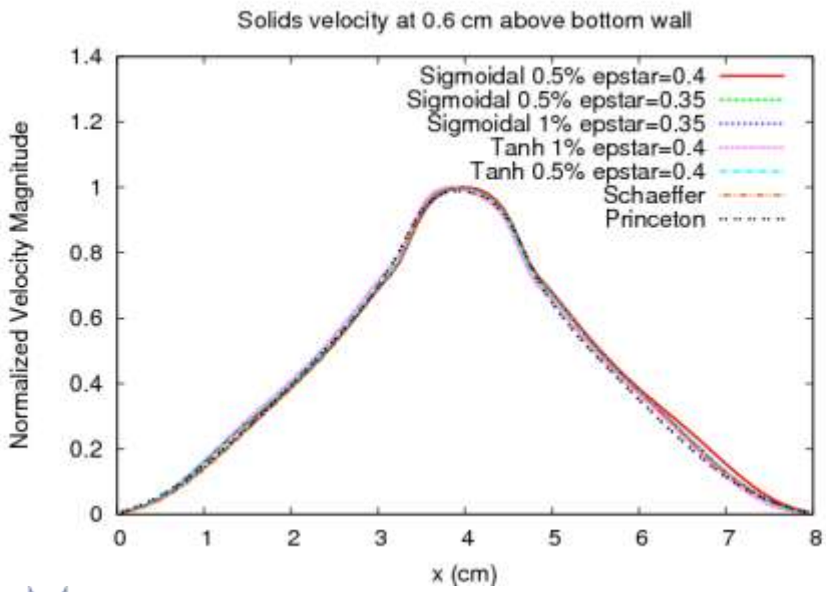
Model	Exponent	Constant
Beverloo Correlation	1.5	0.55-0.65
Princeton	1.35	1.08
Schaeffer Original	1.87	0.61
Schaeffer Blended (truncated and scaled sigmoid - 0.5%)	1.18	0.80
Schaeffer Blended (tanh - 1% and eps = 0.4)	1.36	0.68
Schaeffer Blended (truncated and scaled sigmoid - 1%)	1.3	0.82
Schaeffer Blended (truncated and scaled sigmoid - 0.5% and eps = 0.4)	1.35	0.68
Schaeffer Blended (tanh - 0.5% and eps = 0.4)	1.34	0.70

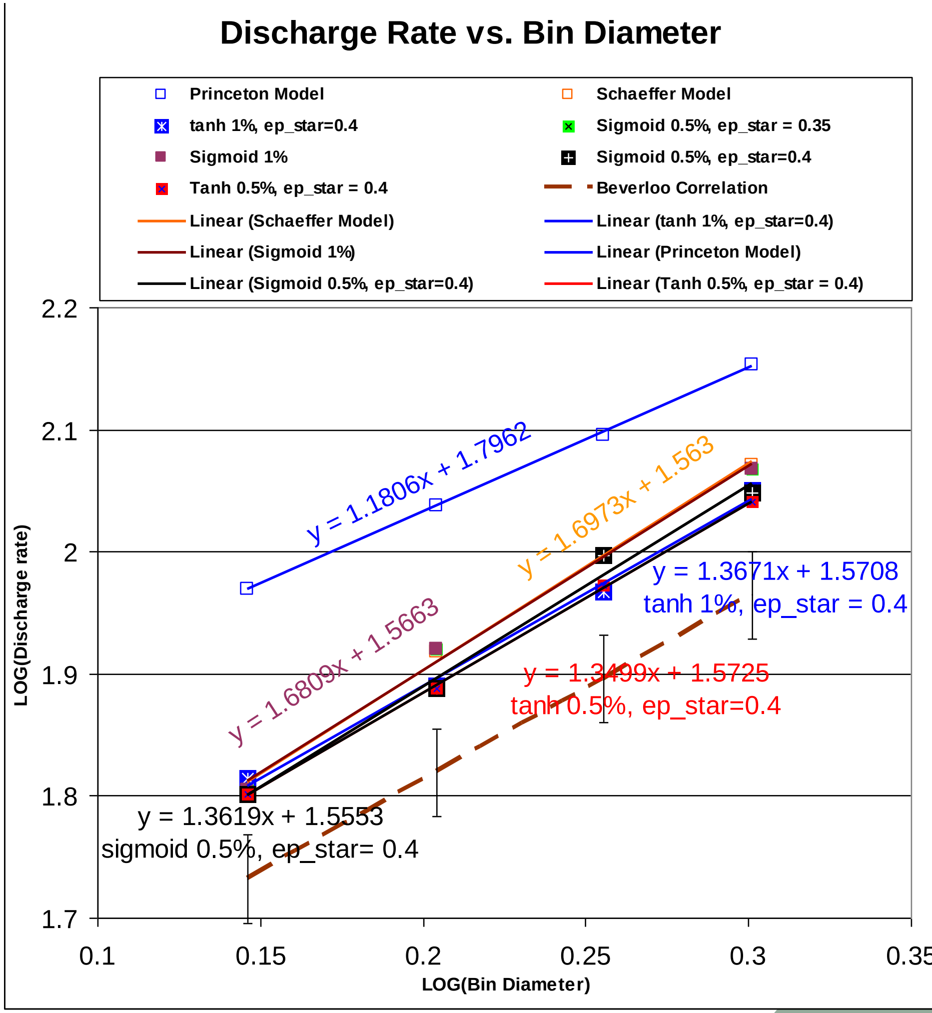




Bin Discharge (without Max_mus)

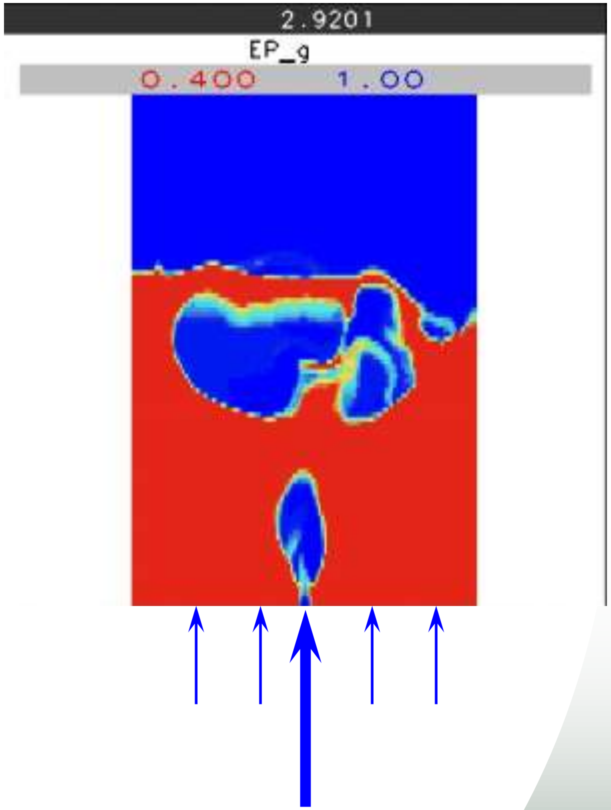
Model	Exponent	Constant
Beverloo Correlation	1.5	0.55-0.65
Princeton	1.18	0.80
Schaeffer Original	1.697	0.67
Blended (Sigmoid - 1% and ε* = 0.35)	1.68	0.68
Blended (Sigmoid - 0.5% and ε* = 0.35)	1.68	0.68
Blended (Sigmoid - 0.5% and ε* = 0.4)	1.36	0.67
Blended (tanh - 1% and ε* = 0.4)	1.37	0.68
Blended (tanh - 0.5% and ε* = 0.4)	1.35	0.68





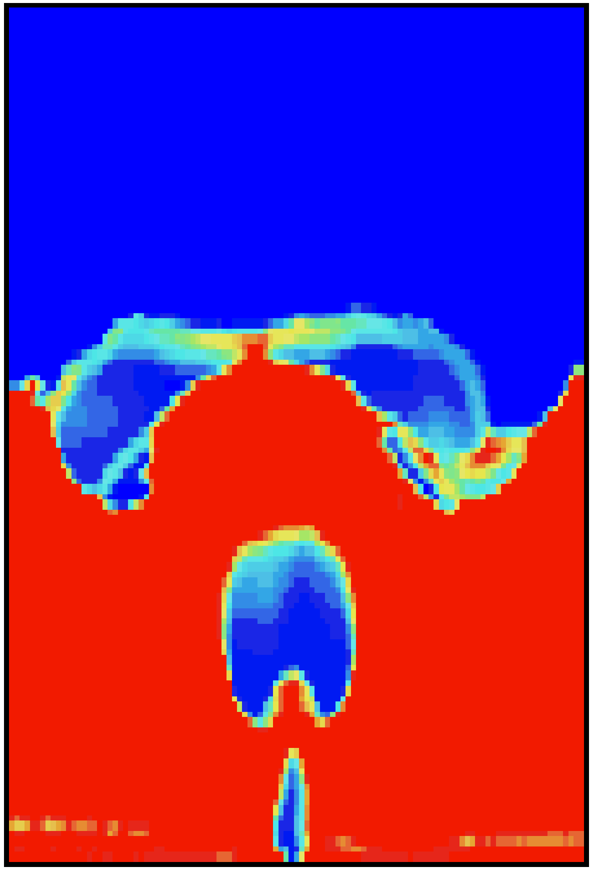
Fluidized Bed with Jet

- Gidaspow (1994)[1]
- 500 & 800 μm sand (2610 kg/m^3)
- Jet velocities: 3.5, 5.77, 9.88 m/s
- 2D bed with a central jet
- 0.39 m width x 0.58 m height
- 124 x 108 cells

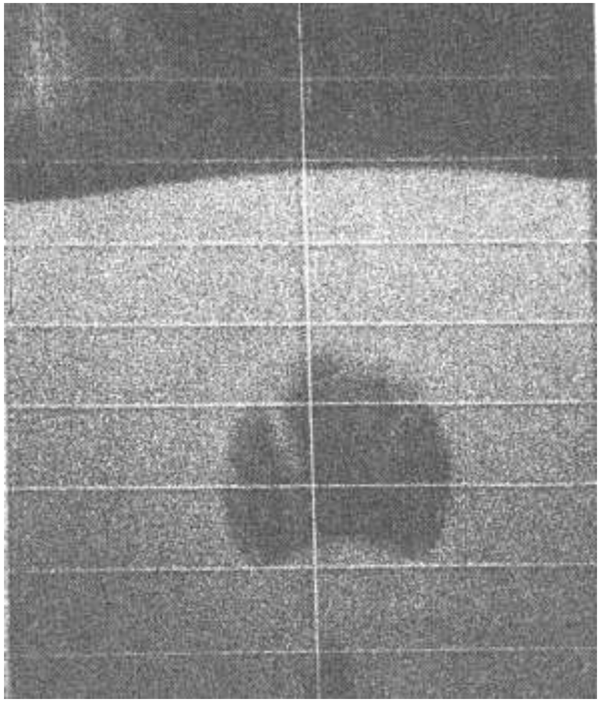


1. Sec.7.8.1; Syamlal (1997)

Bubble Size and Shape

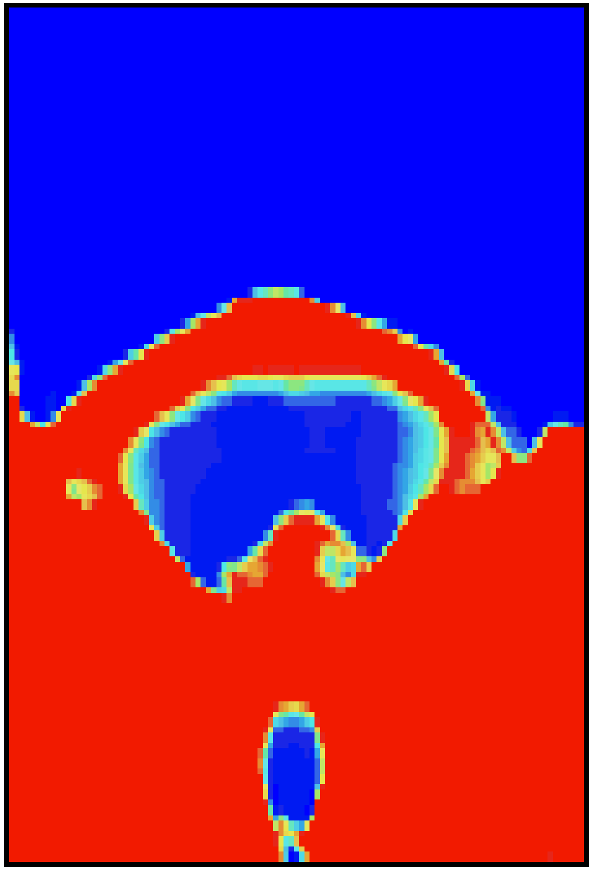


Syamlal (1997)

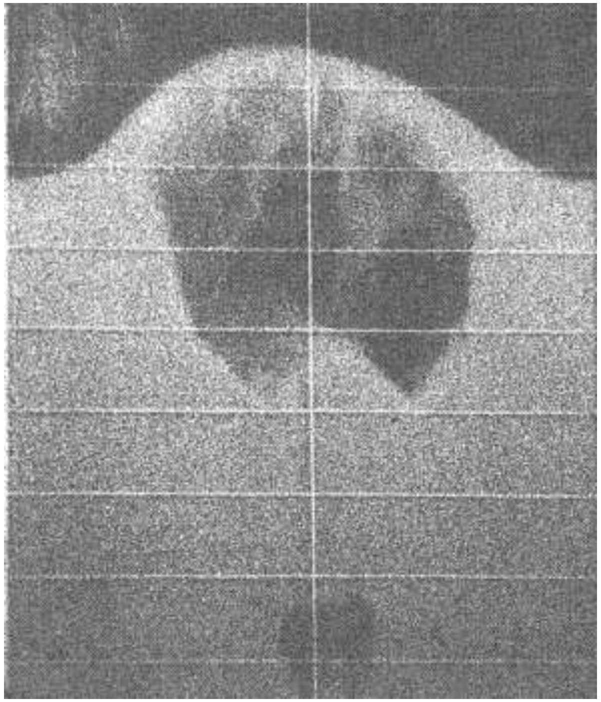


Gidaspow (1994) Fig. 7.10

Bubble Size and Shape

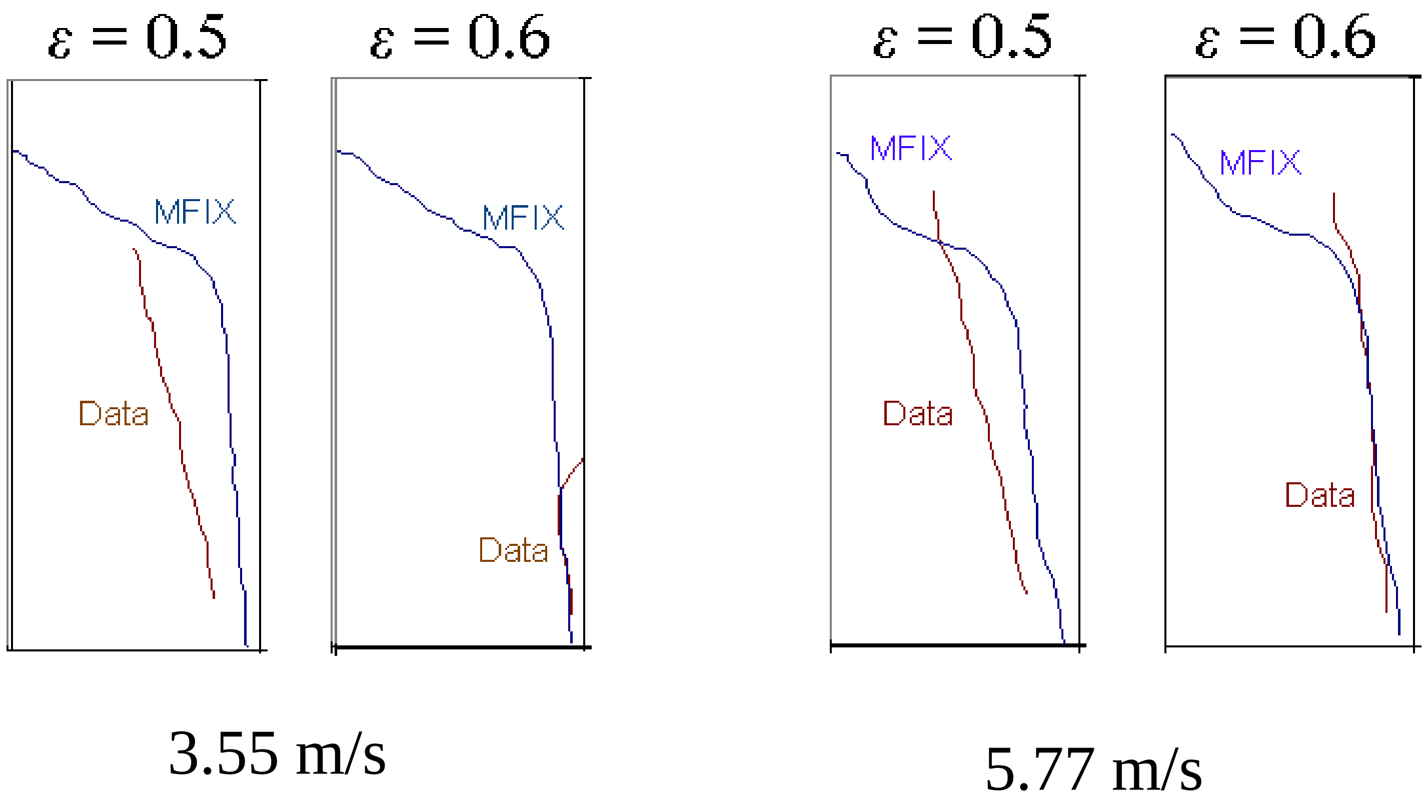


Syamlal (1997)



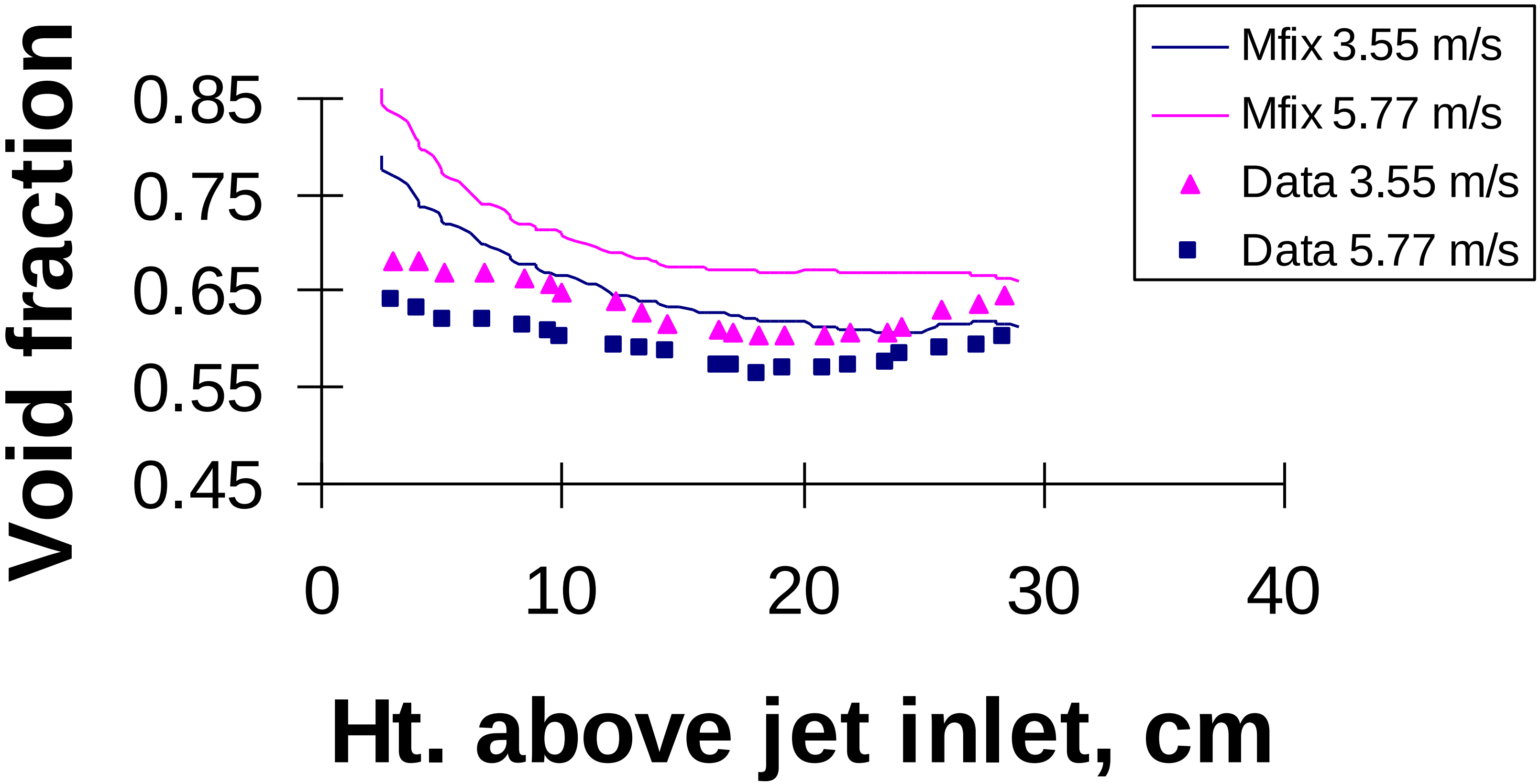
Gidaspow (1994) Fig. 7.11

Voidage Contours time average



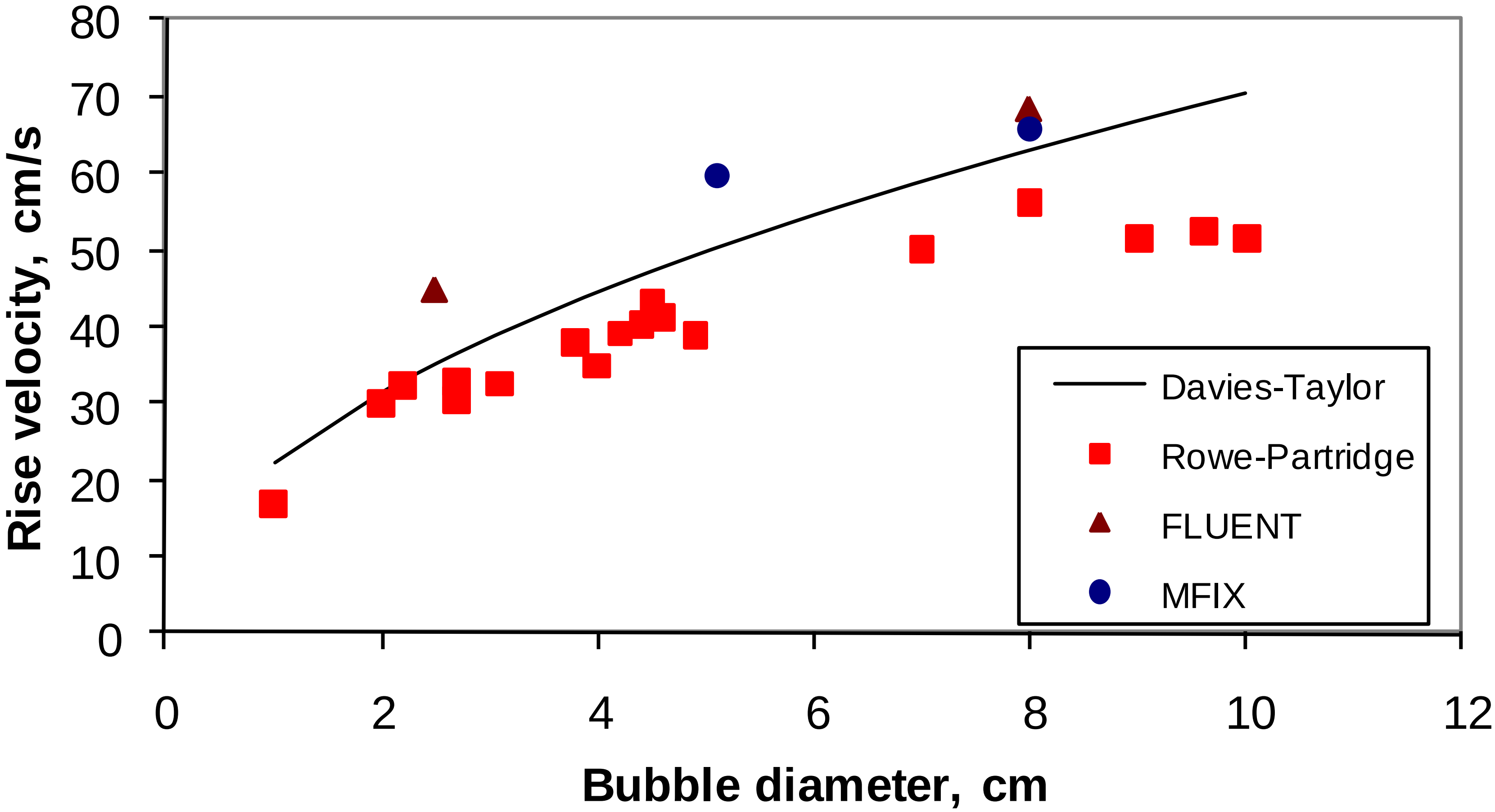
Syamlal (1997); Data - Gidaspow, Lin, and Seo (1983)

Centerline Voidage time average



Syamlal (1997); Data - Gidaspow and Ettehadieh (1983)

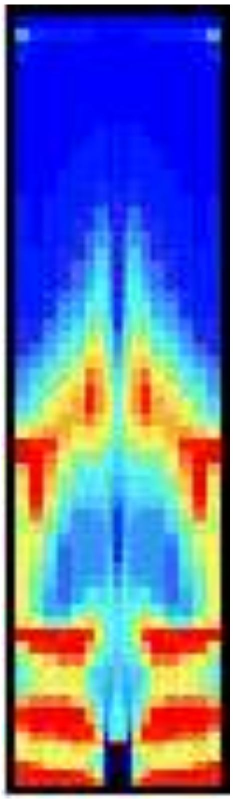
Bubble rise velocity



Rowe and Partridge (1962), Davidson and Harrison (1963), Syamlal and O'Brien (1989)

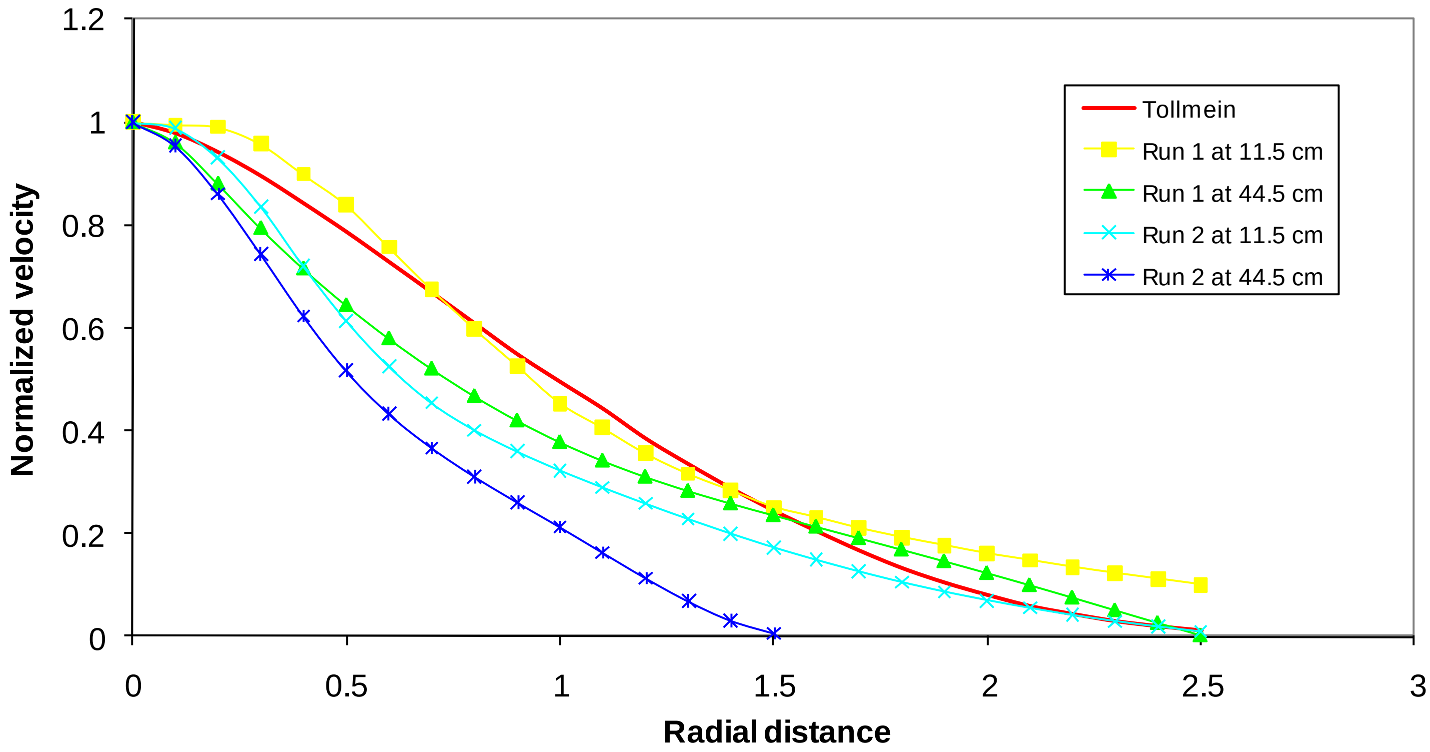
Jetting Fluidized Bed

- Yang and Keairns (1980)
- 0.28 cm Polyethylene (901 kg/m^3)
- Jet velocity 62 m/s, grid velocity 0.96 m/s
- 0.28 m dia x 2.1 m height
- 20x77 cells



Boyle and Sams (1997)

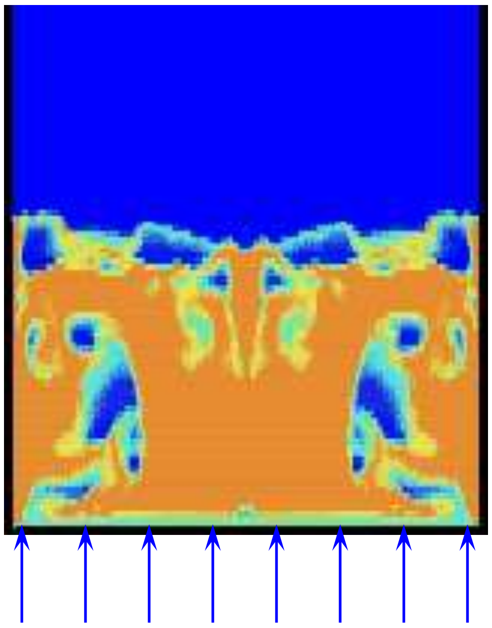
Jet Velocity Profile



Boyle and Sams (1997)

Uniform Fluidization

- **Halow and Nicoletti (1992)**
- **700 μm plastic (1460 kg/m^3)**
- **Uniform flow 1.04 U_{mf} - air**
- **3D cylindrical bed**
- **0.15 m diameter x 0.25 m height**
- **30 x 100 x 16 cells**



Bubble Properties
Average of 9 bubbles

	Data	MFIX
Frequency, s^{-1}	4.2	5.3
Diameter, cm	5.2	2.5
range, cm	(3.4 - 6.9)	(1.5 - 4.0)
Spacing, cm	10.7	4.4
range, cm	(2.4 - 23.)	(2.3 - 9.4)

Data -- Halow and Nicoletti (1992)

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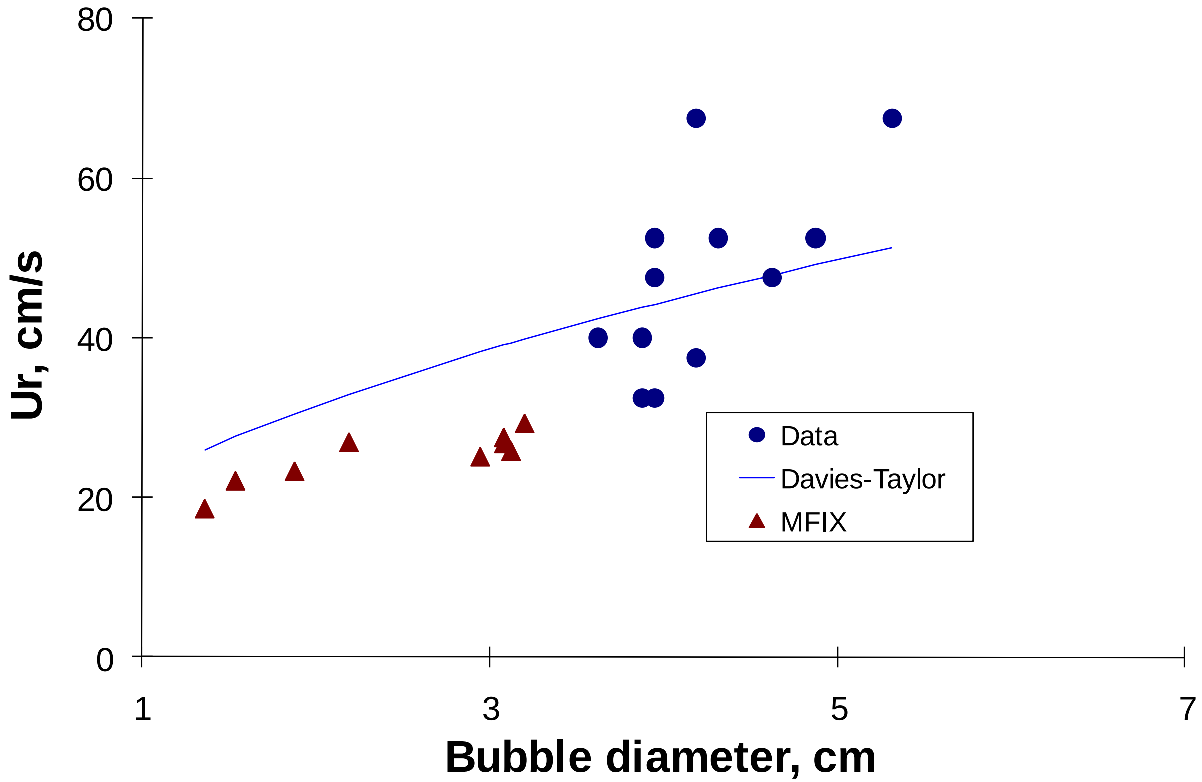
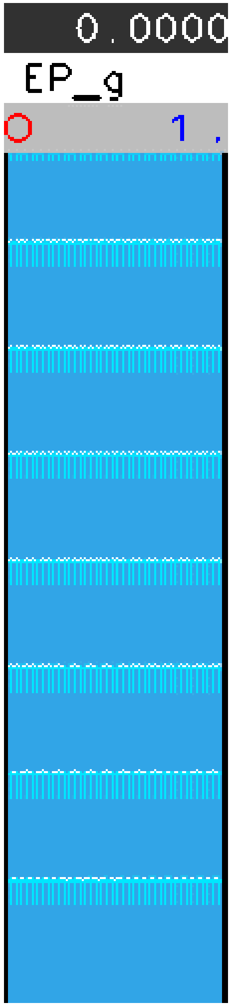
Bubble Rise Velocity



Data -- Halow and Nicoletti (1992)

Circulating Fluidized Bed

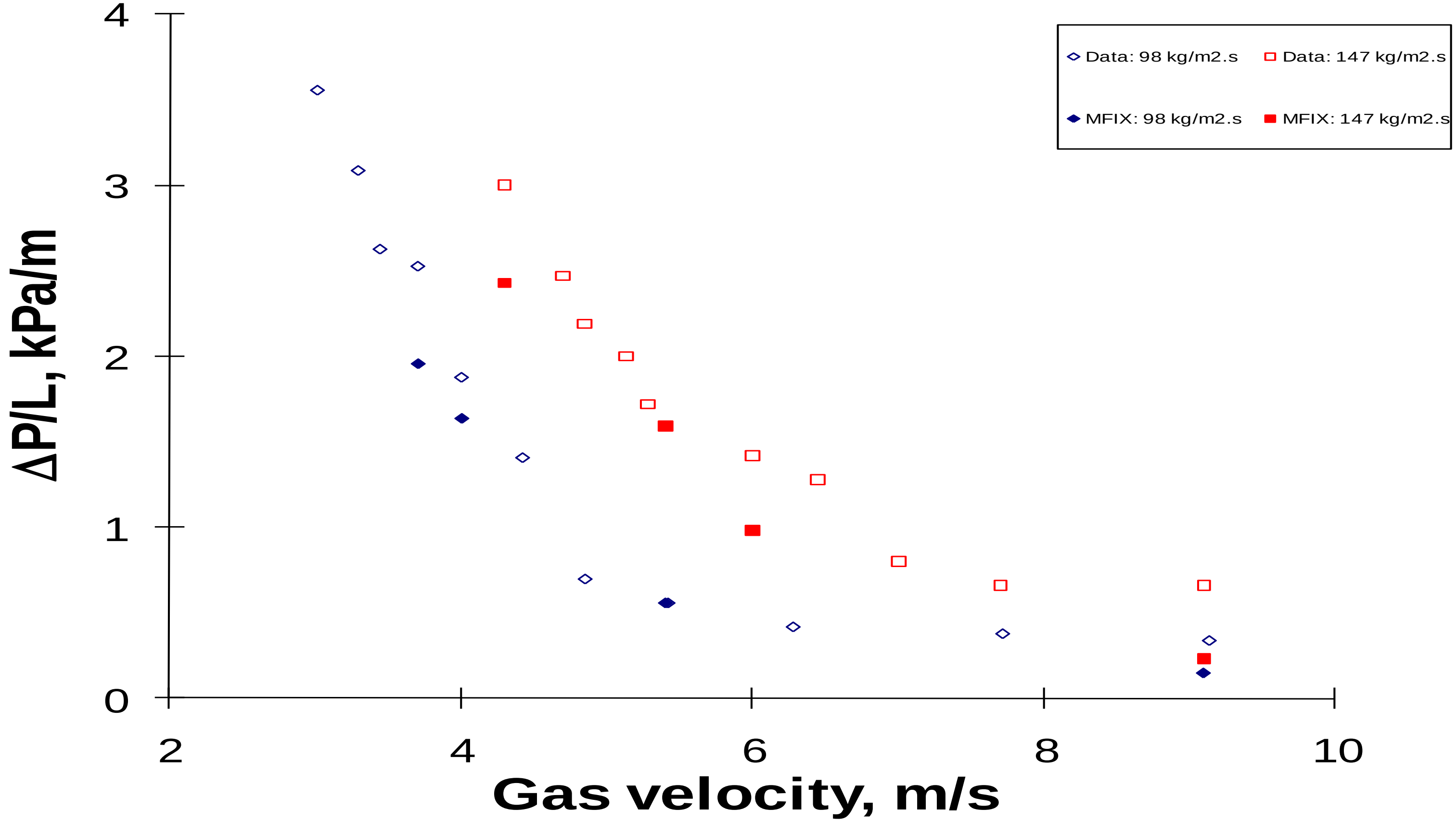
- **Bader, Findlay, and Knowlton (1988)**
- **76 μm FCC catalyst (1714 kg/m³)**
- **Solids flux: 98 and 147 kg/m².s**
- **V_{g0} : 3.7 - 9.1 m/s**
- **0.305 m dia x 12.20 m height**
- **2-D, cyl., 12 x 240 cells**



Periodic channel flow: Solids volume fraction (red-high, blue-low) and velocity vectors (white-gas, light blue – solids). Benyahia, Syamlal and O’Brien, 2005.

O’Brien and Syamlal (1993)

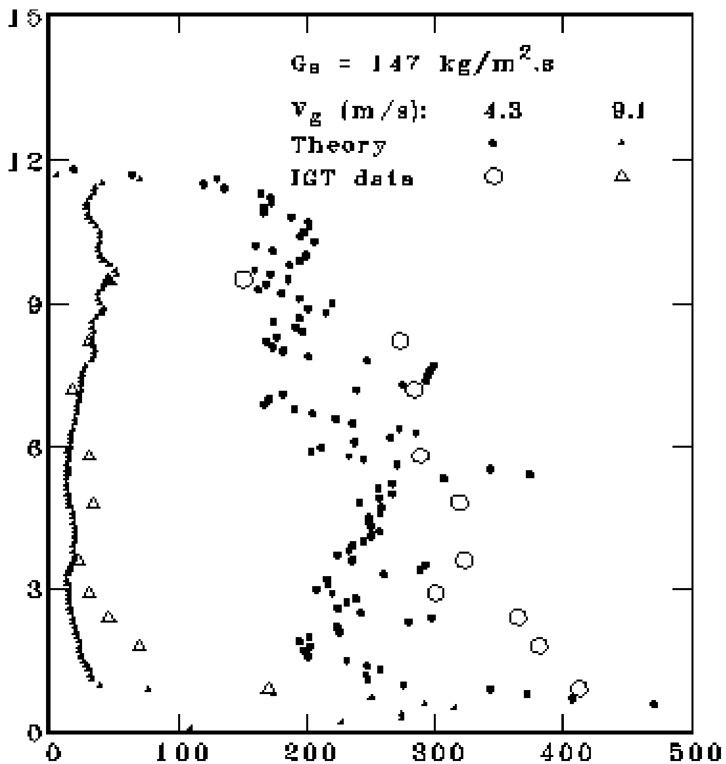
Pressure Drop Across CFB



Data -- Bader et al. (1988)

Solids Distribution in Riser

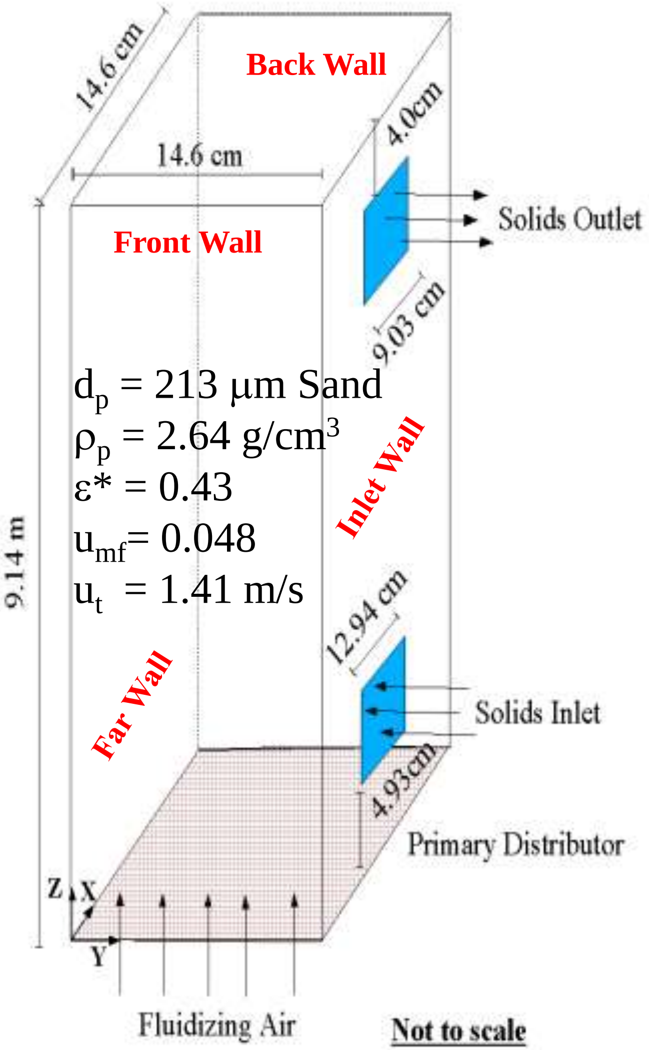
Height, m



Riser Density, kg/m3

Data -- Bader et al. (1988)

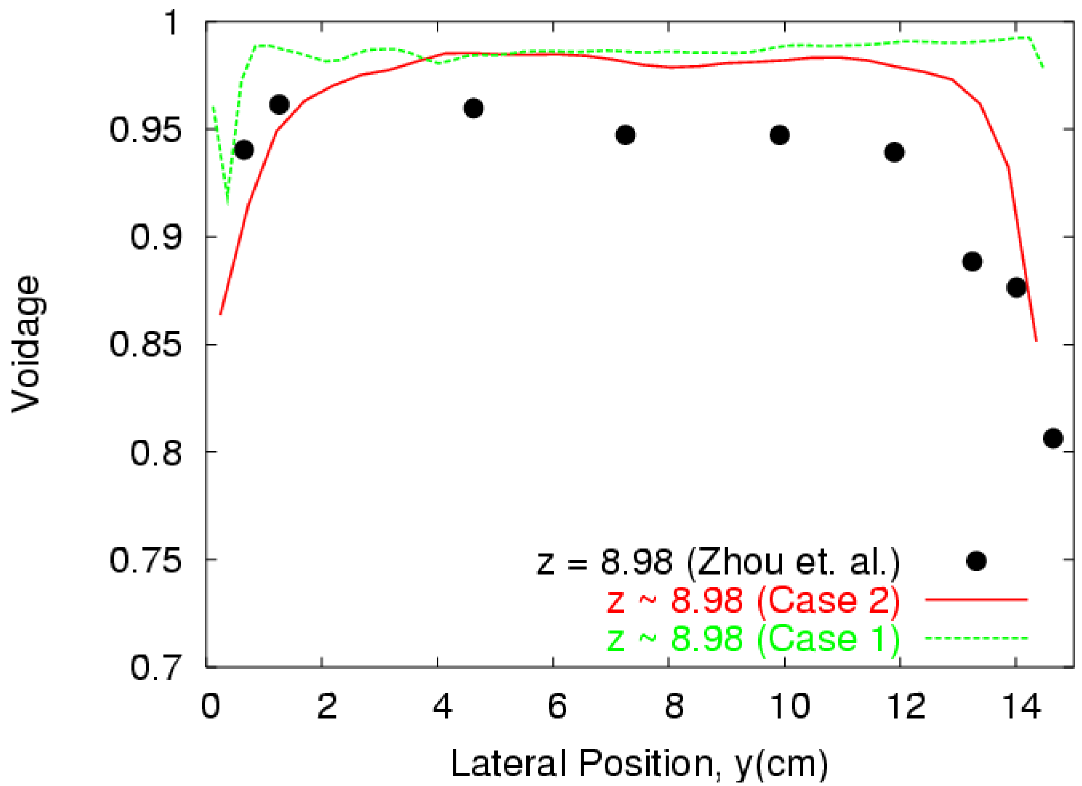
Square CFB



- Similar to the experiments of Zhou et. al. (Chem. Eng. Sci., 49, 3217-3226, 1994)
- Simplified because of Cartesian mesh (circular inlet and outlet are approximated by squares of same area)
- Various cases studied over the years
  - Different resolutions
  - Different drag formulations
  - Multiple particle sizes
  - Medium resolution (~250K cells with clustering at the inlet and outlet seems to work best)

Square CFB -- Lateral profiles of voidage

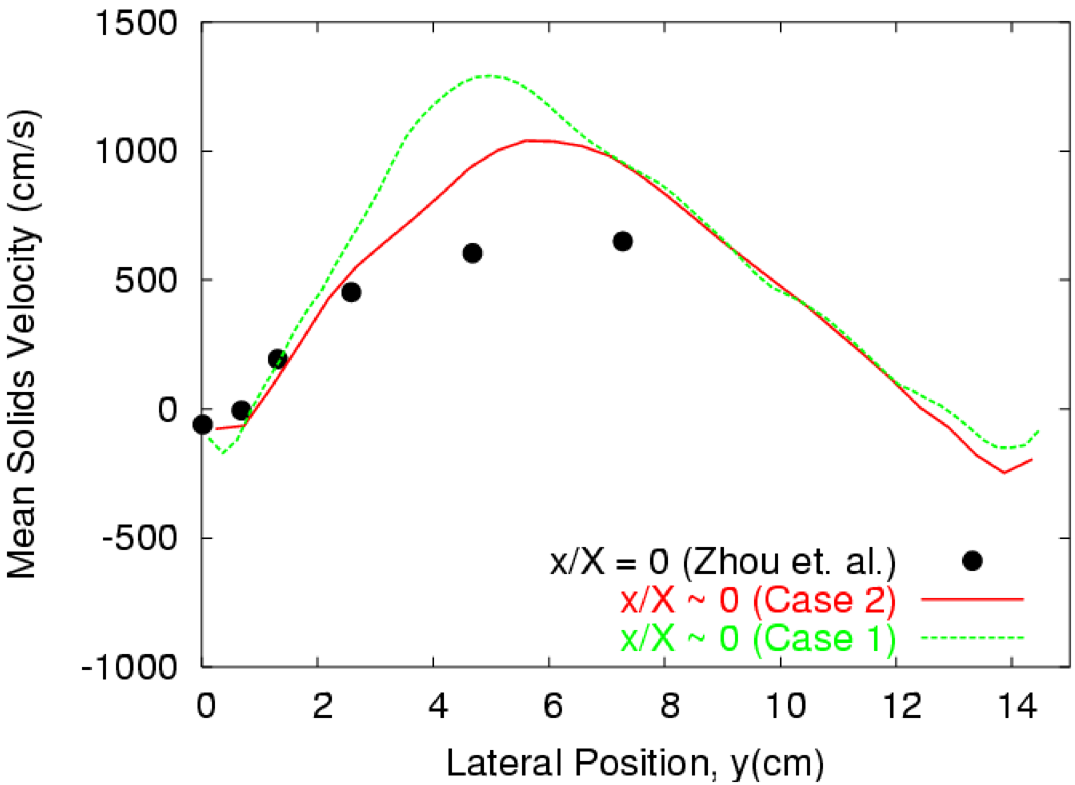
x/X = 0 (CL) – Effect of resolution



Pannala et al. (2003)

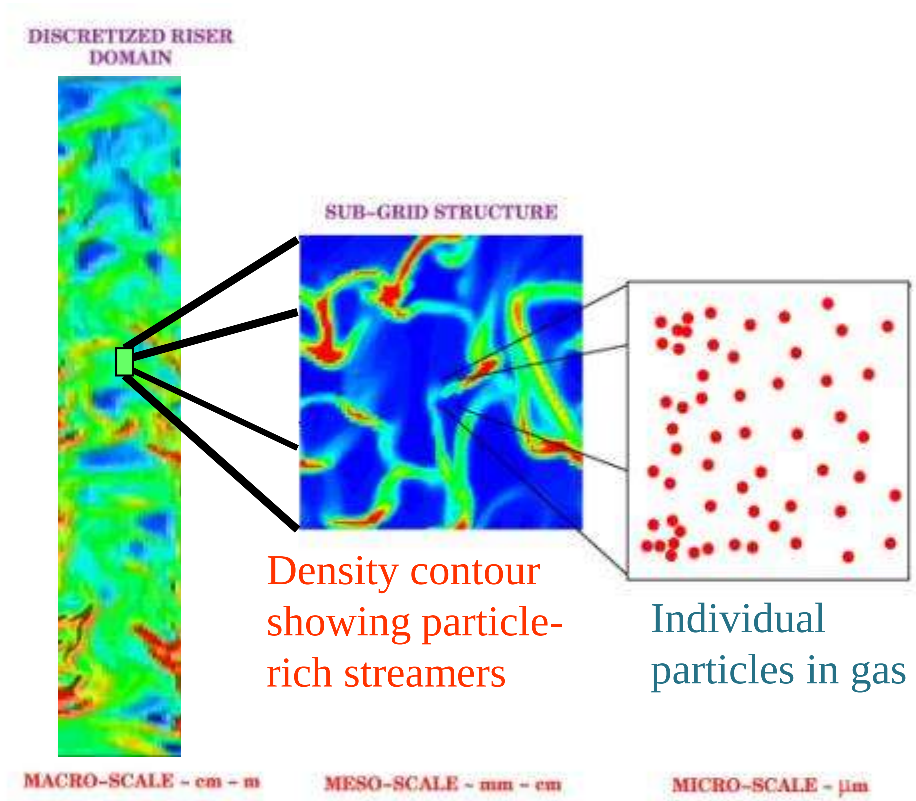
Lateral profiles of solids velocity

Z = 5.13m – Effect of resolution



Pannala et al. (2003)

Coarse-graining of two-fluid models



All the closures for the two-fluid models that we commonly use are for nearly homogeneous mixtures

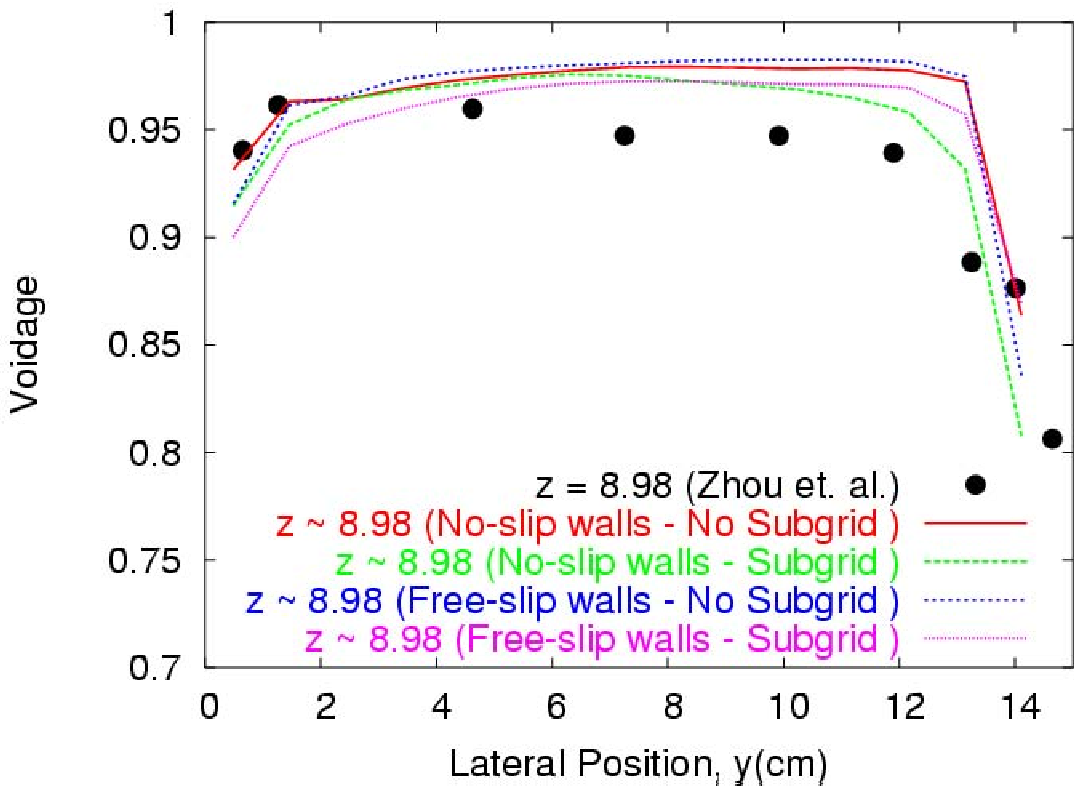
Engineering Need
Tools to probe macro-scale flow features directly

Original two-fluid model → Filtered two-fluid model

Andrews and Sundaresan, 2005

Lateral profiles of voidage

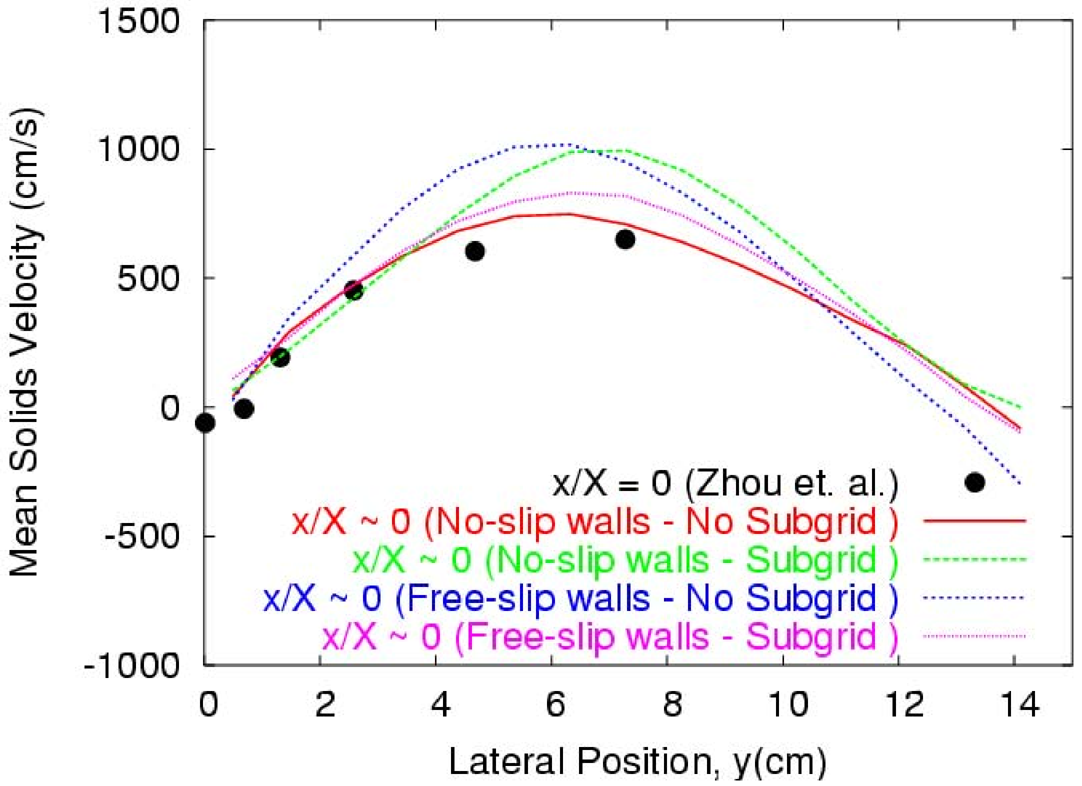
x/X = 0 (CL) – Effect of subgrid model



Pannala et al. (2003)

Lateral profiles of solids velocity

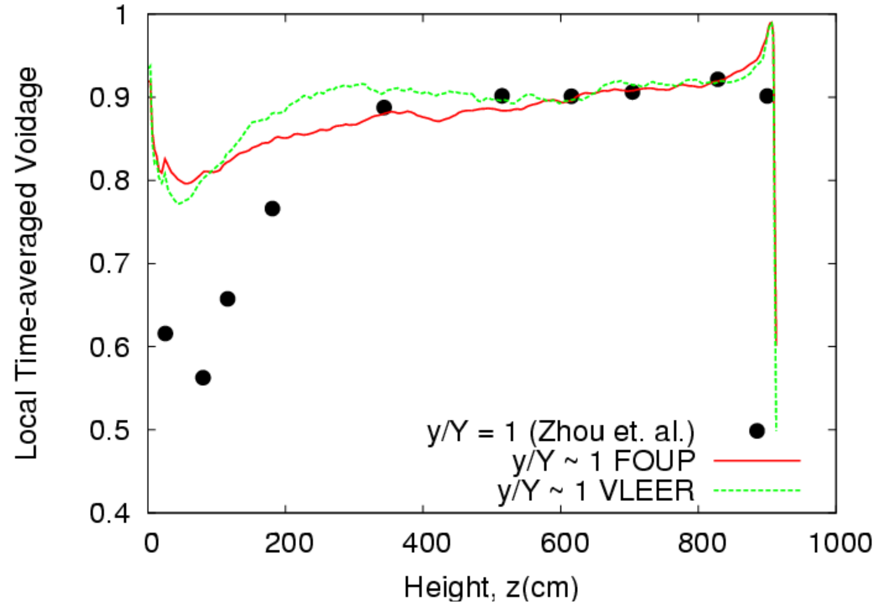
Z = 5.13m – Effect of subgrid model

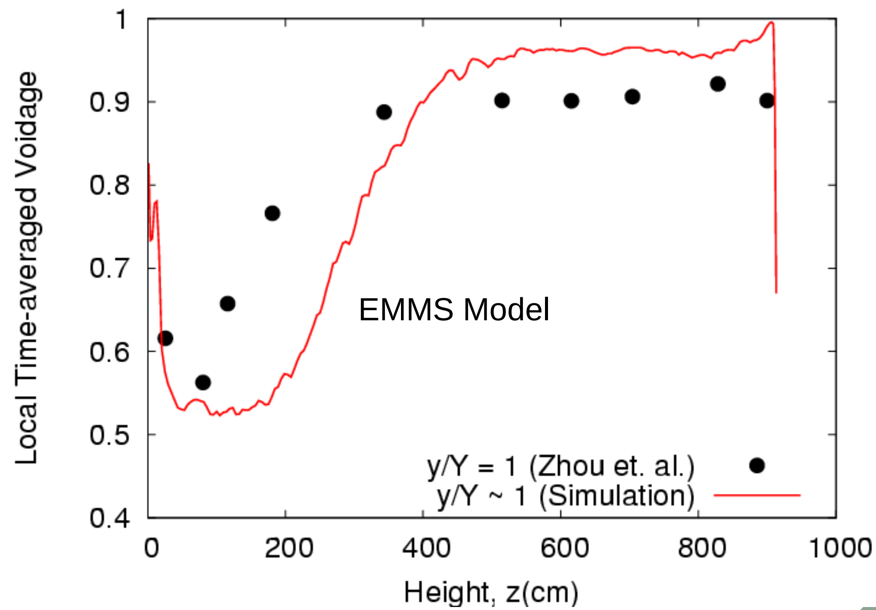


Pannala et al. (2003)

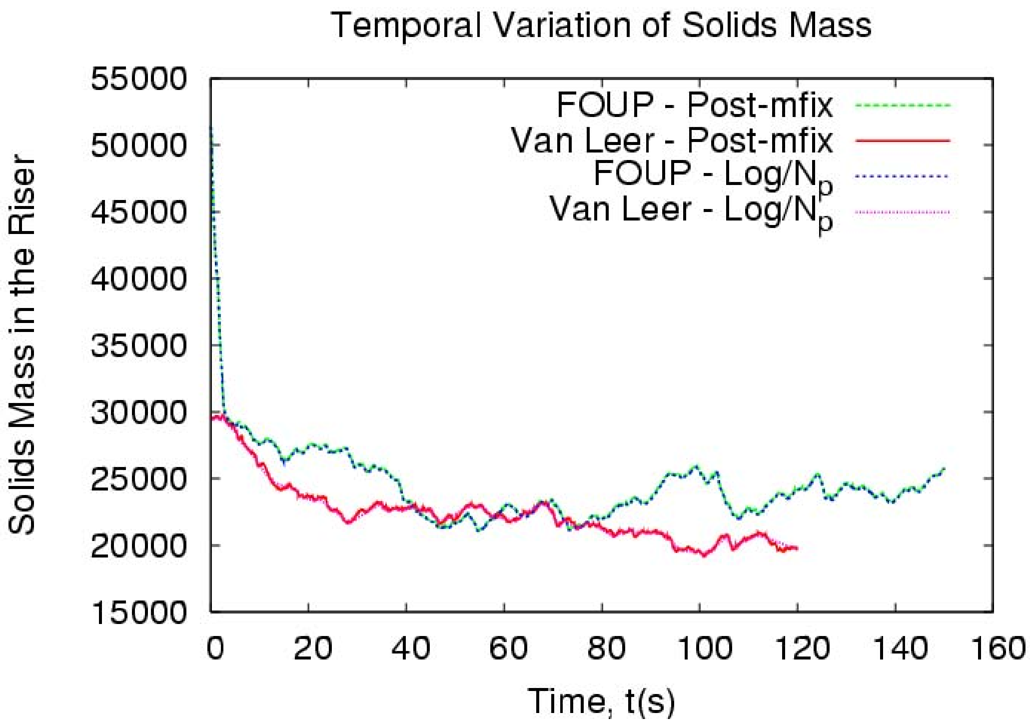
EMMS model

- **This is the only model which seems to give the solids loading similar to the experiments**
- **Currently working on using a revised EMMS model for Group B particles**





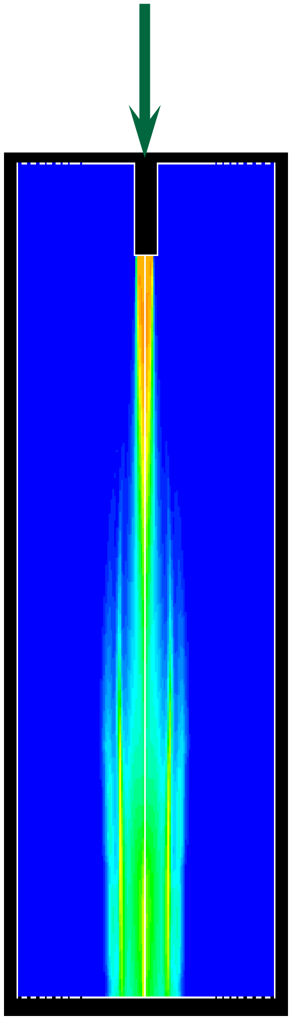
Long-term behaviour of solids loading



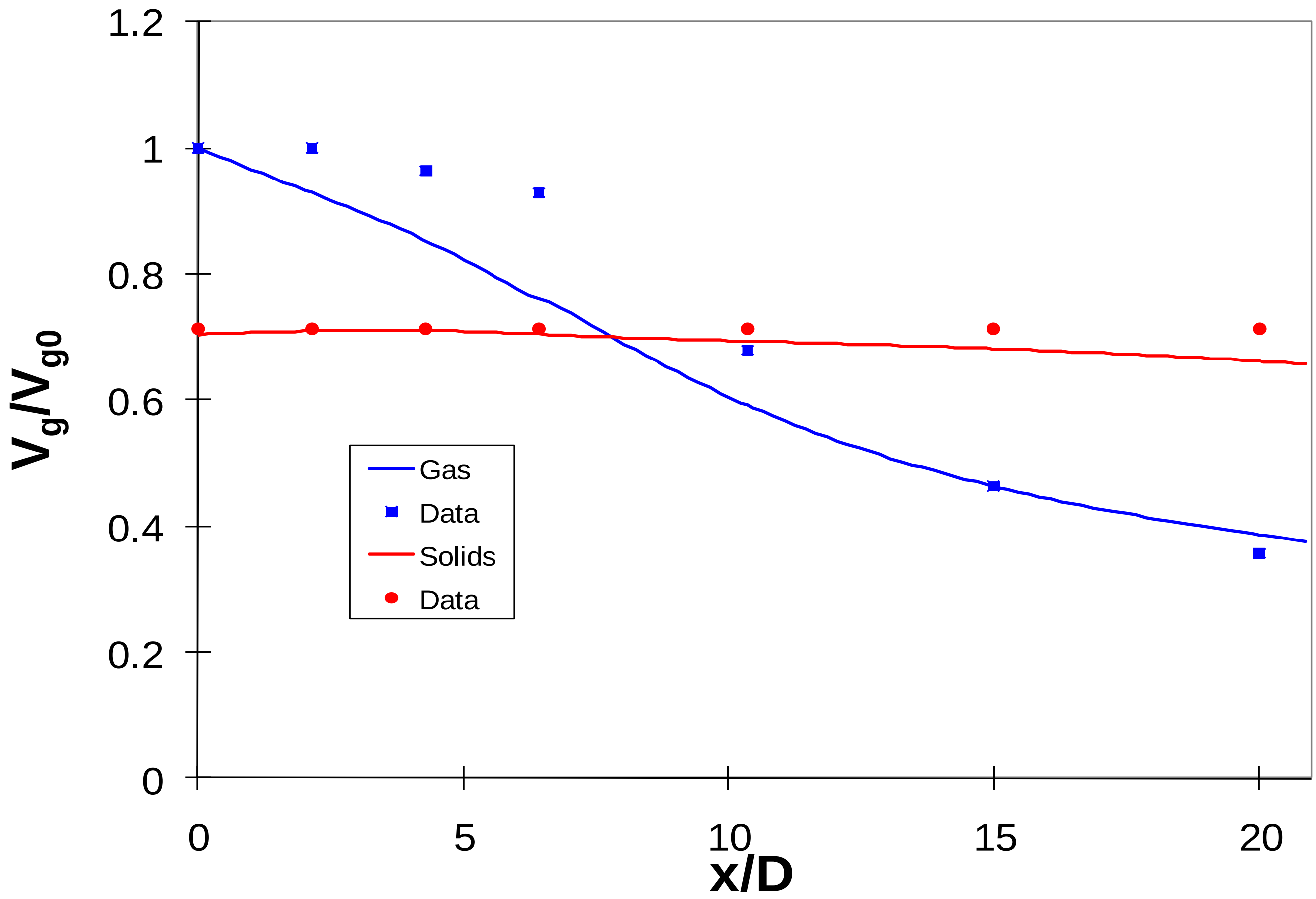
- **Long-term variations in solids holding**
- **Used 50-150 s for getting averaged properties for FOUP**
- **Used 30-120 s for getting averaged properties for Van Leer**

Turbulent Gas-Solids Jet

- Tsuji et al. (1988)
- 2D Axisymmetric cylindrical
- 500 μm polystyrene (1020 kg/m^3) - air
- 24 m/s gas-solids jet
- 20 mm nozzle in 0.3 m dia chamber
- 49 x 259 cells

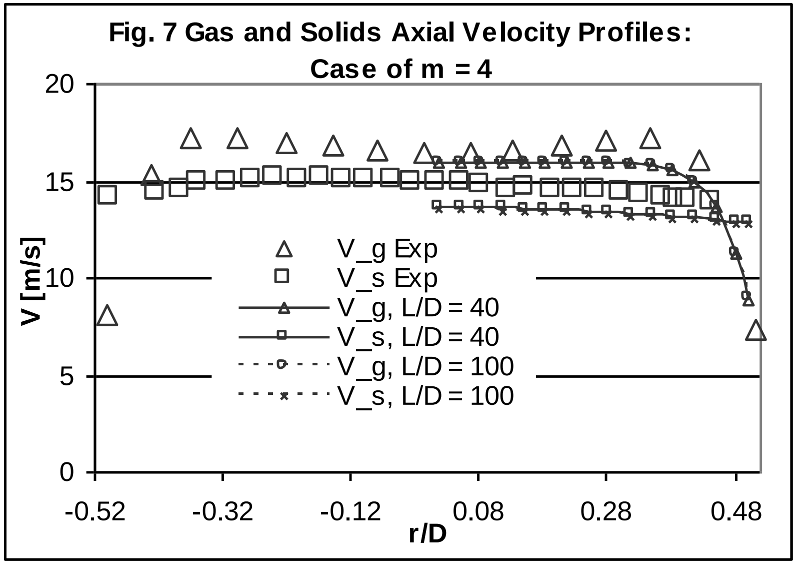


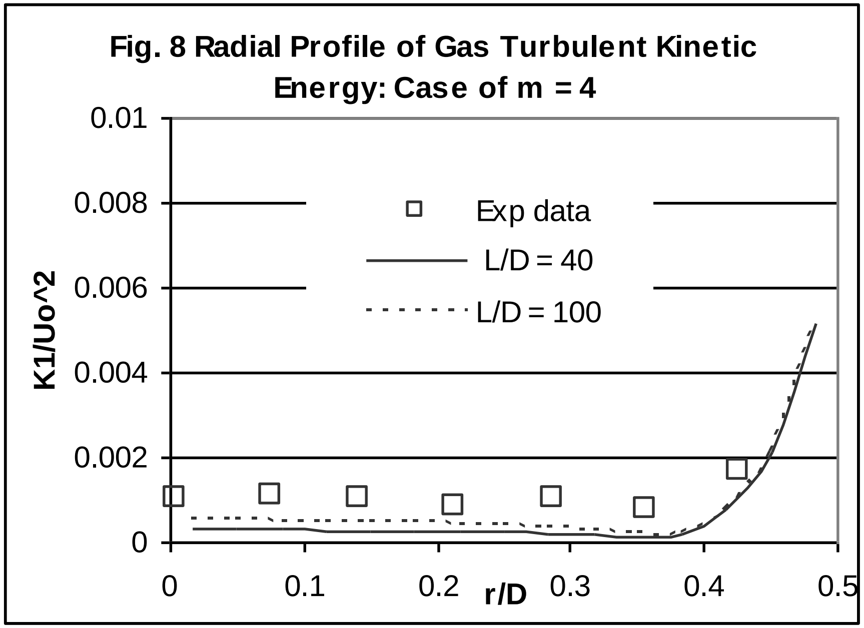
Gas and Solids Velocities Centerline

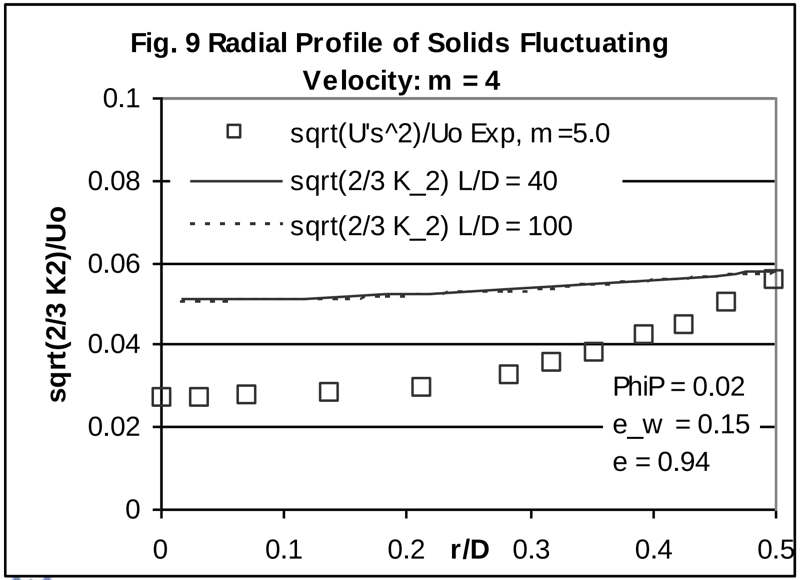


Data -- Tsuji et al. (1988)

Comparison with Jones (2001) Data







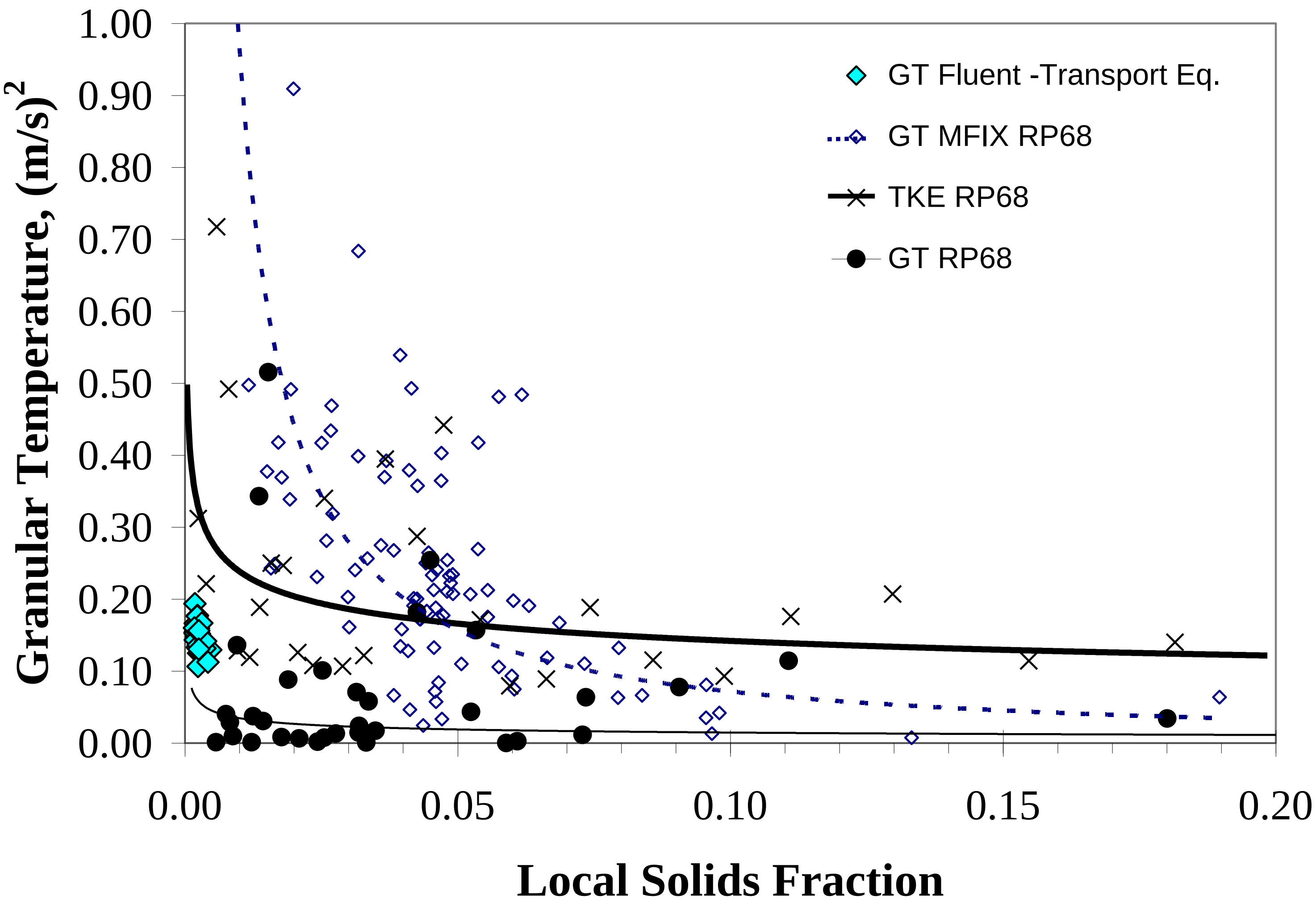
Benyahia et al. (2005), Jones (2001)

NETL CFB data

Vg (m/s)	Gs (kg/s)	ΔP (Pa)	
		Experiment	MFIX
2.3	.20	744	730
3.2	.43	2045	1888
3.2	.51	2018	2412
4.3	.78	2370	2335
4.3	1.10	3121	2894

Guenther et al. (2001)

Granular Temperature



Breault et al. (2005)

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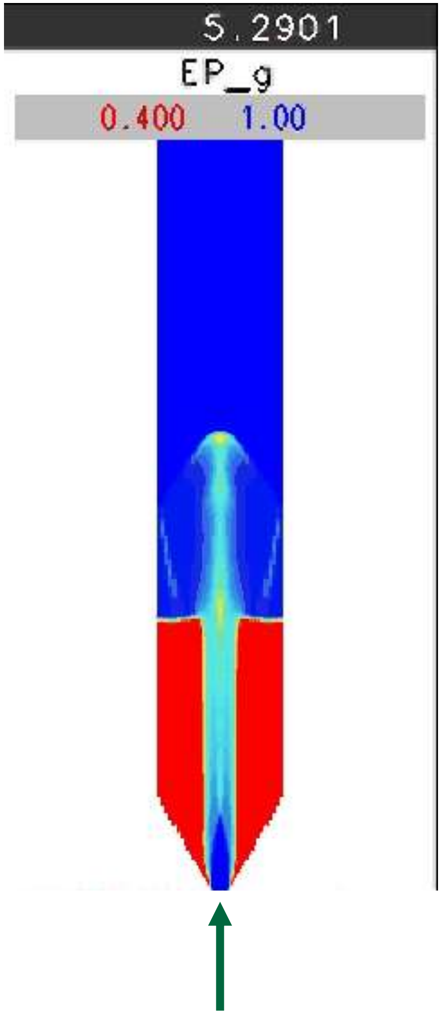
Spouted Bed

- He et al. (1994 a,b)
- 1.41mm, 2503 kg/m^3 glass beads
- 0.152 m dia x 1.4 m height
- Inlet orifice dia: 1.9 cm
- Jet velocity (m/s): 38, 41, 45
- bed height = 0.325 m
- axisymmetric: 49 x 362 cells
- U_{mf} (~ U_{ms})[1] = 0.54 m/s

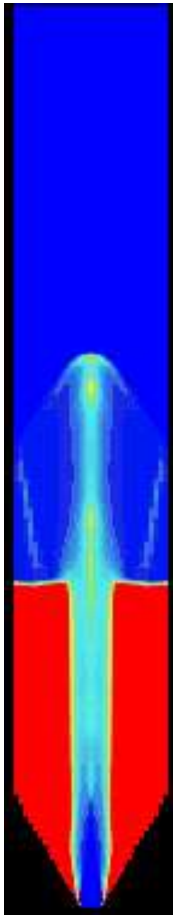


1 Epstein and Grace (1984)

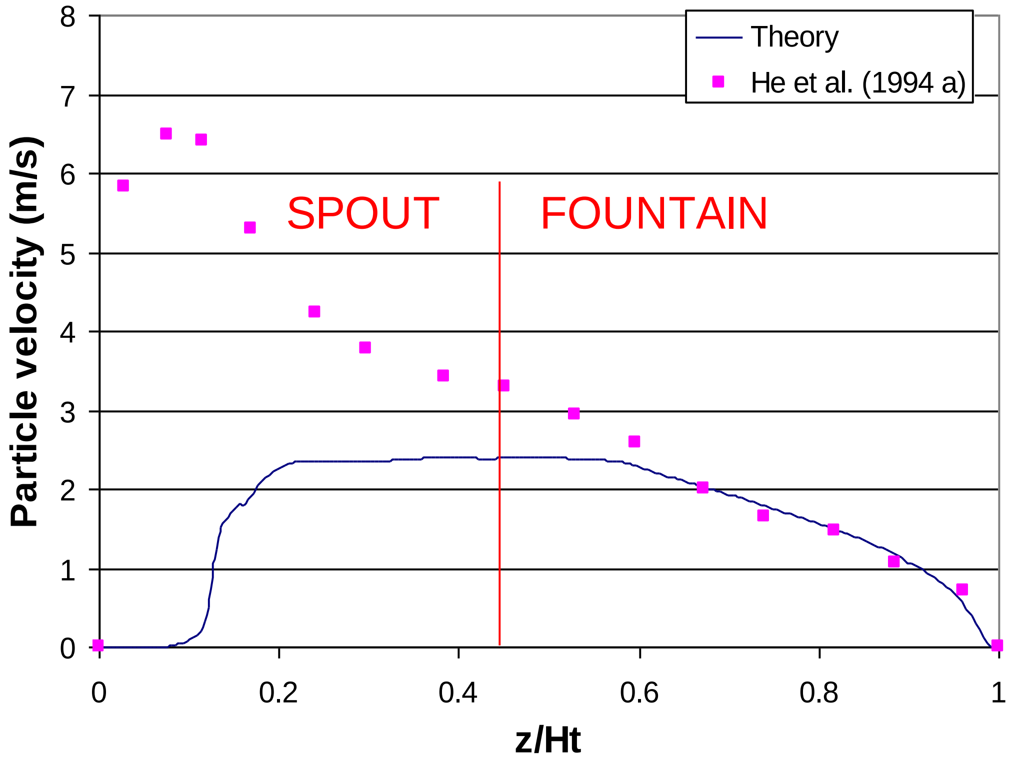
Spouted Bed

- **Gross features: spout, annulus, fountain**
  - **"The fountain core expanded suddenly near the bed surface and then gradually contracted with height" (He et al. 1994a)**

Fountain ht(m) at U/U_{ms}	1.1	1.2	1.3
Theory	0.13	0.18	0.23
Experiment	0.15	0.23	0.37

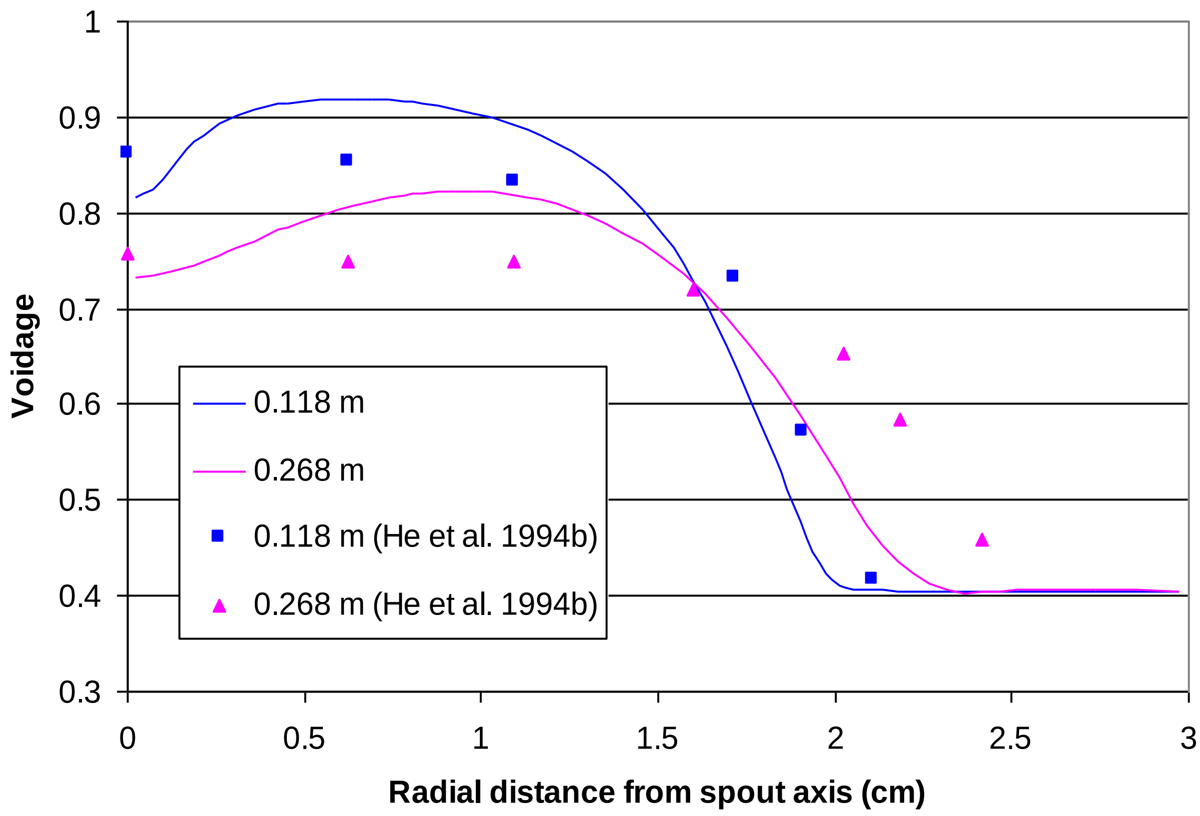


Vertical particle velocities along the axis



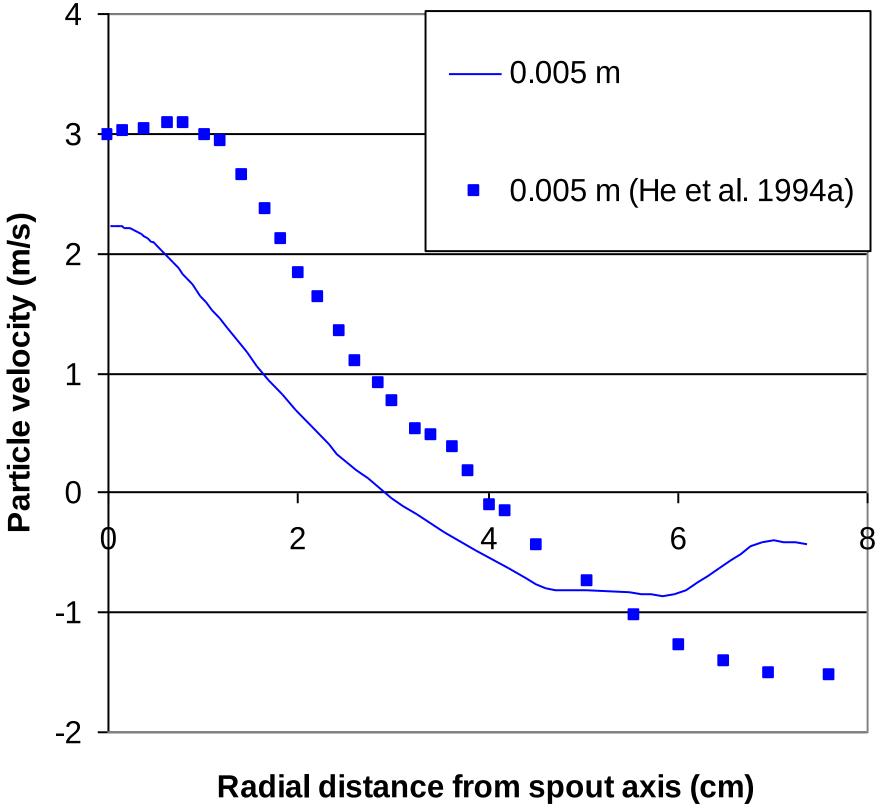
$U/U_{ms} = 1.3$

Voidage profiles in the spout



$U/U_{ms} = 1.3$

Radial profiles of particle velocities in the fountain



$U/U_{ms} = 1.3$

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Simulation Conditions - 1

- Fryer and Potter (1976)
- 117 μm, 2650 kg/m^3 catalyst particles
- 0.229 m dia x static bed ht: 10 to 65 cm
- Gas flow: 2, 4, 6, 8, 10, 12, 14 cm/s
- Used MFIX for simulations
- axisymmetric cylindrical coordinates:
  - 0.318 cm x 0.536 cm (36 x 56)
  - 0.159 cm x 0.268 cm (72 x 112)
  - 0.0795 cm x 0.134 cm (144 x 224)

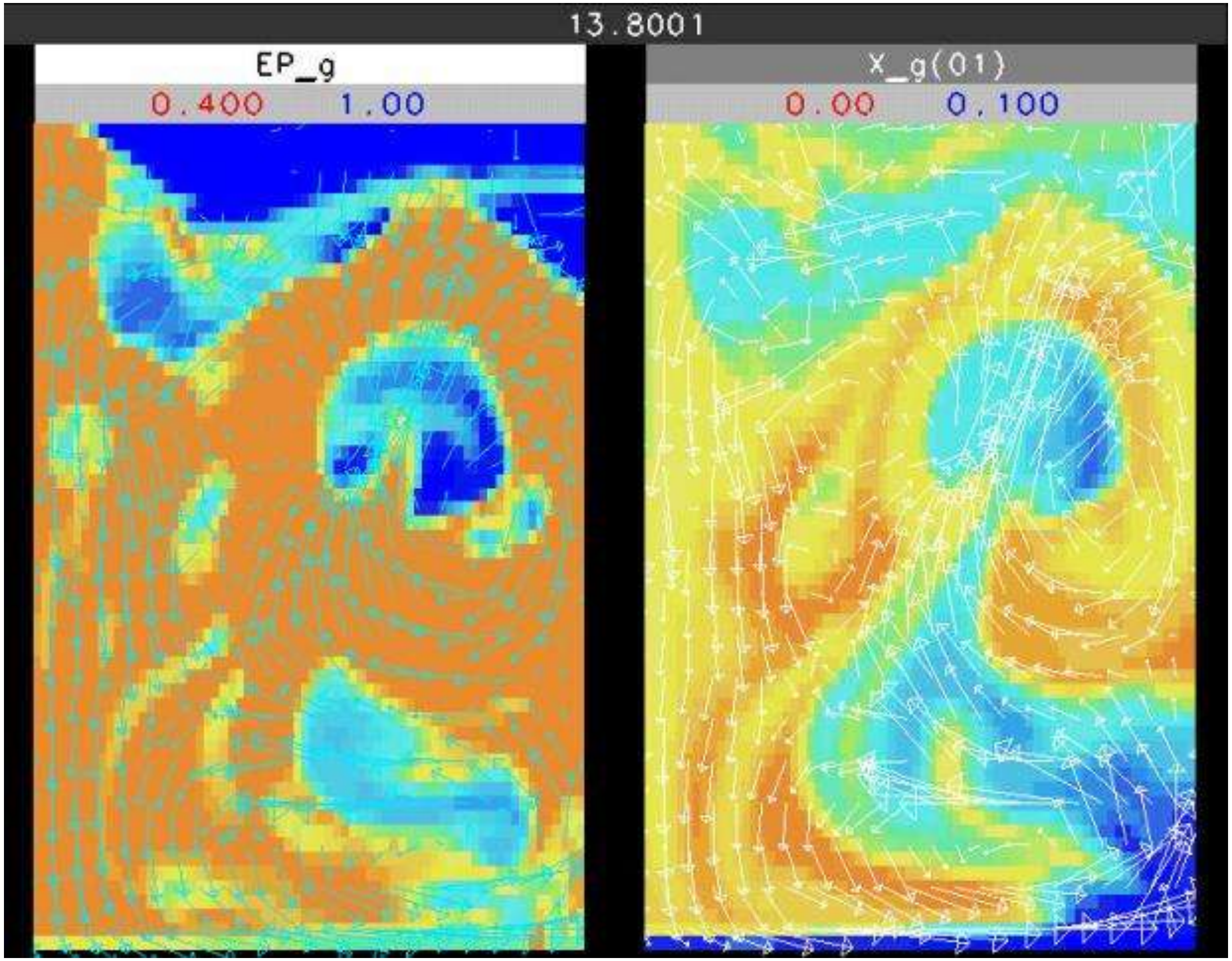
Simulation Conditions - 2

Particle diameter, d_p	117	μm
Sphericity	0.75	
Particle density, ρ_s	2.65	g/cm^3
Coefficient of restitution	0.8	
Angle of internal friction	30	
Minimum fluidization velocity, U_{mf}	1.70	cm/s
Void fraction at U_{mf}, ε_{mf}	0.48	
Parameter c in drag formula	0.765	
Parameter d in drag formula	2.928	
Bed height at U_{mf}, H_{mf}	10 - 65	cm
Fluid viscosity	1.8e-4	g/cm.s
O_3 mass fraction in inlet (O_3-Air) mixture	0.1	

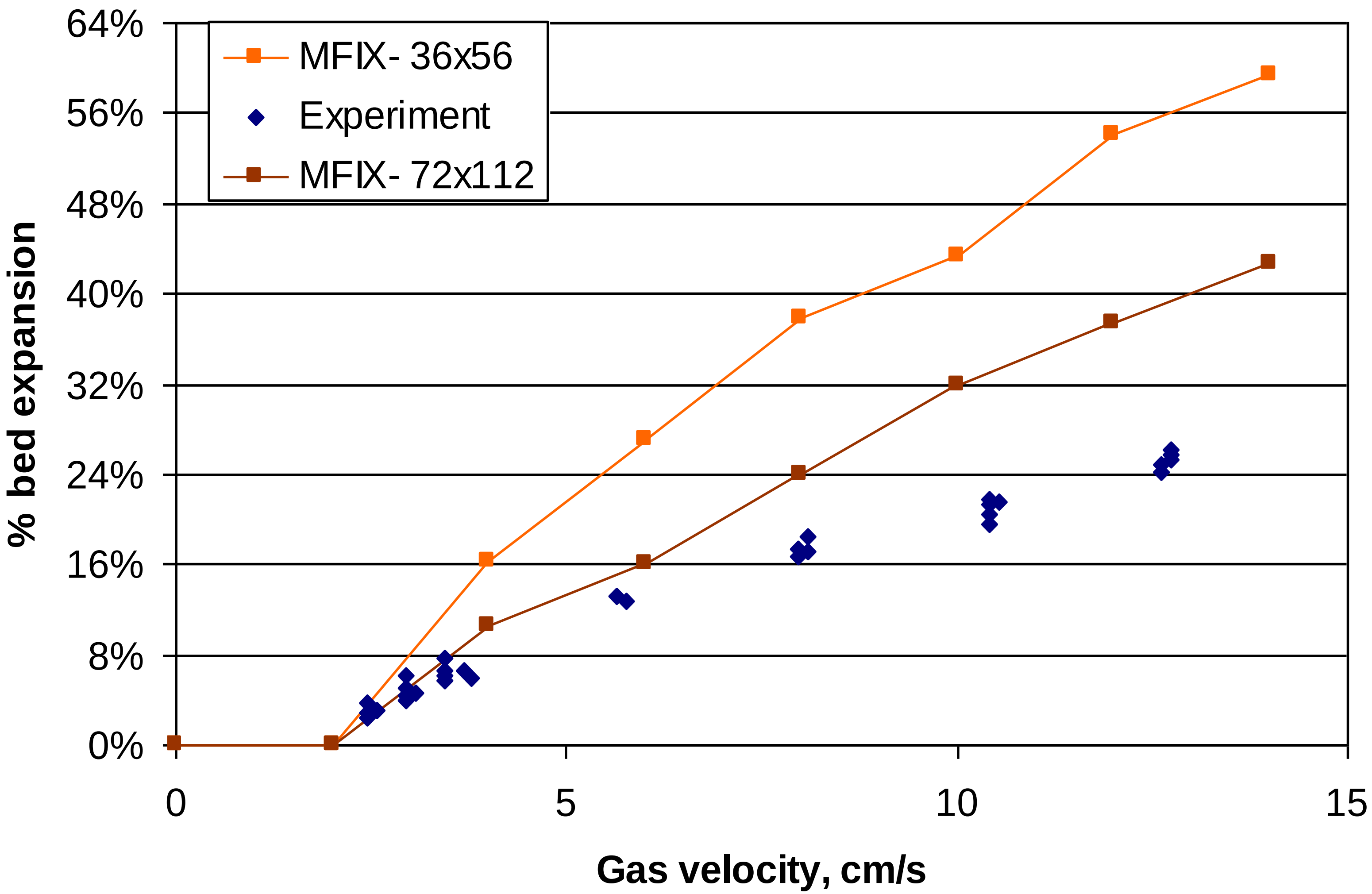
Ozone Decomposition Kinetics

- First order kinetics
  - $O_3 \rightarrow 1.5\ O_2$
- Catalyzed by sand impregnated with iron oxide
- Rate = $k\,(1-\varepsilon)\,[O_3]$ g-mol/($cm^3 \cdot s$)
  - $k = 1.57$ (m^3-gas/m^3-cat $\cdot$ s)

Void fraction, O_3Mass Fraction, Solids and Gas Velocity Vectors

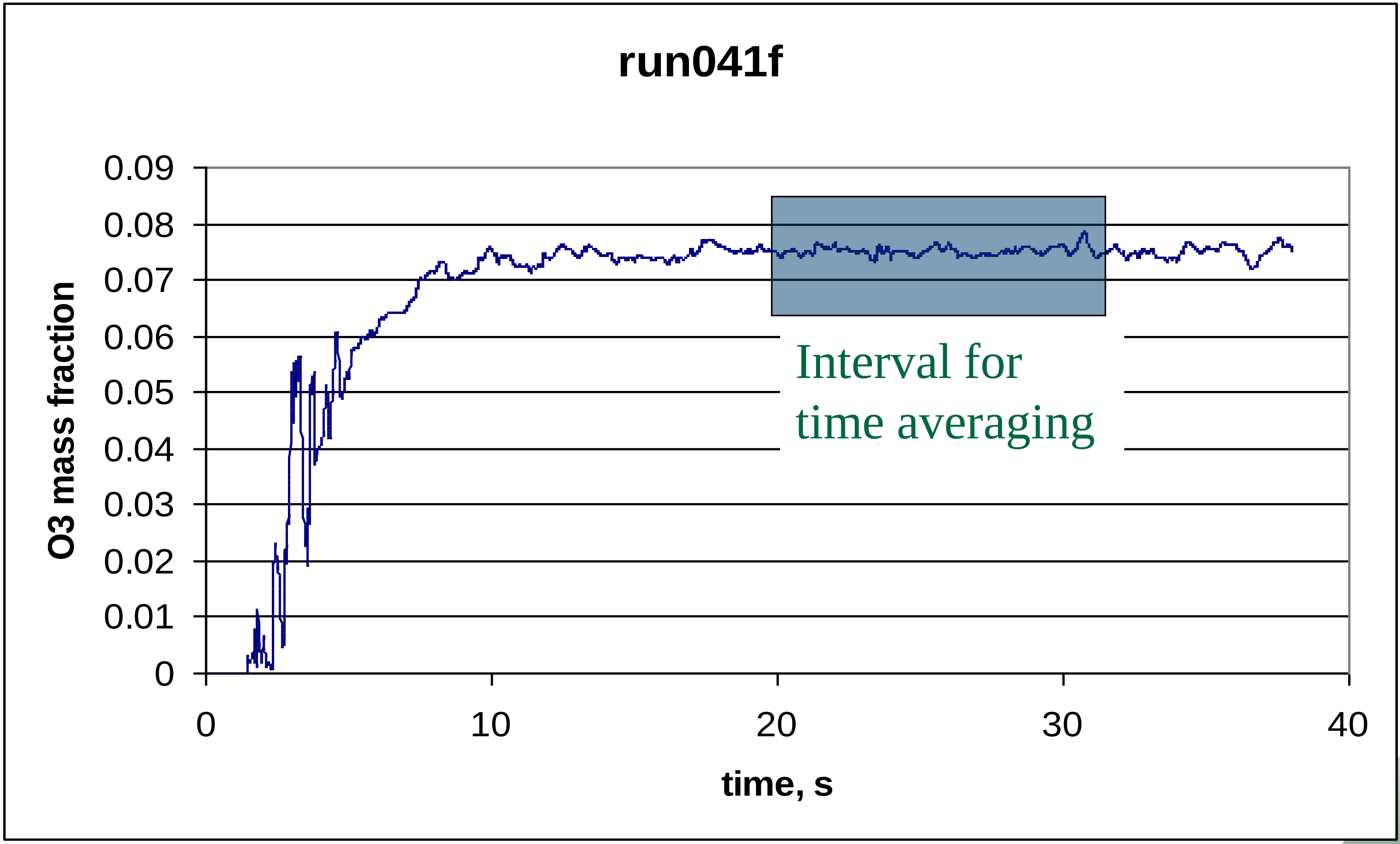


U = 8 cm/s; Hmf = 11.5 cm

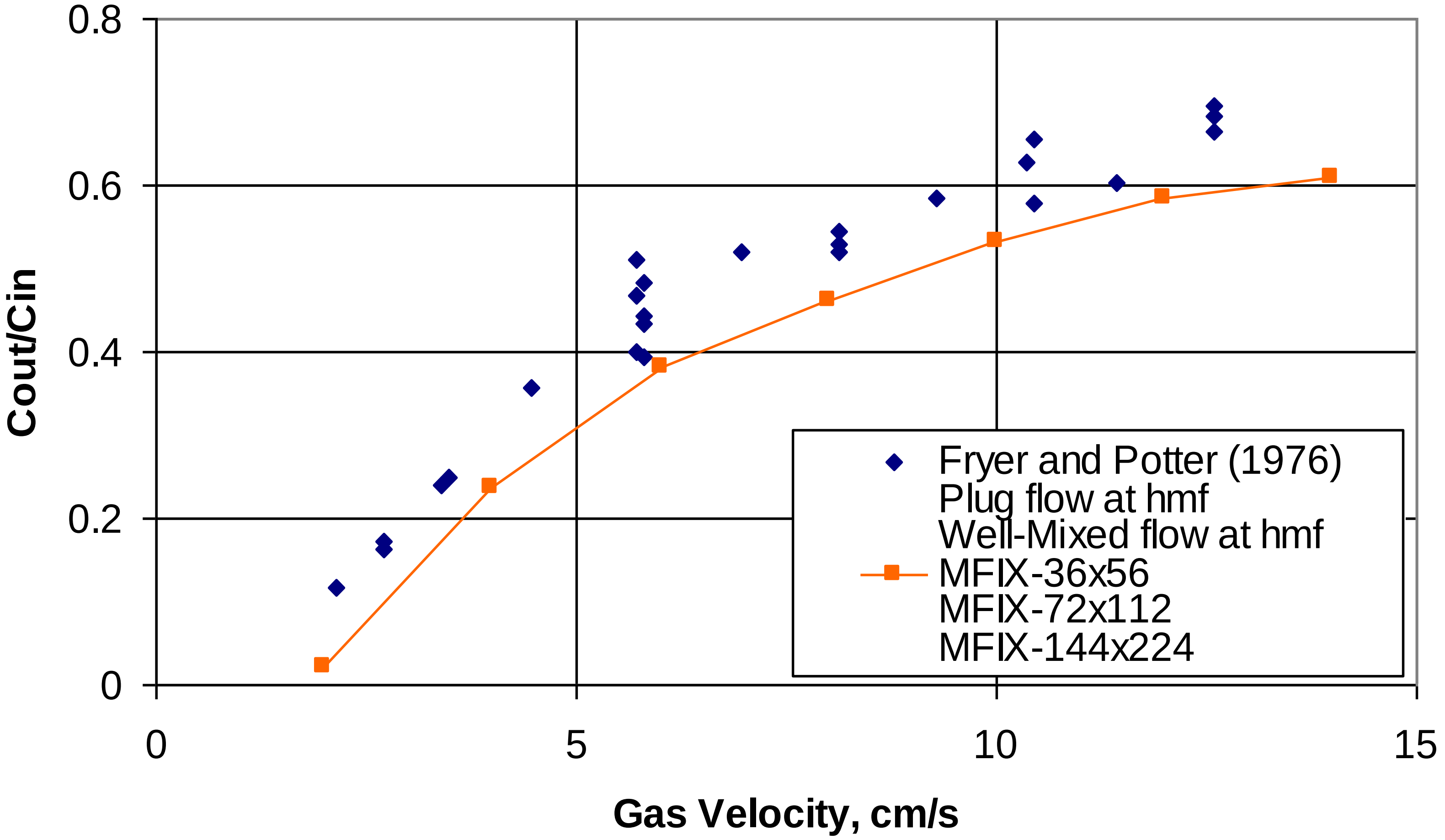


NETL

Oak Ridge National Laboratory

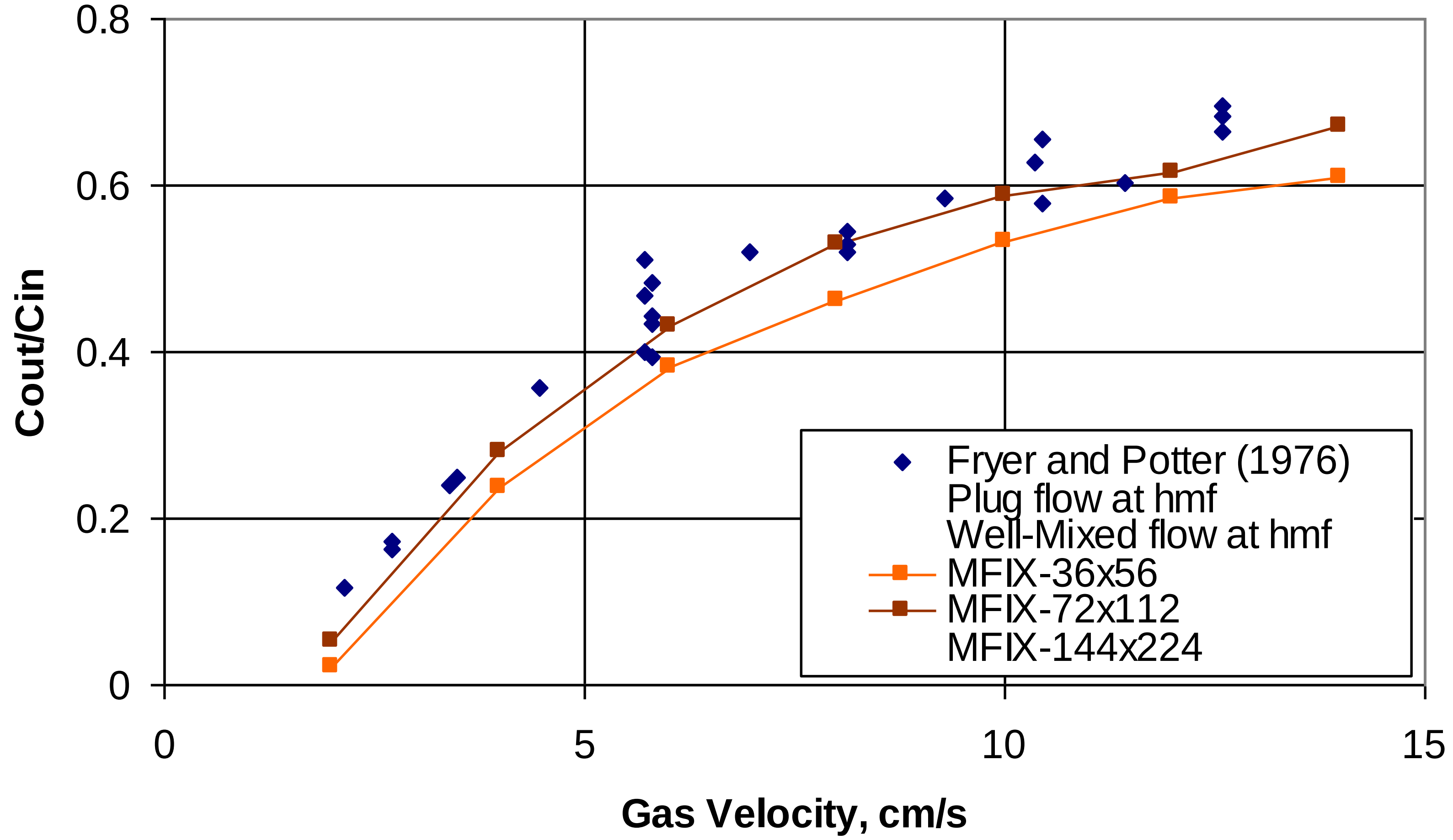

run041f
0.09
0.08
0.07
0.06
0.05
0.04
0.03
0.02
0.01
0
O3 mass fraction
0
10
20
30
40
time, s
Interval for
time averaging

hmf = 11.5 cm



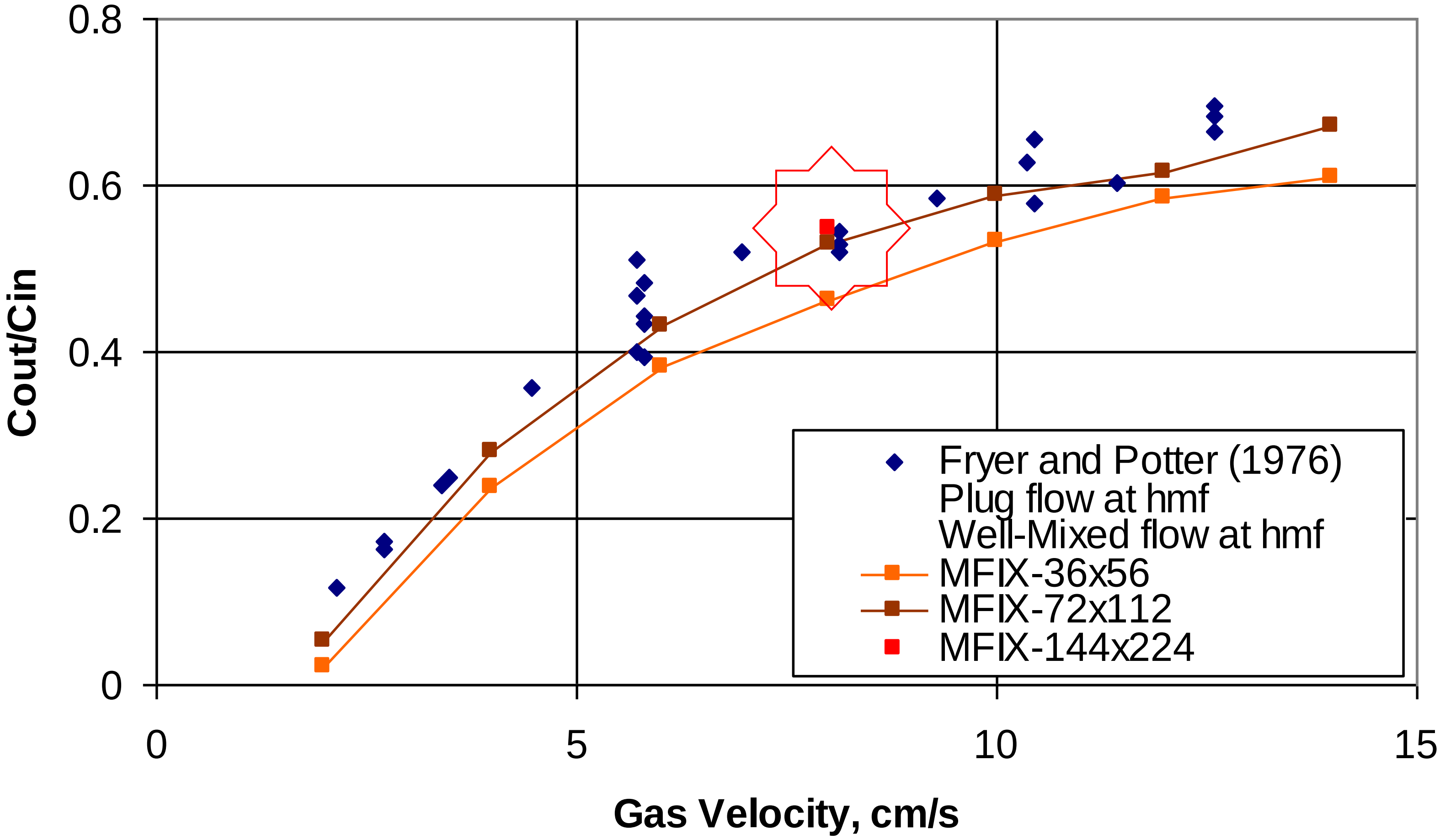
0.8
0.6
0.4
0.2
0
Cout/Cin
0
5
10
15
Gas Velocity, cm/s
Fryer and Potter (1976)
Plug flow at hmf
Well-Mixed flow at hmf
MFIX-36x56
MFIX-72x112
MFIX-144x224

hmf = 11.5 cm



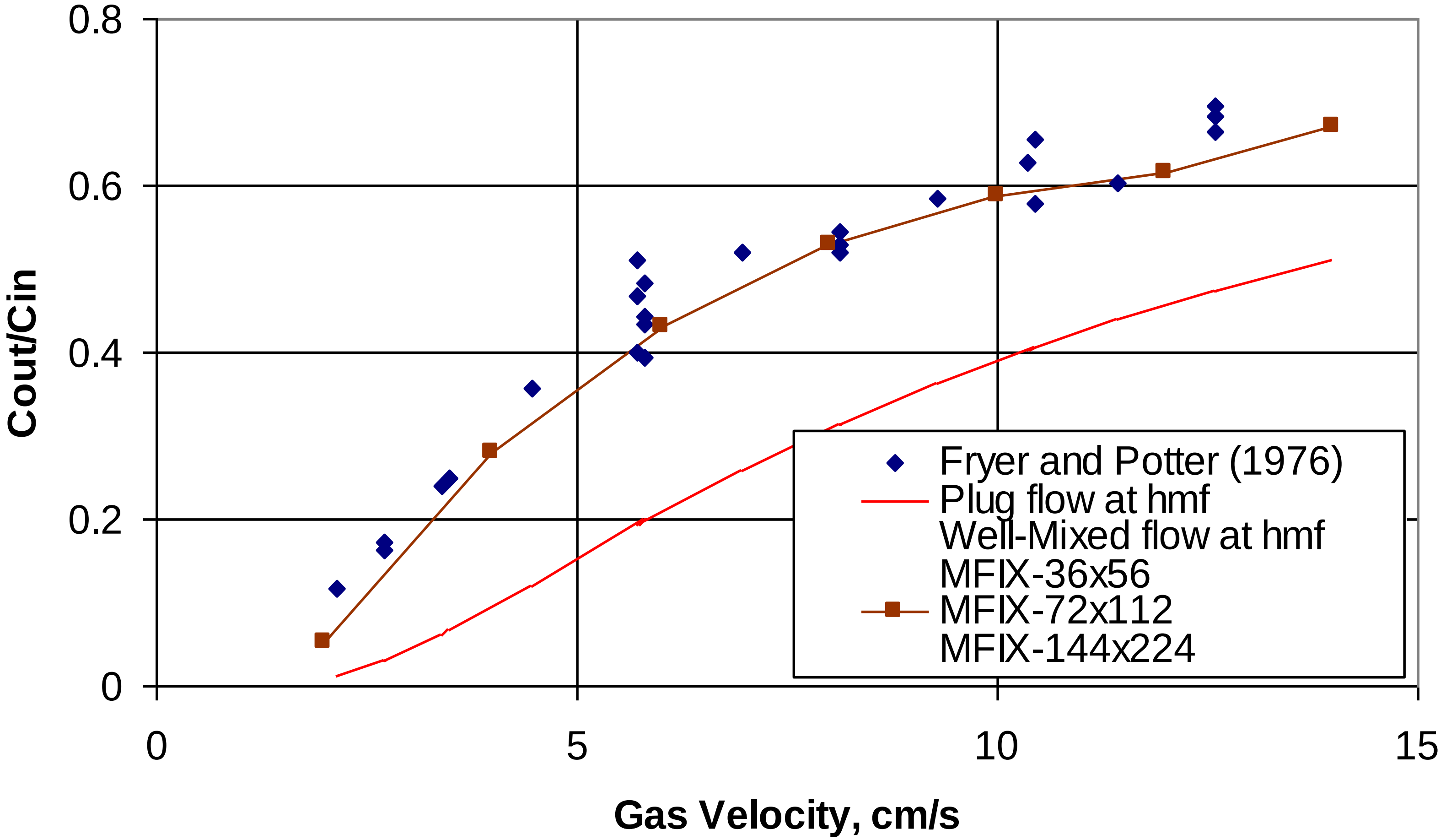
0.8
0.6
0.4
0.2
0
Cout/Cin
0
5
10
15
Gas Velocity, cm/s
Fryer and Potter (1976)
Plug flow at hmf
Well-Mixed flow at hmf
MFIX-36x56
MFIX-72x112
MFIX-144x224

hmf = 11.5 cm



0.8
0.6
0.4
0.2
0
Cout/Cin
0
5
10
15
Gas Velocity, cm/s
Fryer and Potter (1976)
Plug flow at hmf
Well-Mixed flow at hmf
MFIX-36x56
MFIX-72x112
MFIX-144x224

hmf = 11.5 cm



Cout/Cin
0.8
0.6
0.4
0.2
0
0
5
10
15
Gas Velocity, cm/s
Fryer and Potter (1976)
Plug flow at hmf
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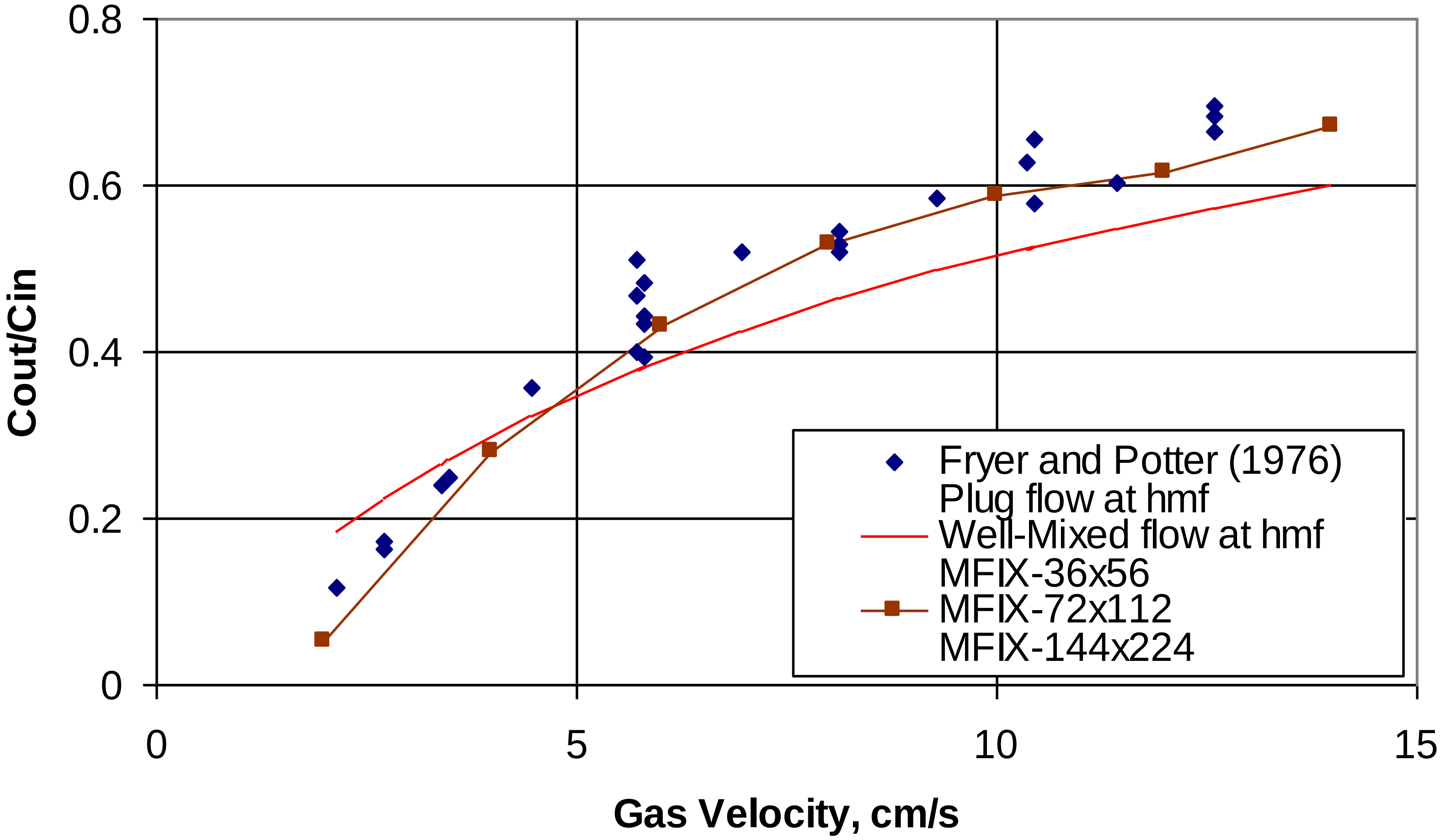
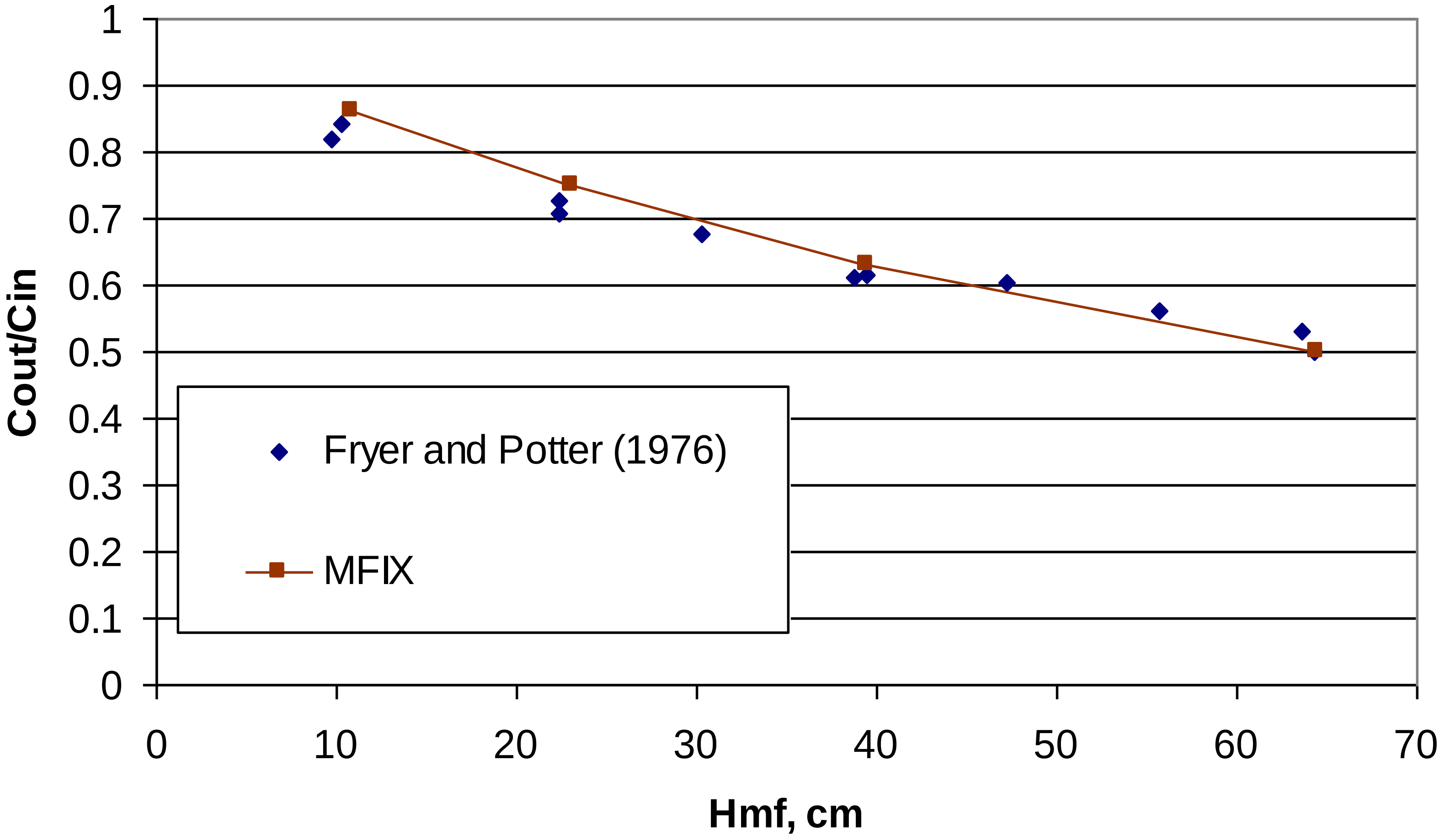
MFIX-36x56
MFIX-72x112
MFIX-144x224

hmf = 11.5 cm



Cout/Cin
0.8
0.6
0.4
0.2
0
0
5
10
15
Gas Velocity, cm/s
Fryer and Potter (1976)
Plug flow at hmf
Well-Mixed flow at hmf
MFIX-36x56
MFIX-72x112
MFIX-144x224

u = 10.4 cm/s



1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
Cout/Cin
0
10
20
30
40
50
60
70
Hmf, cm
Fryer and Potter (1976)
MFIX

Methane Combustion: Motivation

- **Complements ozone decomposition validation**
  - ***reversed role of bubbles*: they promote the reaction unlike in the case of catalysis**
  - **Reaction with heat release**
  - **Solids moderate temperature changes**
  - **Homogeneous chemistry . . . not really?**
- **Coal combustion/gasification: Where does the volatiles and CO burn?**
- **Applications in catalytic partial oxidation (Tomishige et al. 2002, Bharadwaj and Schmidt 1994).**

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Simulation Conditions

- van der Vaart (1992)
- 325 μm, 1460 kg/m^3 sand
- 7 cm dia x 20 cm ht., bed ht = 9 cm
- methane-air mixture velocity: 24 cm/s (6xUmf)
- Two bed temperatures: 1123 K, 1223 K
- axisymmetric cylindrical coordinates
- 40 x 100 cells

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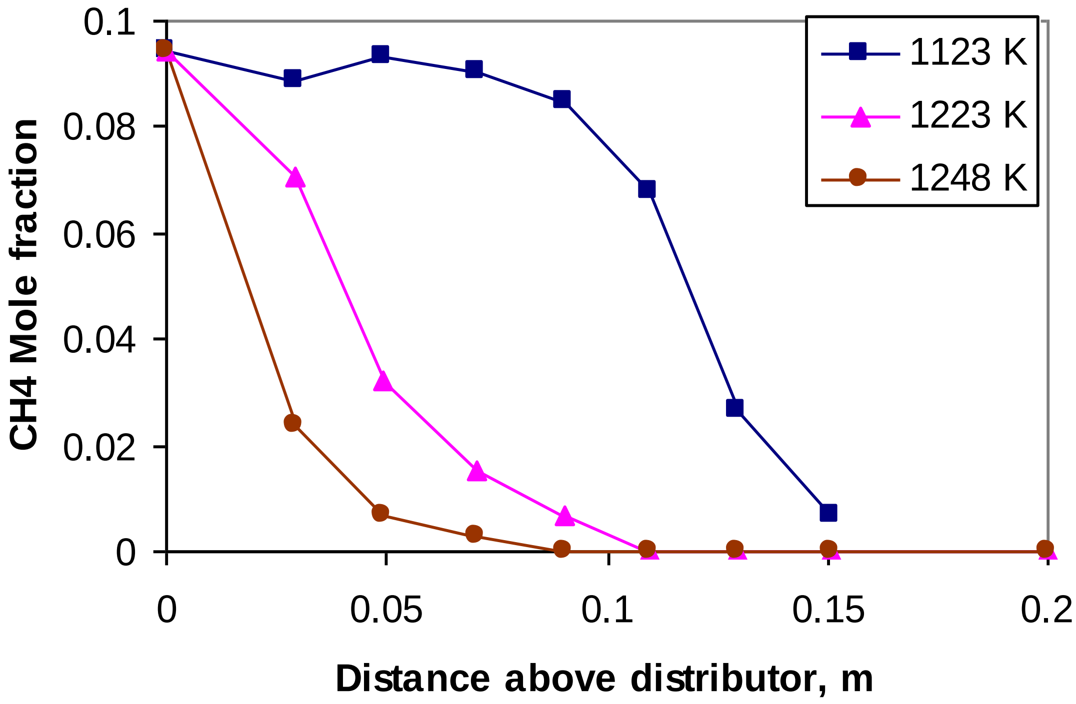
CH_4 Profile Changes with Bed Temperature



Combustion Rate

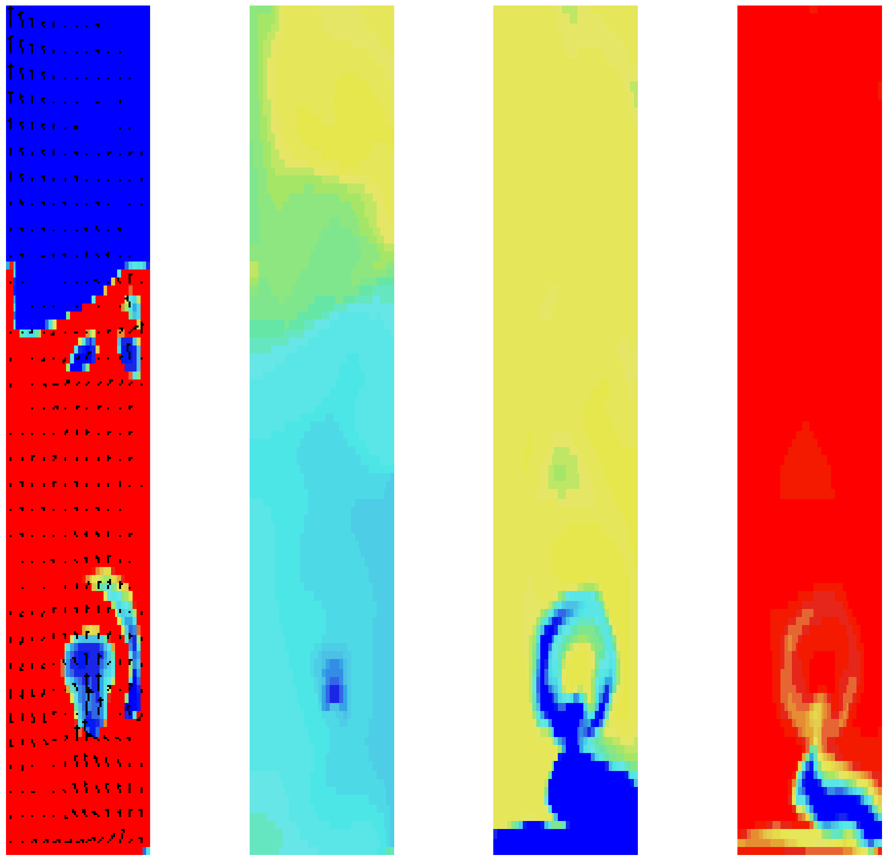
- **Two-step mechanism**
  - $CH_4 + 1.5\ O_2 \rightarrow CO + 2H_2O$
  - $CO + 0.5\ O_2 \rightarrow CO_2$
- **Dryer &Glassman (1973) rate expression**

$$r_{CH4} = \varepsilon_g 10^{13.2} \exp\left(\frac{-24358}{T_g}\right)[\mathrm{CH}_4]^{0.7}[\mathrm{O}_2]^{0.8}$$

$$r_{CO} = \varepsilon_g 10^{14.75} \exp\left(\frac{-21640}{T_g}\right)[\mathrm{CO}][\mathrm{O}_2]^{0.25}[\mathrm{H}_2\mathrm{O}]^{0.5}$$

- **Pre et al. (1998) report good agreement with fluidized bed data**

Preliminary Results - 1



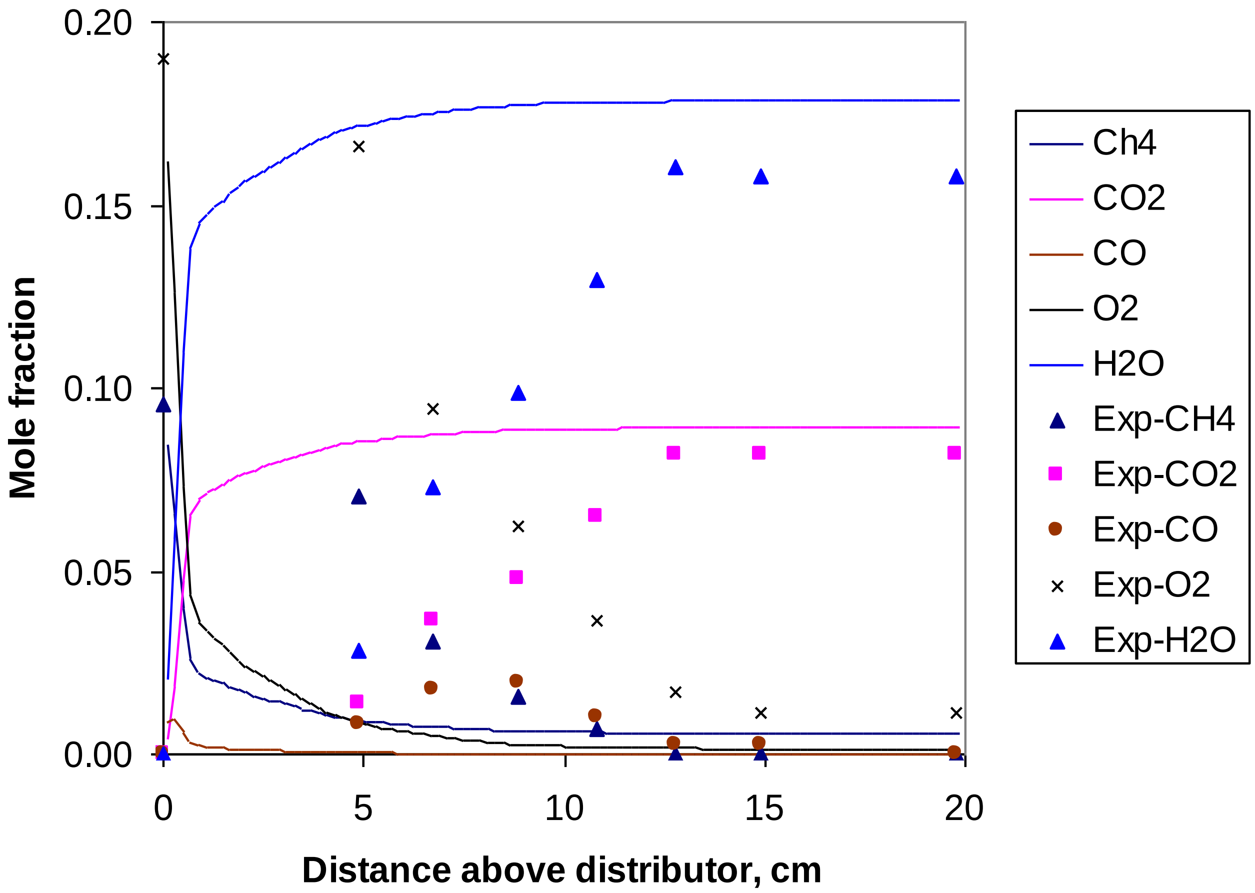
ε_g (0.4 -1)

T_g (300 - 1500 K)

CH_4 (0. - 0.01)

CO (0.4 - 0.01)

Preliminary Results -2



Combustion rate - revisited

- Experimental observations:
  - Volatiles flames are attached to coal particles only as they drop through bubbles[1]
  - CO flames could be seen covering bubble bases[1]
  - Axial CO profiles could be explained only by setting combustion in particulate phase to zero[2]
  - CO conversion decreases with increasing bed height and increasing CO_2 concentration in the feed. This can be explained only in terms of chemical effects and not heat effect[2]
  - Measurements of unsteady temperatures and steady gas concentrations, and comparison of ignition delay times indicate that particulate phase inhibits hydrocarbon combustion[3]

1. Roberts et al. 1987; 2. Hayhurst and Tucker 1990;

3. Hesketh and Davidson 1991

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Combustion rate - revisited

- **Inhibition is caused by recombination of radicals and loss of reactive species O, H, OH, CO* and CO_2* at particulate surfaces[2]**
- **Need to consider the particulate phase inhibition of combustion in fluid bed models[1, 2, 3]**
- **Set CO and CH_4 rate to zero for $\varepsilon_g < 0.9$**

$CO + O_2 \rightarrow CO_2 + O$

$O + CO \rightarrow CO_2^*$

$CO_2^* + O_2 \rightarrow CO_2 + 2O$

$CO_2^* + CO \rightarrow CO_2 + CO^*$

$CO^* + O_2 \rightarrow CO_2 + O$

$CO + O + H_2O \rightarrow CO_2 + H + OH$

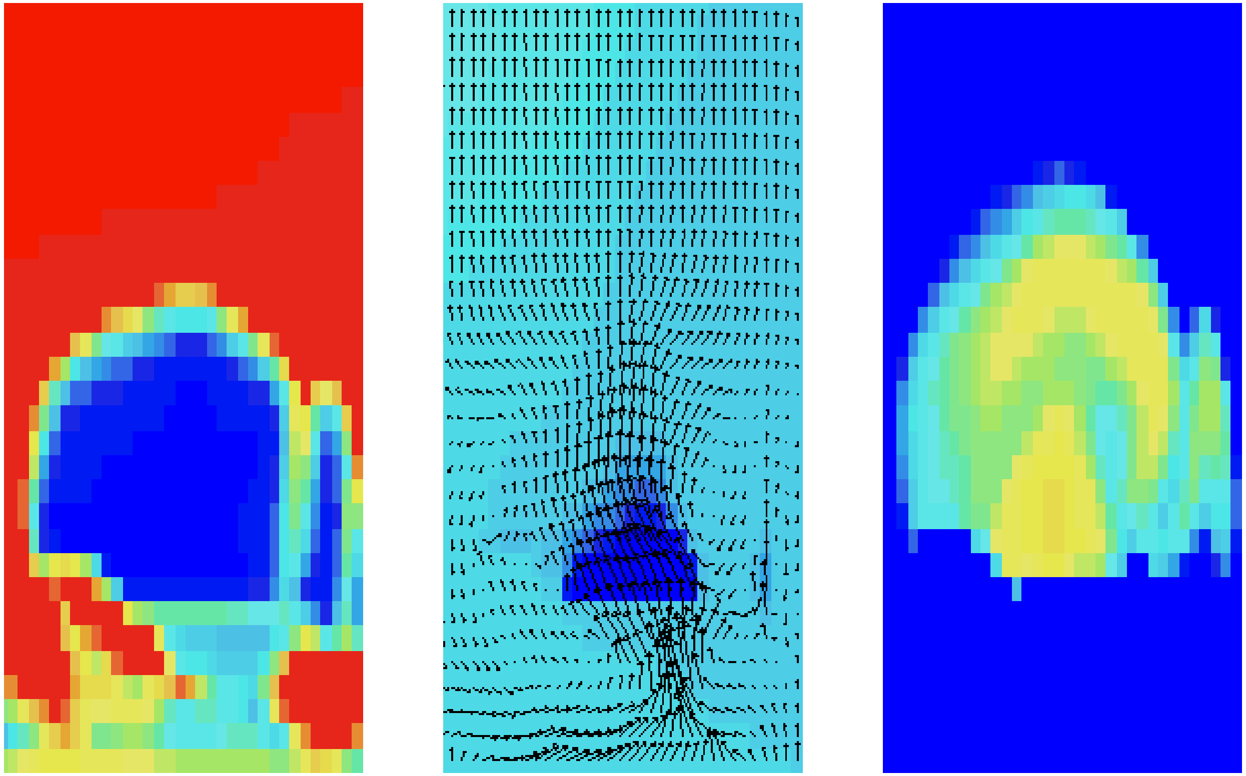
$OH + CO \rightarrow H + CO_2$

$H + O_2 \rightarrow OH + O$

$O + CO_2 \rightarrow O_2 + CO$

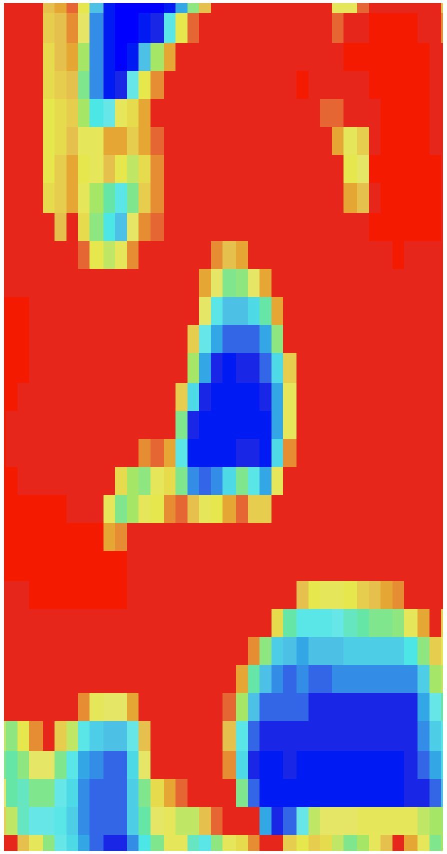
1. Roberts et al. 1987; 2. Hayhurst and Tucker 1990; 3. Srinivasan et al. 1998

Results – 1

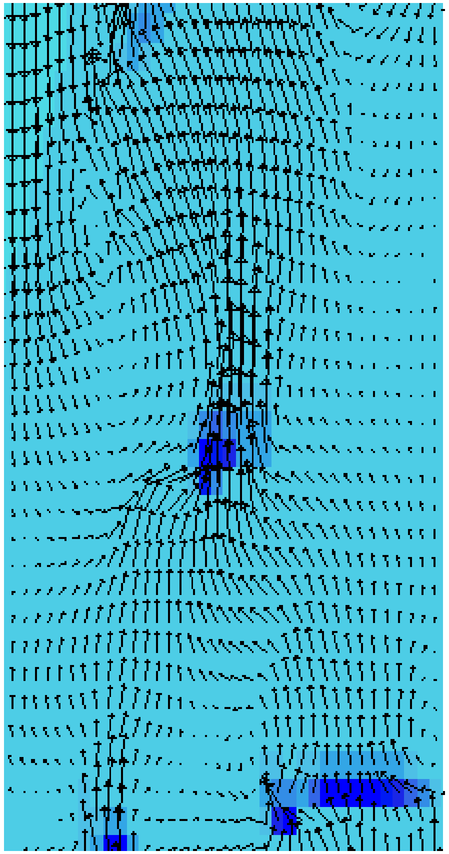


ε_g (0.4 -1) T_g (300 - 1500 K) CH_4 (0.0 - 0.01)

Results – 2

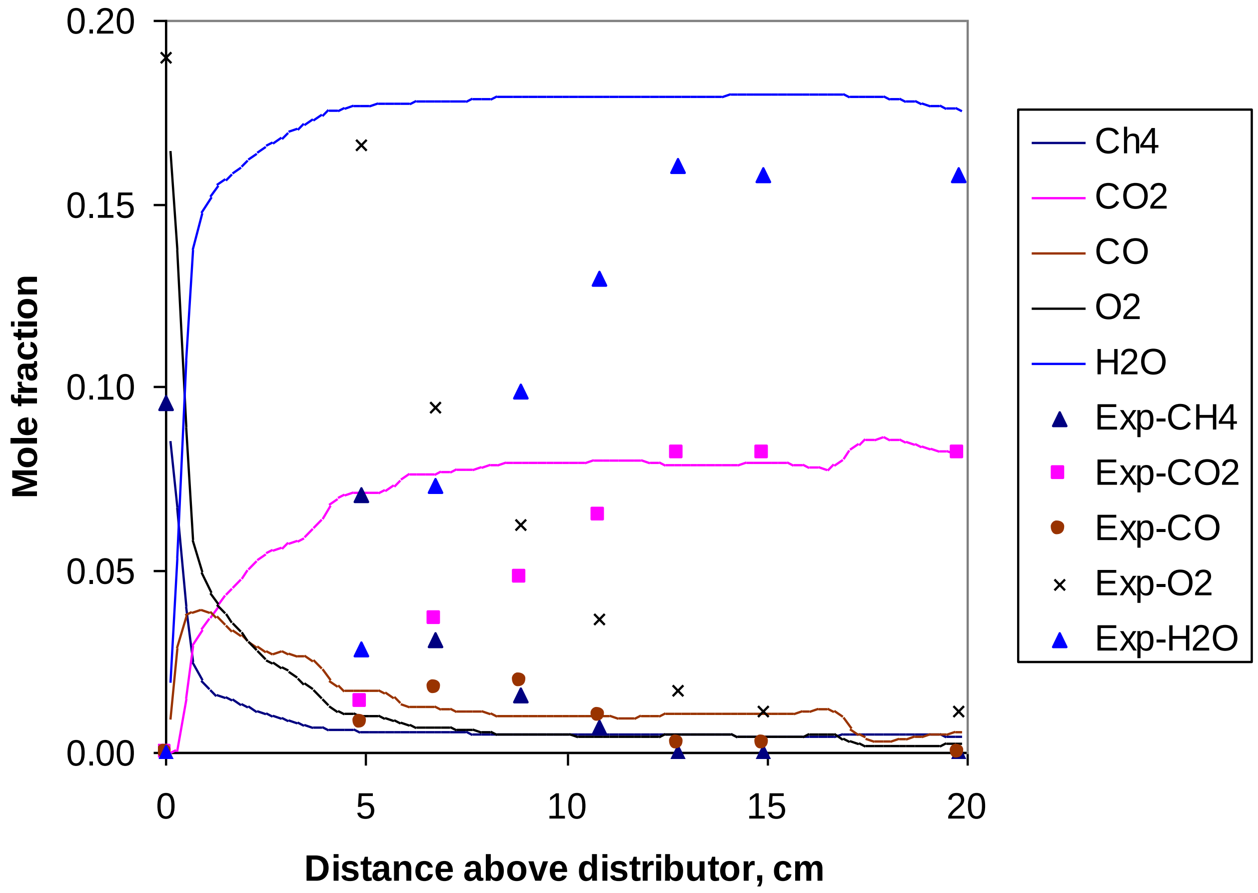


ε_g (0.4 -1)

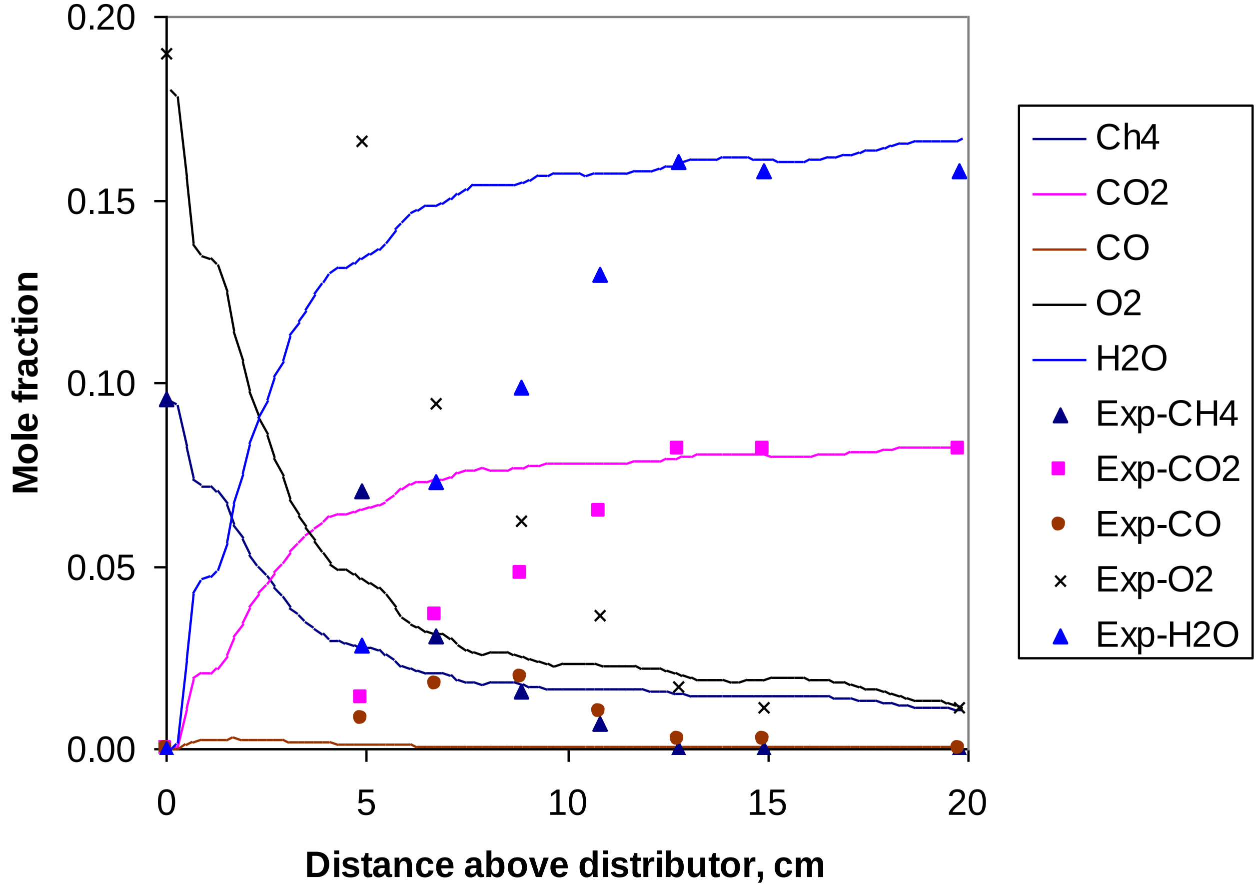


T_g (300 - 1500 K)

Particulate phase CO combustion inhibited



Particulate phase CO/CH_4 combustion inhibited



CH_4 Combustion – Concluding Remarks

- Qualitative features such as enhanced combustion in the bubble phase, gas bypassing between bubbles, and a cloud phase consisting of combustion products agree with experimental observations.
- Quantitative comparison with concentration profile data showed that particulate phase inhibition of combustion must be included in the model.
- Better agreement with experimental data was obtained by turning CO and CH_4 combustion in the particulate phase.

Si Production

- **Produce metallurgical grade Si by reduction of silica in "blast" furnaces**

  $$SiO_2 + C \rightarrow Si\ (m.g.) + CO_2$$

- **Gasify m.g. Si**

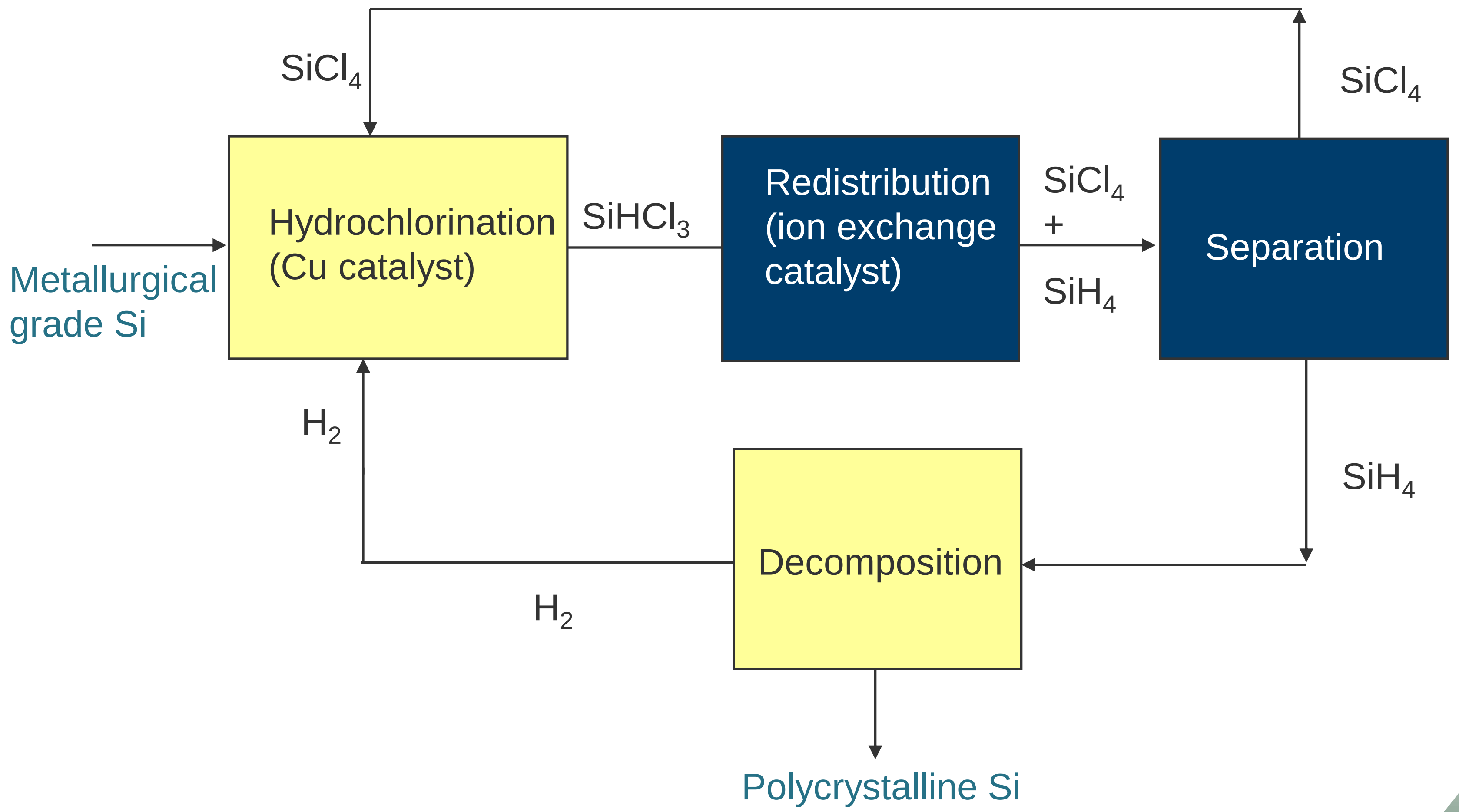
  $$Si\ (m.g.) + 2H_2 \rightarrow SiH_4$$

- **Purify gaseous Si species**

- **Reduce silane (or tetrachlorosilane) on a hot wire filament (Siemens process)**

  $$SiH_4 \rightarrow Si(s) + 2\ H_2$$

Si Purification Process



Hydrochlorination Chemical Kinetics

Step 1 (psuedo-homogeneous, slow):

$SiCl_4 + H_2 \Leftrightarrow SiHCl_3 + HCl$

$$rate = \frac{0.267}{T^{1/2}} e^{-27,680/T} \left[P_{SiCl_4} P_{H_2}^{1/2} - \frac{P_{SiHCl_3} P_{HCl}}{K_{EQ} P_{H_2}^{1/2}} \right]$$

Step 2 (Heterogeneous, fast):

$Si(s) + 3HCl \Rightarrow SiHCl_3 + H_2$

$$rate = 1.698 \times 10^{-3} \left(\frac{6(1-\varepsilon)}{d_p} \right) e^{-11,575/T} \left[P_{HCl} \right]^{1/2}$$

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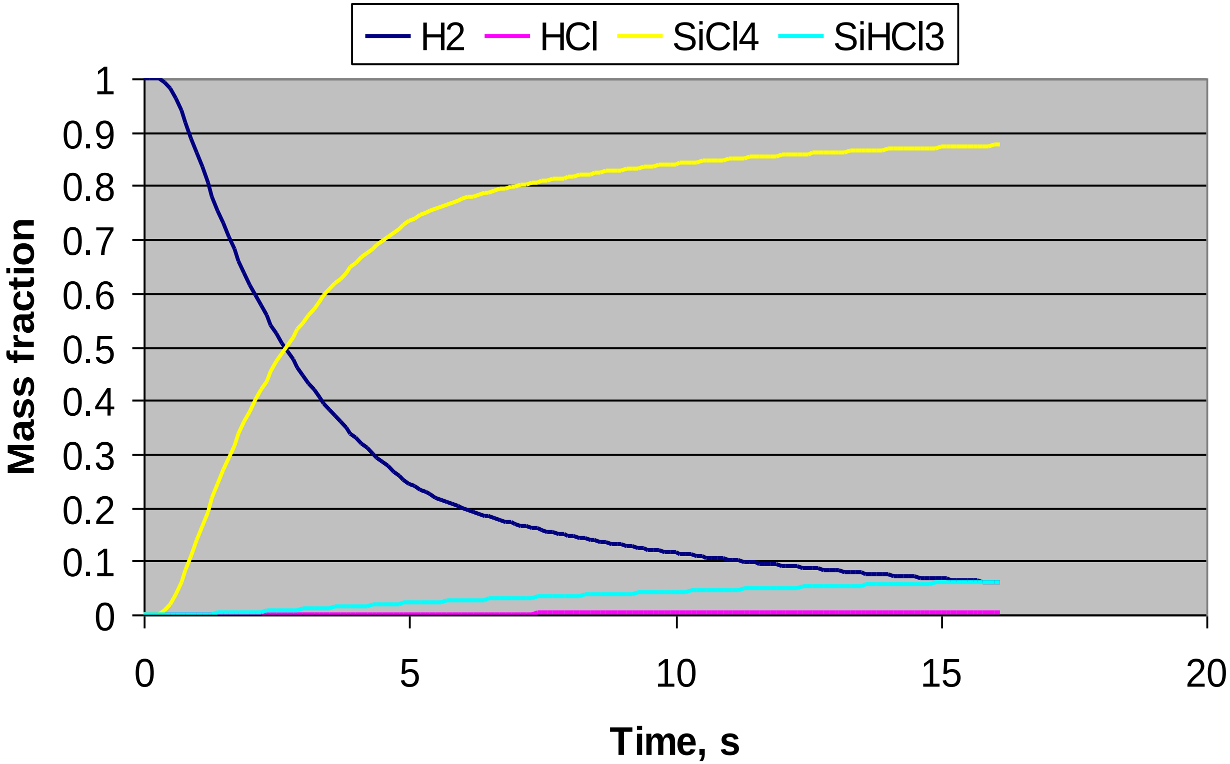
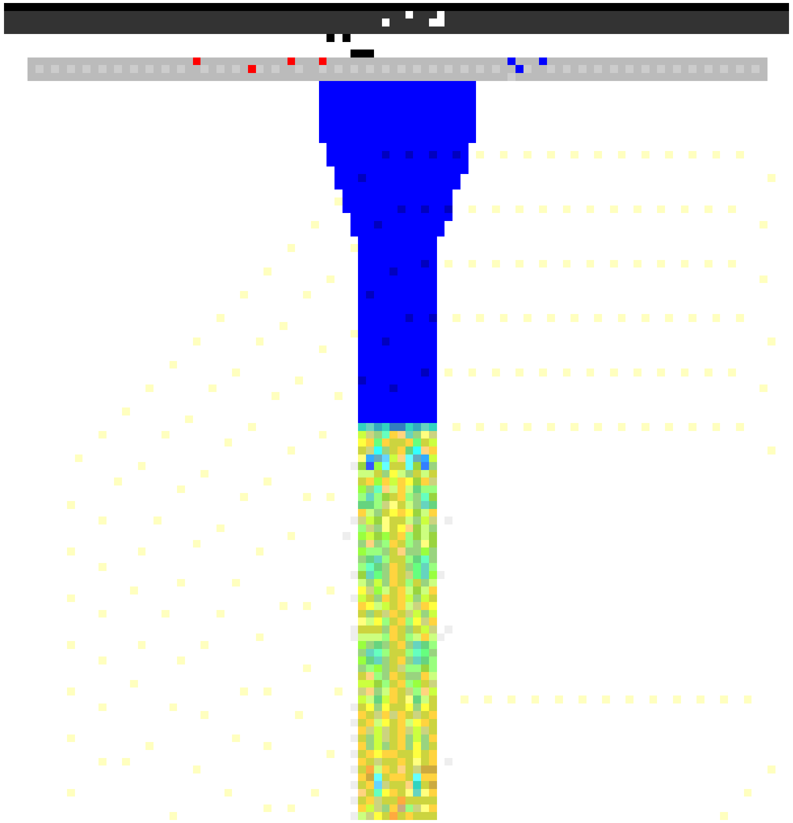
Outlet Concentration



Gas phase species, as a function of time, in the exit stream simulating the chlorination of a bed of metallurgical grade silicon by reaction with H_2 and $SiCl_4$.

Toulouse Experiments Facility

- **Stainless steel cylinder**
  - **5.3 cm (ID), 63 cm tall**
- **Sloping transition**
  - **1.2 cm tall**
- **Expansion section**
  - **10 cm (ID), 17.7 cm tall**
- **Restricted center outlet**
  - **2 cm (ID)**
- **Distributor:**
  - **cooled (< 450 °C),**
  - **stainless steel perforated plate**



Caussat, Hémati, and Couderc, 1995.

SiH_4 Pyrolysis

Scheme I (global kinetics):

$$SiH_4 \rightarrow Si + 2\,H_2$$

$$\left(\frac{d[SiH_4]}{dt}\right)\left(\frac{\text{mol}}{\text{cm}^3\cdot s}\right) = -\frac{k_{V0}[SiH_4]}{1+K_U P_{H_2}} - \left(\frac{6}{d_p}\frac{1-\varepsilon}{\varepsilon}\right)\frac{k_{S0}[SiH_4]}{1+K_{H_2}P_{H_2}+K_{SiH_4}P_{SiH_4}}$$

$$k_{V0} = 2.14 \times 10^{13}\ (1/\text{s})e^{-26{,}620(\text{K})/T}$$

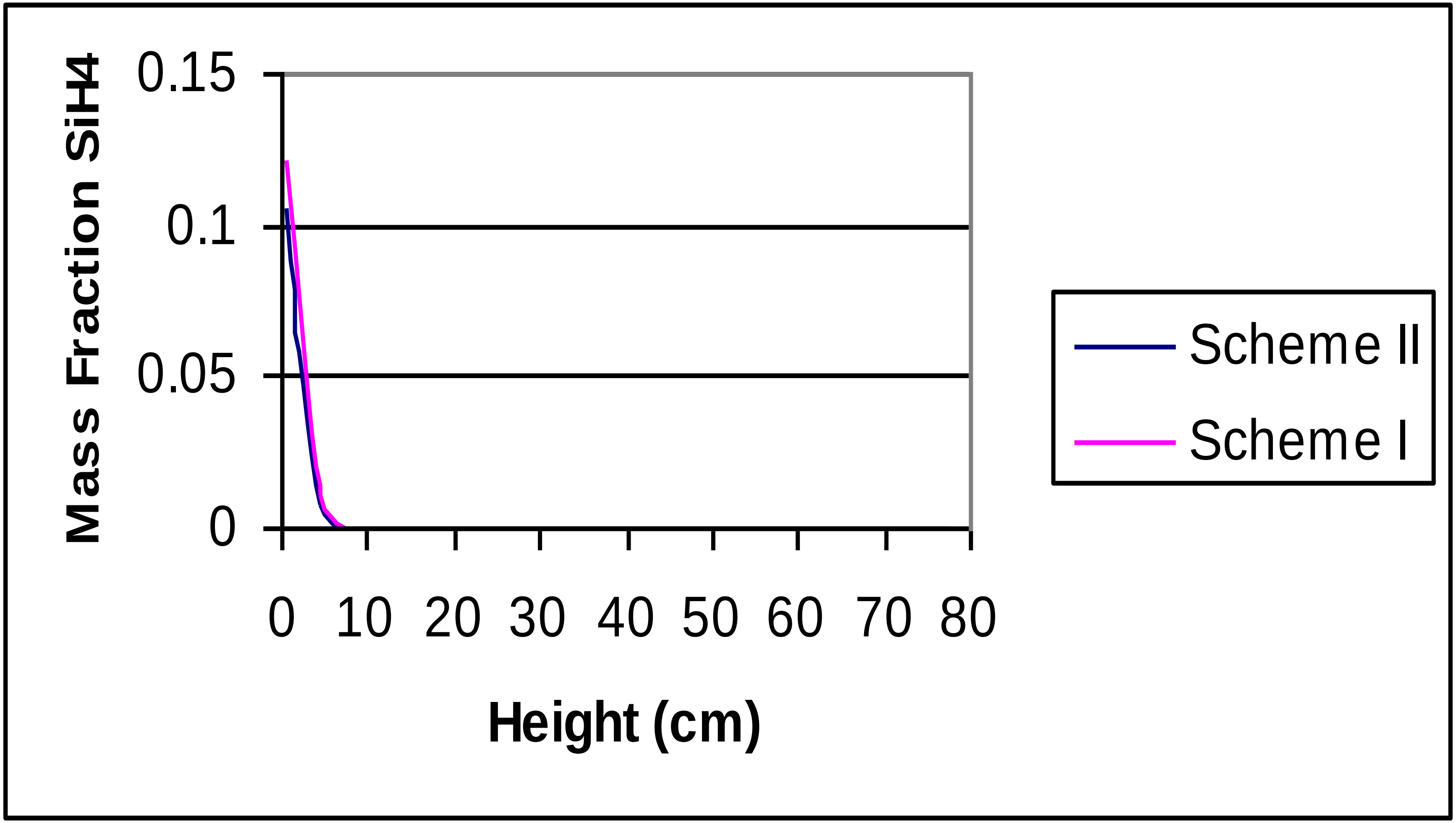
$$K_U = 0.50\ (1/kPa)$$

$$k_{S0} = 2.15 \times 10^{10}\ (\text{cm/s})e^{-23{,}030(\text{K})/T}$$

$$K_{H_2} = 0.034\ (1/kPa)$$

$$K_{SiH_4} = 7.6 \times 10^{-3}\ (\text{cm/s})e^{+3960(\text{K})/T}$$

Furusawa, Kojima, Hiroha, 1988.



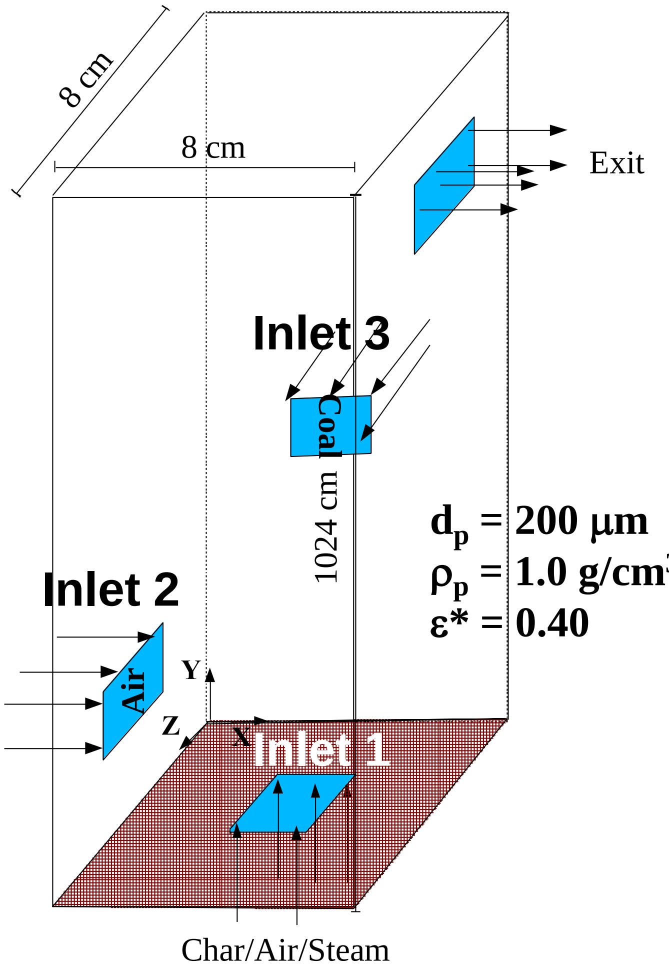
Mass Fraction SiH4
0.15
0.1
0.05
0
0
10
20
30
40
50
60
70
80
Height (cm)
Scheme II
Scheme I

Gasifier Simulations

- Develop a systematic procedure to understand the interaction between different non-linear processes (convection, reactions, diffusion, phase change, heat & mass transfer)
  - Cause and effect?
  - Is it even possible to unravel the behavior of such complex systems?
- Critical for design
  - The desirable conversion is dependent on the time-scales of the various processes but also the spatiotemporal evolution of the field variables
    - Exothermic reactions, solids distribution, thermal expansion etc.
  - The effect of inlets and boundary conditions
  - What is the optimal size of the reactor?
    - Reactor height, location/area/mass-flow of the inlets etc.
  - Insights into scaling?
- Enormous amount of data from large simulations
  - Knowledge discovery
  - Aid development of reduced-order models
  - Aid experiments
  - Current evaluation of accuracy might be limiting

Pannala, Guenther, Gel, Galvin and Syamlal,
CFD CRE V, 2008

Simulation Configuration



d_p = 200 μm
ρ_p = 1.0 g/cm^3
ε* = 0.40

Not to scale

- Char/Air/Steam inlet and Exit - 4x4 cm
- Coal and Air inlets – 2x2 cm
- Cartesian mesh
- Cases Studied:
  - Case A: Ozone decomposition
  - Case B: Char combustion
  - Case C: Complex gasification chemistry
- Different resolutions
  - 0.25M cells: Cases A, B, and C
    - 2-3 weeks run-time for 15s on 16-32 processors (AMD Cluster)
  - ~2M cells: Case C
    - 10-days run-time for 15s on 256-512 processors (CRAY XT4)
  - ~10M cells: Case C
    - 1-week run-time for 5s on 1024-2048 processors (CRAY XT4)

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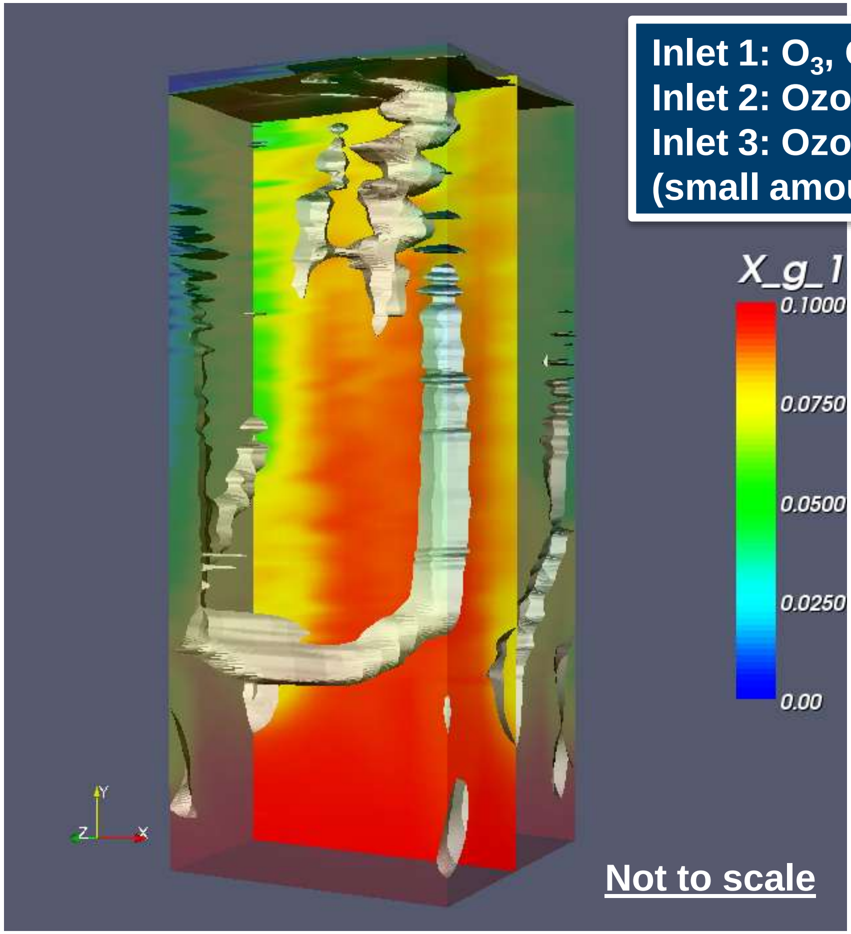
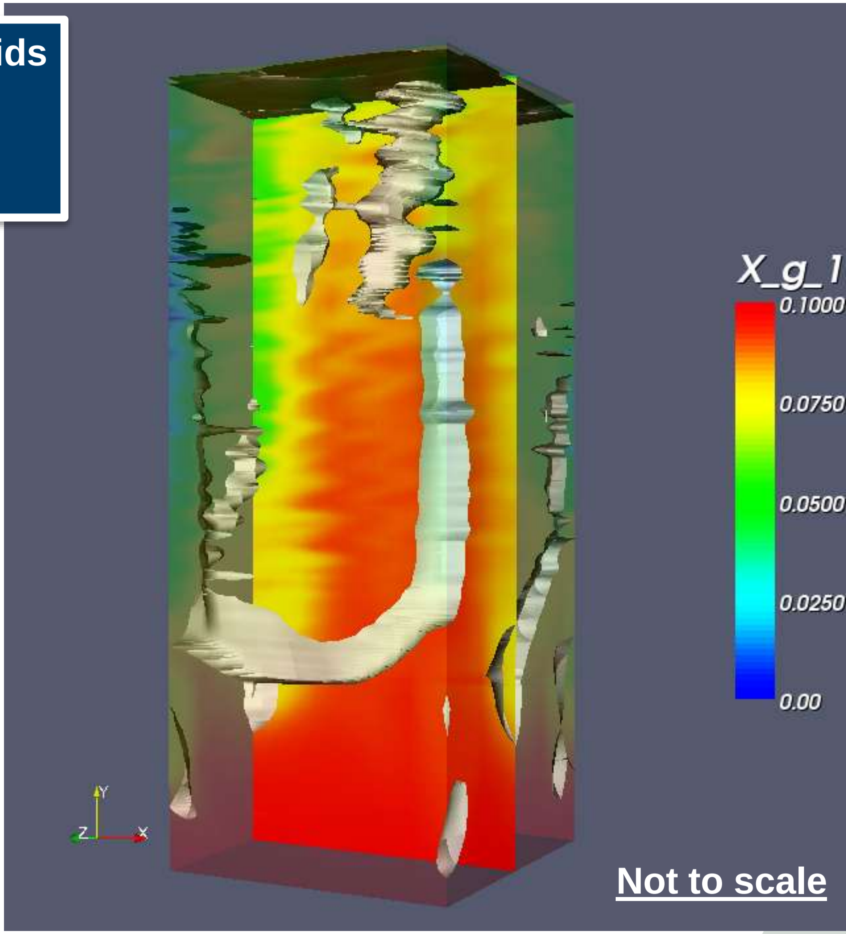
Ozone concentration along with solids contours (Case A – Ozone Decomposition)

Inlet 1: O_3, O_2, N_2, Solids
Inlet 2: Ozone
Inlet 3: Ozone, solids (small amount)





- **Solids accumulate primarily at corners and top**
- **Ozone conversion is strongly correlated to solids presence**

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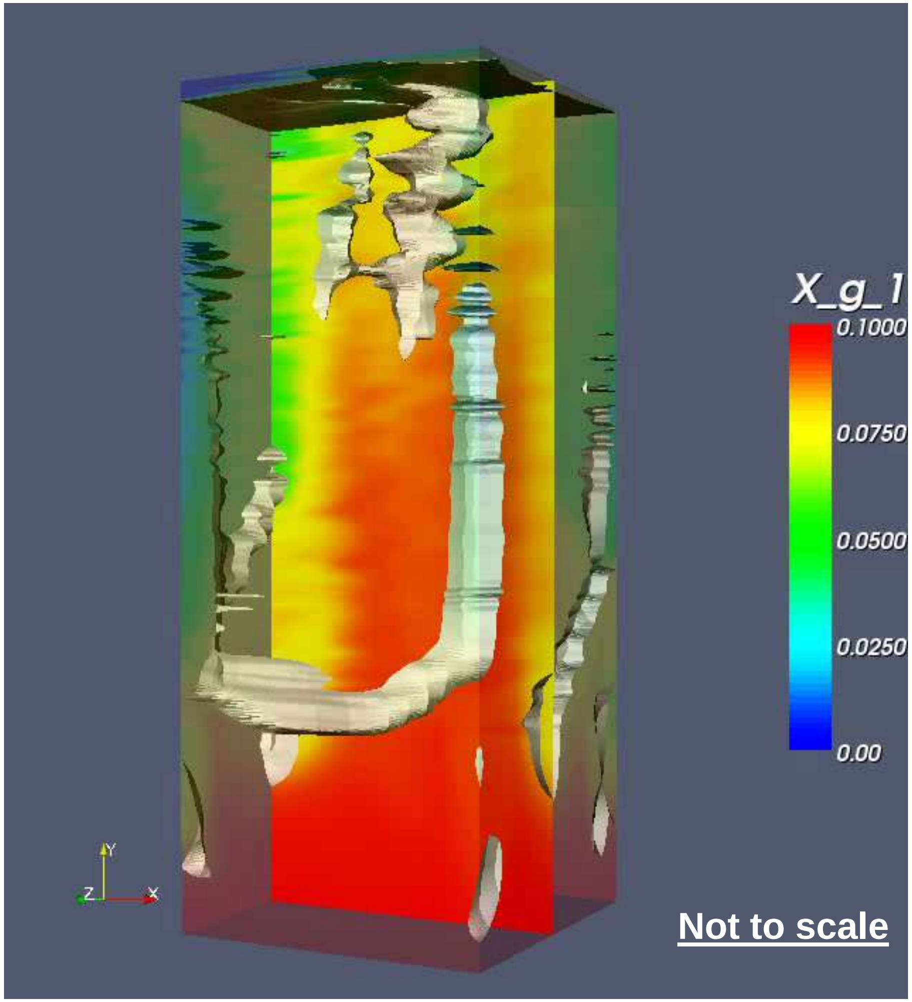
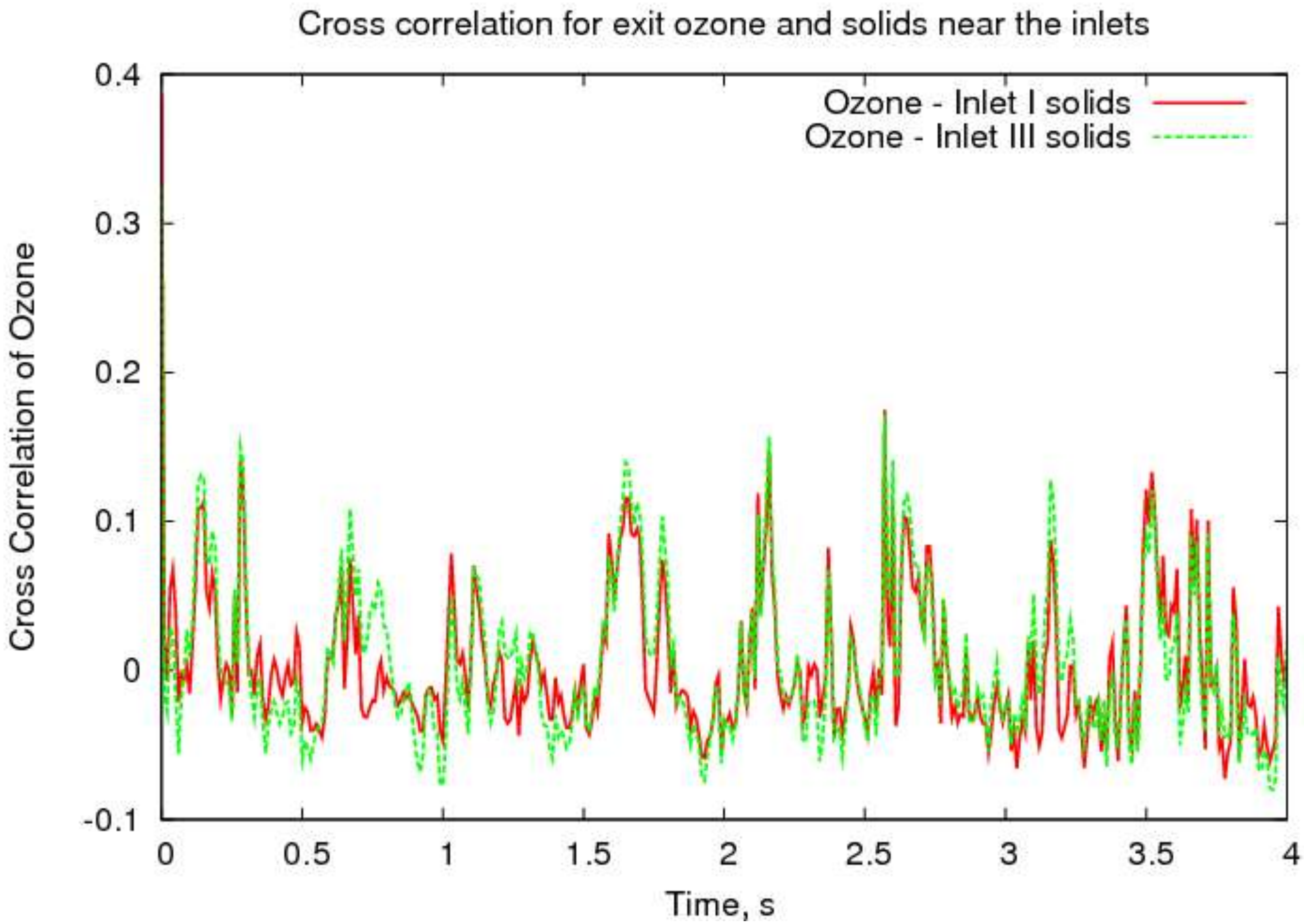
Ozone concentration along with solids contours (movie)



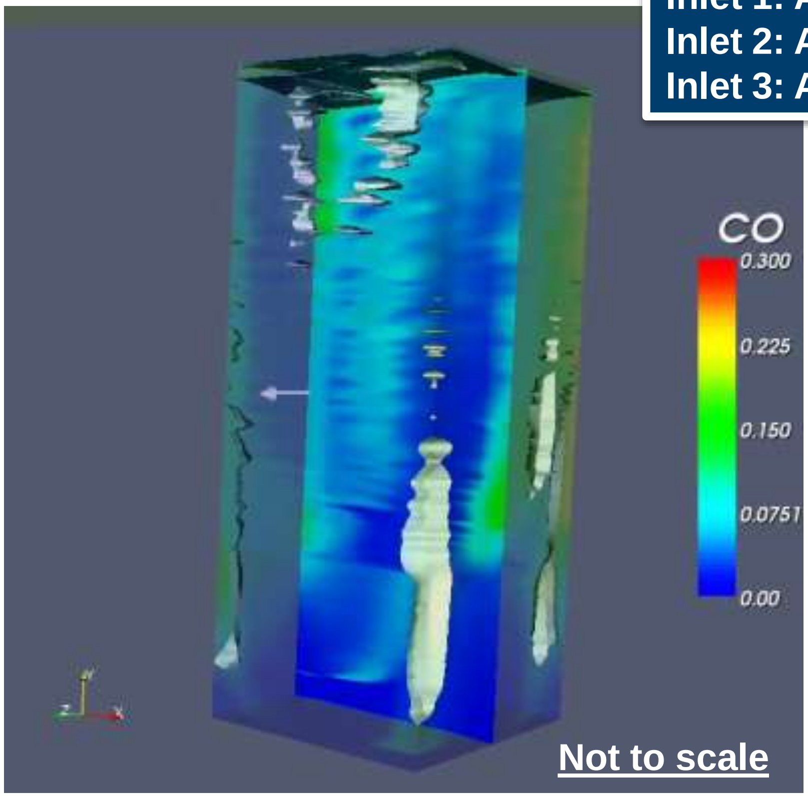
Cross-correlation

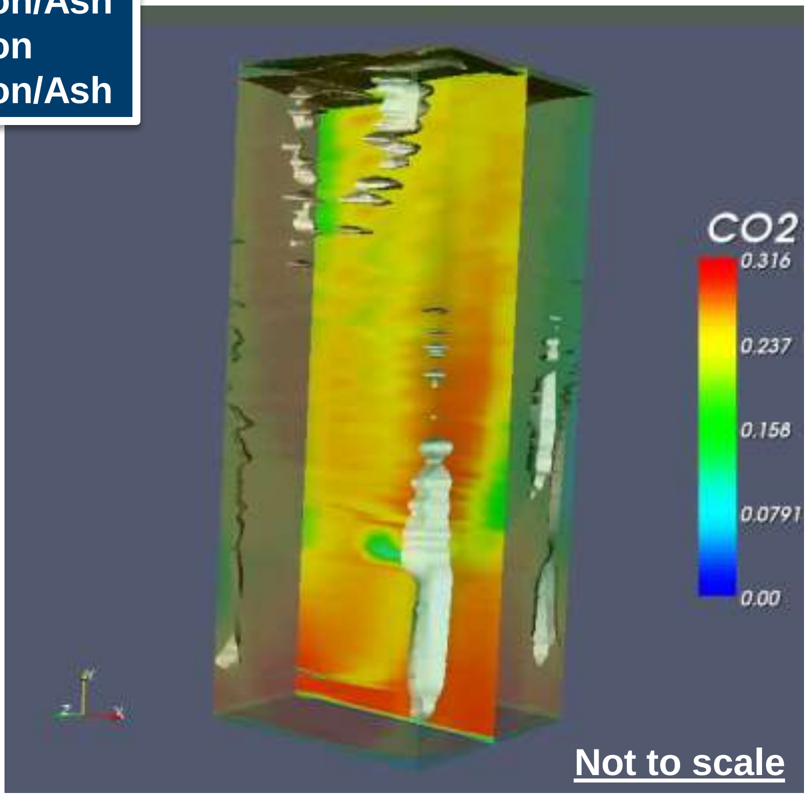


- **Weak correlation between the exit ozone and inlet solids**
- **Too many complex interactions in the reactor**

CO and CO_2 along with solids contours (Case B – Char Combustion)

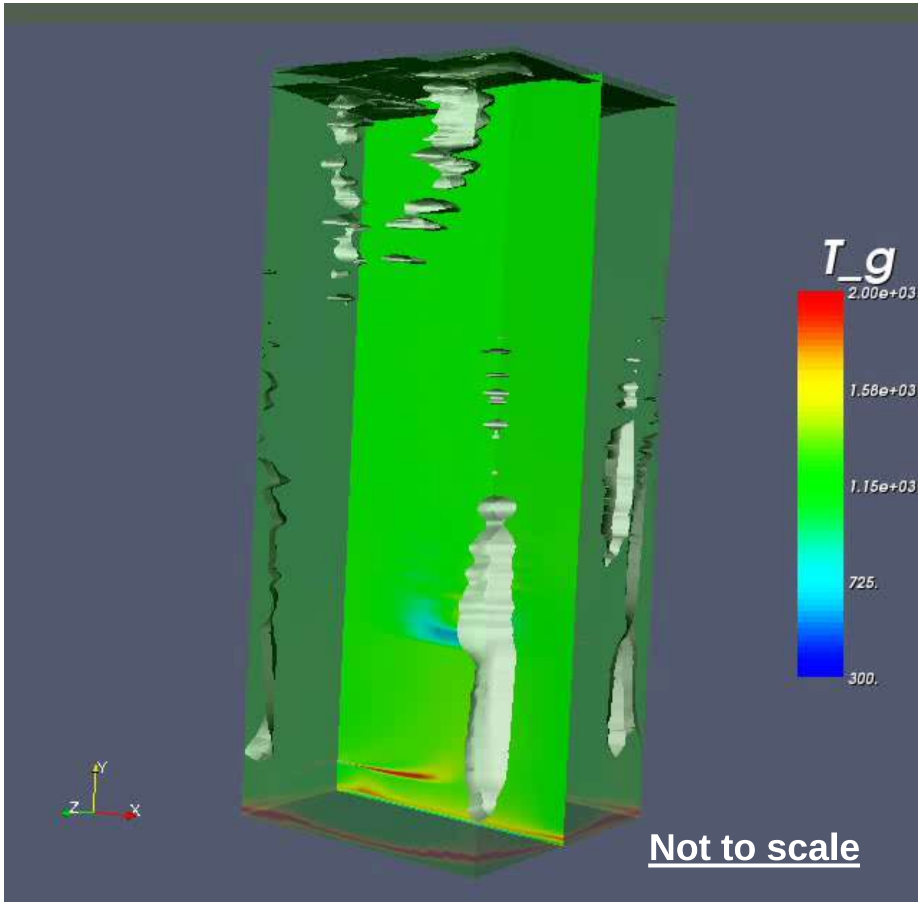
Inlet 1: Air, Carbon/Ash
Inlet 2: Air, Carbon
Inlet 3: Air, Carbon/Ash





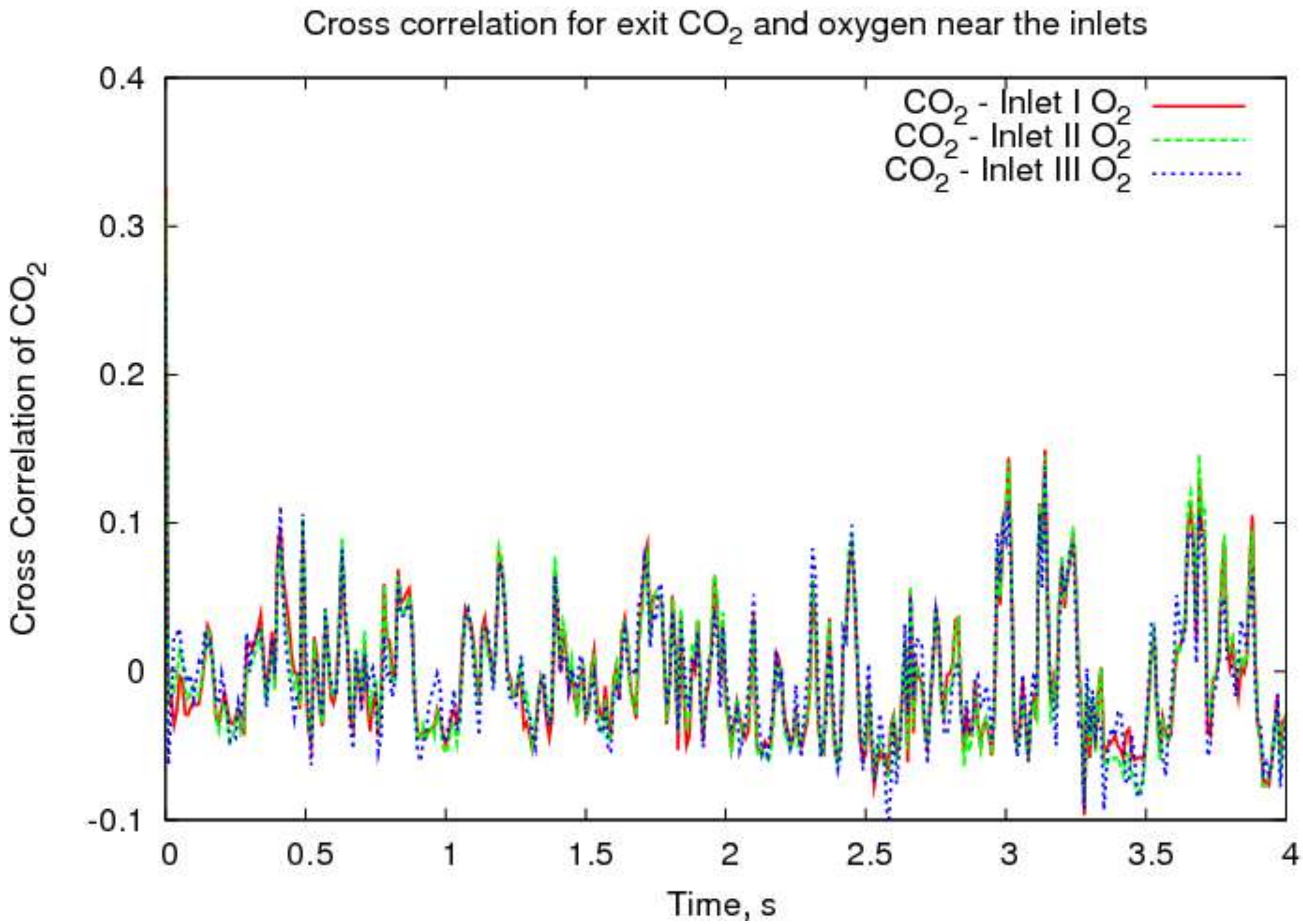
- Solids accumulate primarily at corners in the lower domain and top wall
- Higher CO and lower CO_2 in the vicinity of solids

Gas Temperature along with solids contours (Case B – Char Combustion)



- **Solids accumulate primarily at corners in the lower domain and top wall**
- **Weak correlation between the solids and gas-temperature**

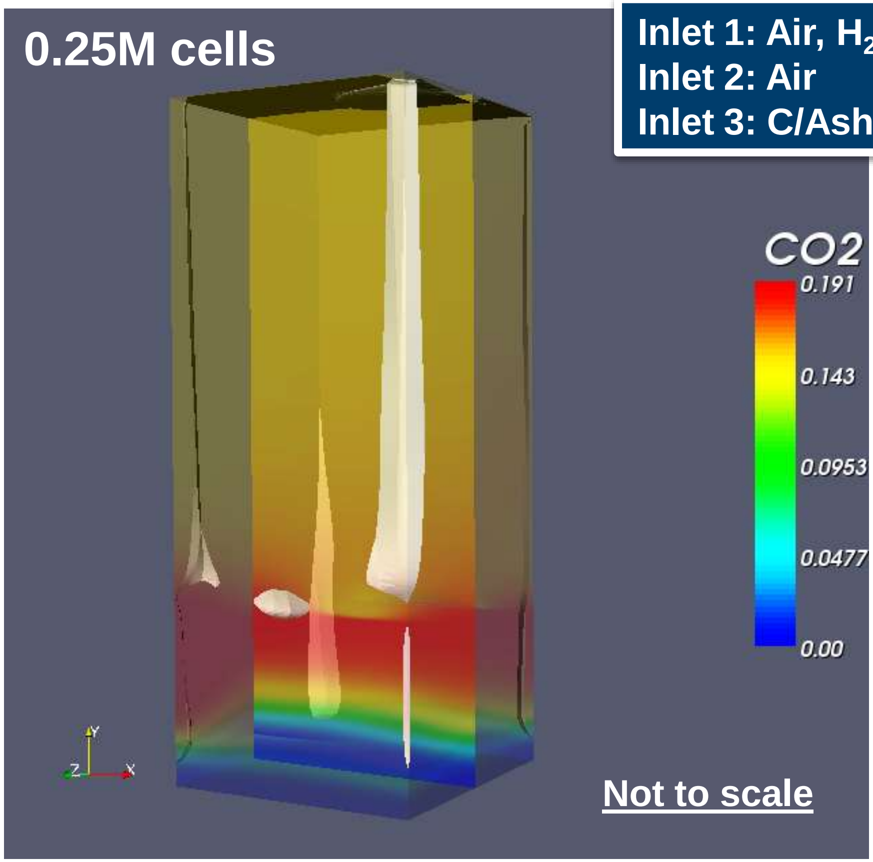
Cross-correlation

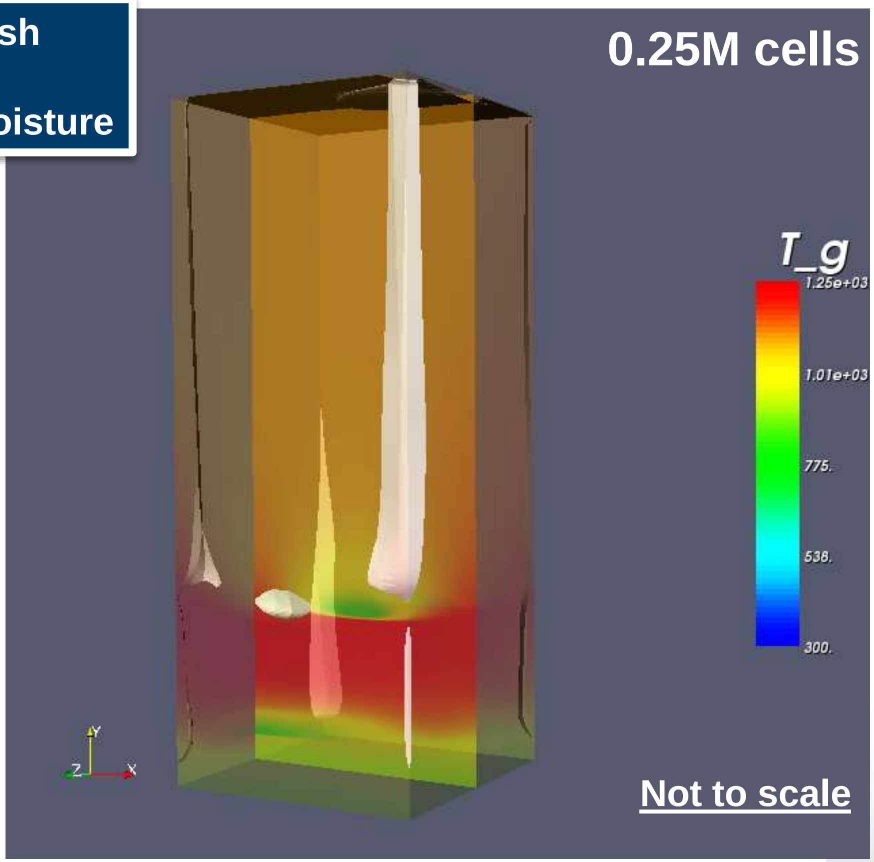


- **Weak correlation between the exit CO_2 and inlet O_2**
- **Too many complex interactions in the reactor**
- **Correlation seems to be weaker than O_3**

Gas Temperature and CO_2 along with solids contours (Case C - C3M Module)

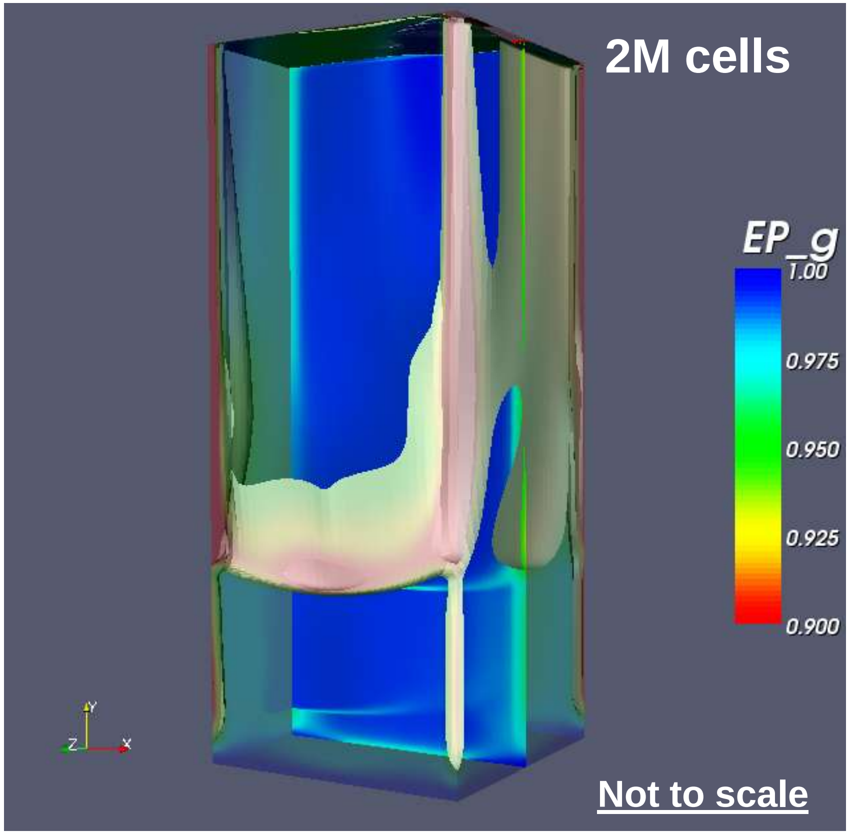
Inlet 1: Air, H_2O, C/Ash
Inlet 2: Air
Inlet 3: C/Ash/VM/Moisture

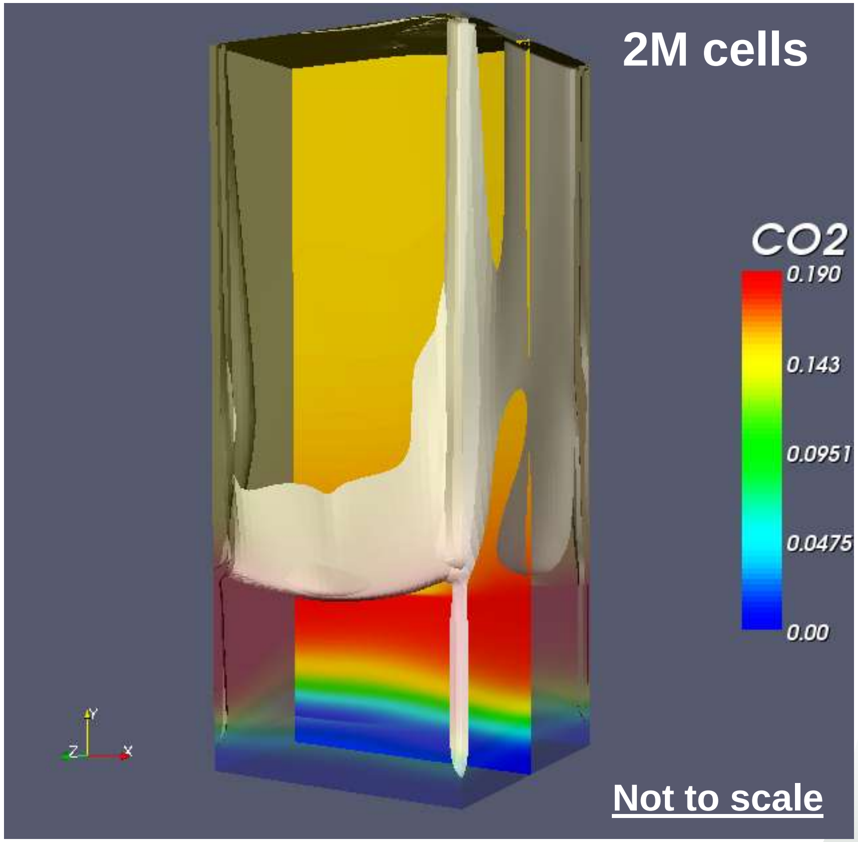




- Solids accumulate primarily at the corners and top wall
- Gas temperature and CO_2 are strongly correlated

Void Fraction and CO_2 along with solids contours (Case C - C3M Module)





- **Resolution provides better details**
- **Qualitative trends remain the same except for higher solids loading at the walls**

Outline of Presentation

- Introduction to Fluidization
  - Phenomena and Terminology
- Multiphase CFD
  - Introduction
  - Hydrodynamic Equations
  - Interphase Forces
  - Granular Stress
  - Gas-solids turbulence
  - Energy balance
  - Species balance
  - Numerical techniques
- MFIX Code
- Validation of hydrodynamics
  - Bubbling Fluidized Bed
  - Circulating Fluidized Bed
  - Spouted bed
- Fluidized bed reactors
- Industrial application of multiphase CFD

Where can CFD help?

- Troubleshoot existing devices
- Gain insight about design options
- Evaluate preliminary designs
- Select optimum design
- Discover new designs

Guidelines for Applying CFD – 1

- Problem definition
  - Clearly define the objectives of the simulation
  - Check whether CFD modeling is appropriate for the problem at hand
  - Clearly define the area of primary interest (domain) for the CFD calculation
  - Identify the local/global quantities that are needed from the simulation
    - CFD's strength is in giving insight into local phenomenon
    - Global quantities (e.g., over all conversion) are used for validation
  - Determine the accuracy requirements

Guidelines for Applying CFD – 2

- **Information required**
  - Geometry
  - boundary conditions
  - Initial conditions
  - Physical properties
  - Chemical reaction kinetics
- **Choices made by CFD Analyst**
  - The domain that is being modeled
  - Physical Models
  - Numerical grid
  - Numerical parameters (under relaxation factors, convergence criteria, …)

Guidelines for Applying CFD – 3

- Be aware of the errors and uncertainties
  - Model errors – Use valid physical models
  - Discretization error – Strive for grid-independent solution
  - Iteration or convergence error – May need to reduce residual tolerance and recheck solution
  - Round-off error
  - Ensure that a stationary state has been achieved
  - Uncertainties in specifying the problem – Work closely with design engineers
  - User errors – Double check user input
  - Code errors

Guidelines for Applying CFD – 4

- Checking results
  - Check over all mass balance; e.g. check MFIX log
  - Ensure that gas velocities are reasonable
  - Ensure that the over all pressure drop is reasonable, usually roughly equal to bed weight
- Model validation
  - At a minimum do global validation of quantities such as over all conversion, exit concentration etc.
  - Strive to do as much detailed validation as possible (e.g., velocity, pressure, mass fraction profiles)
  - Ensure that proper averaging technique is used
  - Use error bars on experimental data

Guidelines for Applying CFD – 5

- Communication of model results
  - Team with design engineers and pilot plant engineers and make the expectations clear
  - Educate them about the basis of the models
  - Provide evidence regarding the validity of the models
  - Communicate results frequently to design engineers and seek feedback
  - Communicate CFD results so that designers can gain insight. Animations and computer graphics greatly help.

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Day 2: Getting Started with MFIX

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presented at

Coal Gasification Short Course

Criciúma, Santa Catarina, Brazil
May 10-14, 2010

Outline

- **Day 1**
  - **Install Cygwin, MFIX, Paraview**
  - **Reacting multiphase flows**
  - **Volume averaged equations, closures, code walk through**
- **Day 2**
  - ~~**Volume averaged equations, closures, code walk through (contd..)**~~
  - **Hands-on training: Hydrodynamics cases**
- **Day 3**
  - **Hands-on training: Study the effect of grid resolution, numerical schemes etc.**
  - **Hands-on training: Cartesian grid**
- **Day 4**
  - **Hands-on training: Add heat and mass transfer, chemical reactions**
- **Day 5**
  - **Hands-on training: Put all the things learned to a case with hydrodynamics, heat and mass transfer and chemical reactions**
  - **Close with future pointers**

This is tentative and subject to change based on the feedback, pace, etc.,

Cygwin Installation

- Download Cygwin (setup.exe) from http://cygwin.org/. A nice summary is available at http://www.physionet.org/physiotools/cygwin/.
  - You can use google translator: http://translate.google.com/# if needed
  - http://translate.google.com/translate?js=y&prev=_t&hl=en&ie=UTF-8&layout=1&eotf=1&u=http%3A%2F%2Fwww.physionet.org%2Fphysiotools%2Fcygwin&sl=auto&tl=pt
- Once downloaded, click on setup.exe
- Choose a download site close to you
- Under devel tab, choose ‘gcc4-fortran’, ‘make’, ‘gdb’
- Under docs tab, choose ‘xpdf’ – to view pdf files (optional)
- Under edit, choose ‘vim’ and ‘nedit’ – nedit is a simple editor like note pad but provide syntax coloring, etc. – editing the files using note pad can insert windows characters and make them unworkable
- Under Graphics, choose ‘gnuplot’ and ‘ImageMagick’ (optional)
- Under X11 (see http://x.cygwin.com/docs/ug/setup-cygwin-x-installing.html), choose whatever is most appropriate for your needs – cygwin can be used as an x-terminal similar to exceed but it is also needed if you want to use nedit, etc. (optional) – xorg-server, xterm, xinit
- After you choose the above config options you can proceed with the installation. It might take an hour or so to download and install cygwin.

fortran, make, gdb, xpdf, nedit, gnuplot, xinit, xorg-server, xterm, vim

MFIX Installation

- Download mfix from https://mfix.netl.doe.gov/members/download_develop/mfix.tar.gz
- Place it in your home directory on cygwin. If you installed cygwin at c:\cygwin, the home directory would be c:\cygwin\home\your_user_name
- Open the cygwin terminal – click on the shortcut on the desktop
- If you want X support, just type in 'startx' and you should get a new terminal which supports X or using the links Cygwin-x under program menu. If you have any problems, try to follow the steps at: http://x.cygwin.com/docs/ug/setup-cygwin-x-installing.html
- To begin with you will be in your home directory. If you have mfix.tar.gz at that location, at the command prompt, type: tar xzvf mfix.tar.gz – this should create the directory mfix
- From now on you can follow the instructions in the Readme for Linux installations. Here is a quick summary:
  - cd mfix/tutorials/fluidBed1 (just picking this as an example)
  - sh ../../model/make_mfix
  - Choose the default settings for compilation options and for the compiler, chose gfortran (option 2)
  - After the compilation is successful, type ./mfix.exe and this should run the case
  - You could download visit (https://wci.llnl.gov/codes/visit/) or paraview (http://paraview.org/) for windows and use it to visualize the data generated directly

What is in mfix directory

- CHANGES – lists changes from previous versions
- Readme.pdf – very important file to get started
- doc – various documents, another good resource in addition to the documents online
- Tutorials – good cases to run and to get familiar with the code and capabilties
- ani_mfix – if you want to use this for visualization – I prefer Paraview and that is what I will show today
- model – all the code lies here
- tests – good set of cases to go through
- cartesian_grid_tutorials – if you are interested in cartesian grid
- post_mfix – set of post-processing tools to analyze data – maybe we will get a chance to use this
- tools – various tools, e.g. to generate make files if you add new source files in the model directory

Readme version 2010-1 1

MFIX

Multiphase Flow with Interphase eXchanges
Version MFIX-2010-1 (Date: 02/02/2010)

Notice

Neither the United States Government nor any agency thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed or represents that its use would not infringe privately owned rights.

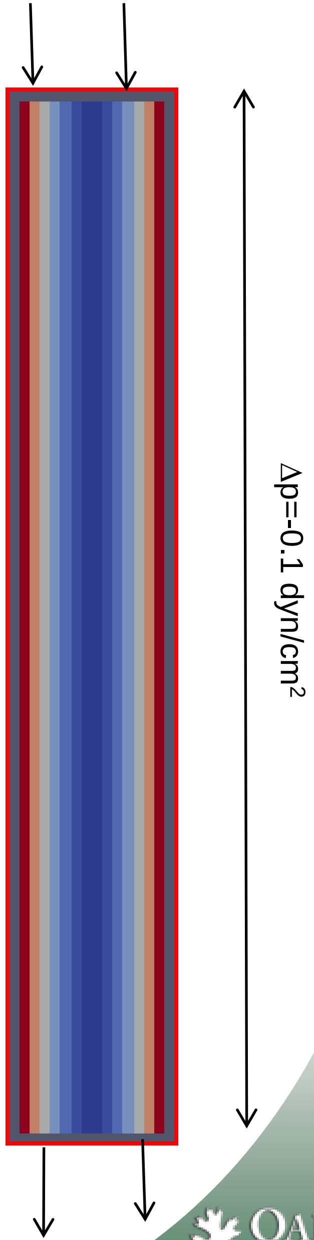
- MFIX is provided without any user support for applications in the user's immediate organization. It should not be redistributed in whole or in part.
- The use of MFIX is to be acknowledged in any published paper based on computations using this software by citing the MFIX theory manual. Some of the submodels are being developed by researchers outside of NETL. The use of such submodels is to be acknowledged by citing the appropriate papers of the developers of the submodels.
- The authors would appreciate receiving any reports of bugs or other difficulties with the software, enhancements to the software, and accounts of practical applications of this software.

Table of Contents

Pipe flow – single phase with pressure drop

- **We only solve for ½ the domain – axisymmetric**
- **Length: 100 cm; Width: 7 cm (radius)**
- **Grid: 100 x 7**

$$V_g(x) = \Delta P_y * x^2 / (4 * \mu_g * Y)$$



Let us look at the mfix.dat file

```
#
#  developed flow -- use cyclic condition
#
#  F.B. Modeler                   9-6-94
#
#  V_g(2,j,k) = delp_y * XLENGTH^2/(4*mu_g0*YLENGTH) (BSL p.46)
#
#
# Run-control section
#
  RUN_NAME = 'COL01'
  DESCRIPTION = 'developed laminar flow'
  RUN_TYPE = 'new'  !  'restart_1' !
  UNITS = 'cgs'
#   TIME  =0.0  TSTOP = 1.0E-4   DT = 1.0e-4   DT_MAX = 1.0e-4   OUT_DT = 1.0e-4
  ENERGY_EQ = .FALSE.
  SPECIES_EQ = .FALSE.    .FALSE.
  MOMENTUM_X_EQ(1) = .FALSE.
  MOMENTUM_Y_EQ(1) = .FALSE.
  LEQ_IT(1) = 20
  LEQ_IT(3) = 50
  LEQ_IT(4) = 50
!  UR_FAC(3) = 0.7  LEQ_METHOD(3) = 2
!  UR_FAC(4) = 0.7  LEQ_METHOD(4) = 2

  GRAVITY = 0.0
#
# Geometry Section
#
  COORDINATES = 'cylindrical'

  XLENGTH  =   7.0    IMAX =  7
  YLENGTH  = 100.0    JMAX = 10

  NO_K      = .TRUE.
  CYCLIC_Y_PD = .TRUE.
  delp_y = -0.1

  MAX_NIT = 3000
  TOL_RESID  = 1.E-4


#
# Gas-phase Section
#
  RO_g0 = 1.0
  MU_g0 = 0.01
  MW_avg = 29.
#
```

NETL

Oak Ridge National Laboratory

Let us look at the mfix.dat file

```
# Solids-phase Section
#
  MMAX          = 0


#
# Initial Conditions Section
#
       !
  IC_X_w            =  0.0
  IC_X_e            =  7.0
  IC_Y_s            =  0.0
  IC_Y_n            = 100.0

  IC_EP_g           =  1.0

  IC_U_g            =   0.0
  IC_V_g            =  0.0



#
#  Output Control
#
  RES_DT = 0.01
  OUT_DT = 10.
        !
        ! EP_g P_g       U_g  U_s  ROP_s     T_g  X_g
        !      P_star    V_g  V_s            T_s1 X_s
        !                W_g  W_s            T_s2
  SPX_DT = 0.01 0.1      0.1  0.1  100.      100. 100.    100.   100.

  NLOG   = 25
  RESID_STRING = 'P0'  'U0' 'V0'
  FULL_LOG = .TRUE.

# DMP control

  NODESI = 1  NODESJ = 1   NODESK = 1
```

Code compilation

```
DISCRETE:developed_pipe_flow% sh ../../model/make_mfix


*******************************************
* Creating the MFIX-executable mfix.exe   *
*               Version 2010-1               *
*******************************************



MFIX directory is /cygdrive/c/Users/8sx/Documents/8sx-cyg/MFIX/support/brazil/co
urse_material/mfix/model

Do you need SMP version? (y/n) [no]

Do you need DMP version? (y/n) [no]
Do you need debug version? (y/n) [no]

Force re-compilation of source files in run directory? (y/n) [no]




CYGWIN on Windows Detected

==============================================================
MFIX Compilation directives available for following compilers:
==============================================================
 [1] g95
 [2] gfortran

Select the compiler to compile MFIX? [2]
```

Successful compilation

```
    source_ghd_granular_energy.o \
    thermal_conductivity.o \
    thermal_diffusivity.o \
    thermal_mobility.o \
    transport_coeff_ghd.o \
    get_values.o \
    readTherm.o \
  -o mfix.exe odepack.a blas90.a dgtsv90.a
\nPlease wait . . .
make -f mfix_l_not.make mfix.exe
make: `mfix.exe' is up to date.

*******************************************

 Compilation successful: mfix.2010-1 created
 To run MFIX type: mfix.exe
*******************************************
```

- **mfix.exe is created only when you have successful compilation**

Running the code

- ./mfix.exe

```
DISCRETE:developed_pipe_flow% ls
AUTOTEST  mfix.dat  mfix.exe
DISCRETE:developed_pipe_flow% ./mfix.exe

 MFIX (2010-1    ) simulation on computer: discrete
 Run name: COL01                  Time:  3:45                   Date:  5-11-2010
 Memory required:    9.11 Mb

------------------------------------------------------------------------
           0           1


 Starting solids mass = 0.0000        CPU time left =     0.000 s
  Nit      P0        U0        V0    Max res
    1   2.        0.        0.      P0
    2  0.4      3.3E-02  0.6      V0
    3  0.3      1.6E-02  0.3      V0
    4  0.2      9.0E-03  0.2      V0
    5  0.1      5.7E-03  0.2      V0
    6  3.7E-02  2.7E-03  0.1      V0
```

Files in the run directory

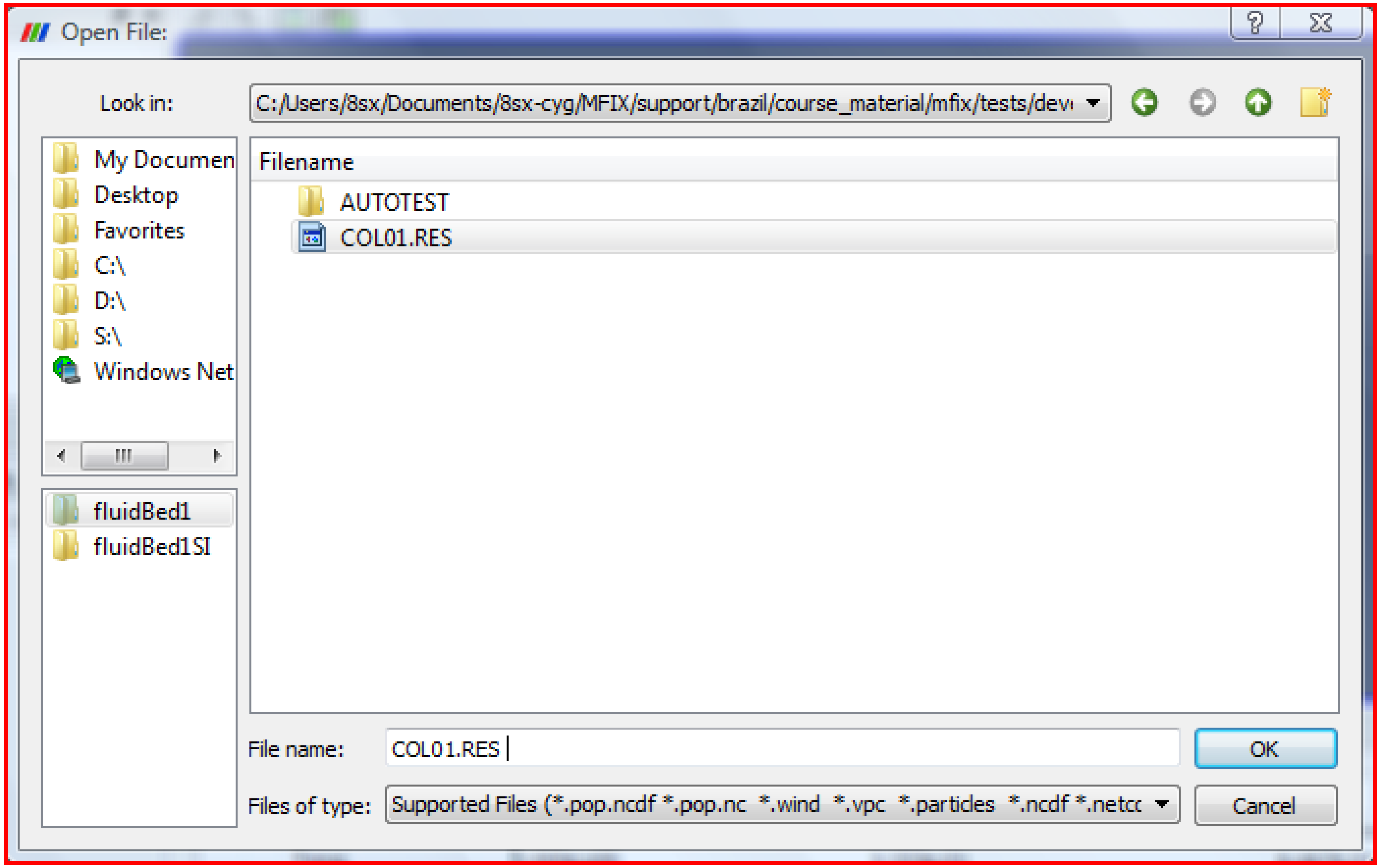
```
DISCRETE:developed_pipe_flow% ls
AUTOTEST    COL01.RES   COL01.SP3   COL01.SP6   COL01.SP9   mfix.dat
COL01.LOG   COL01.SP1   COL01.SP4   COL01.SP7   COL01.SPA   mfix.exe
COL01.OUT   COL01.SP2   COL01.SP5   COL01.SP8   COL01.SPB   scr00000
```

- ***.LOG files and *.OUT are very important files – you want to look at them whenever you run into a problem**

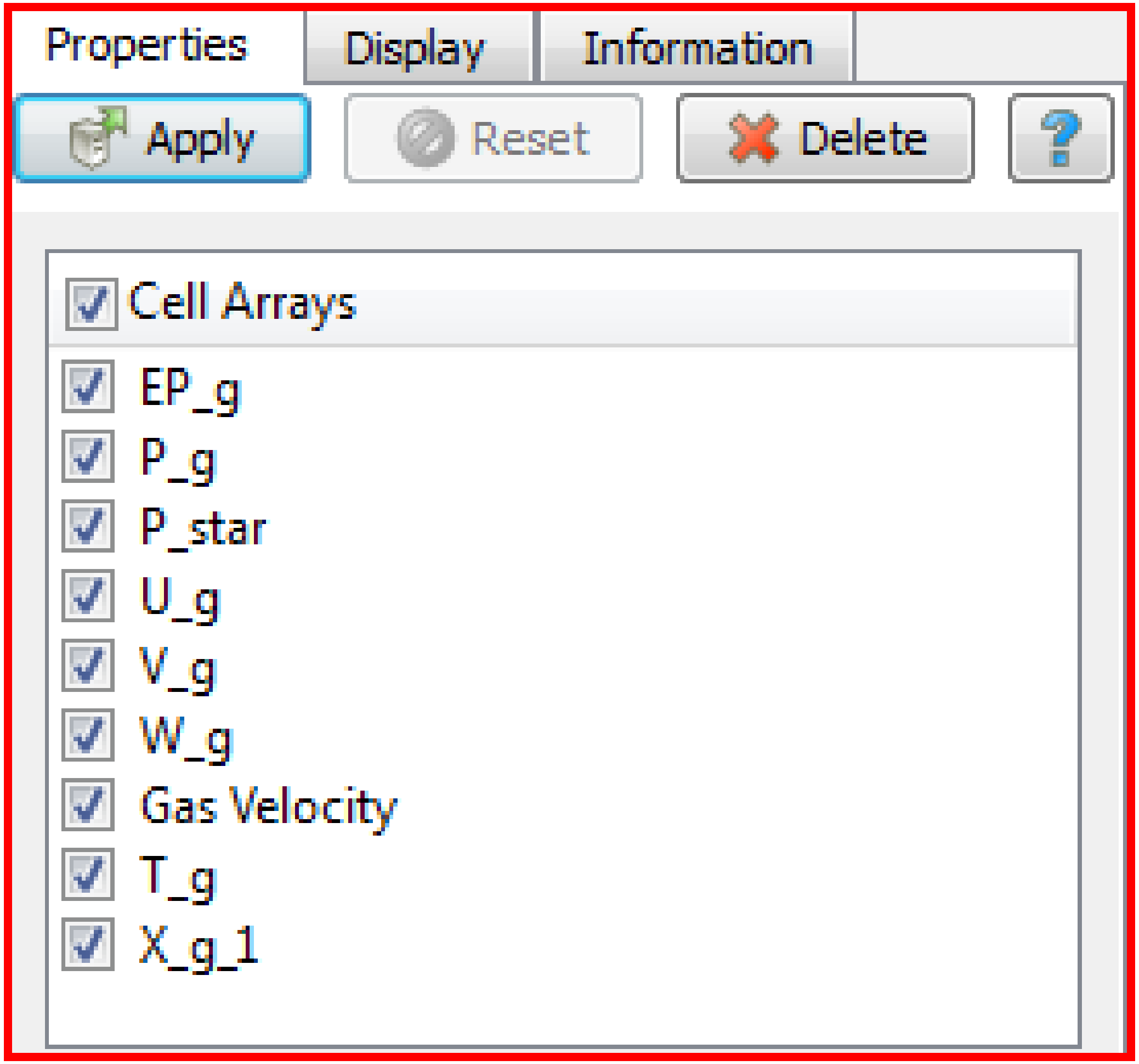
COL01.OUT

Visualizing the results

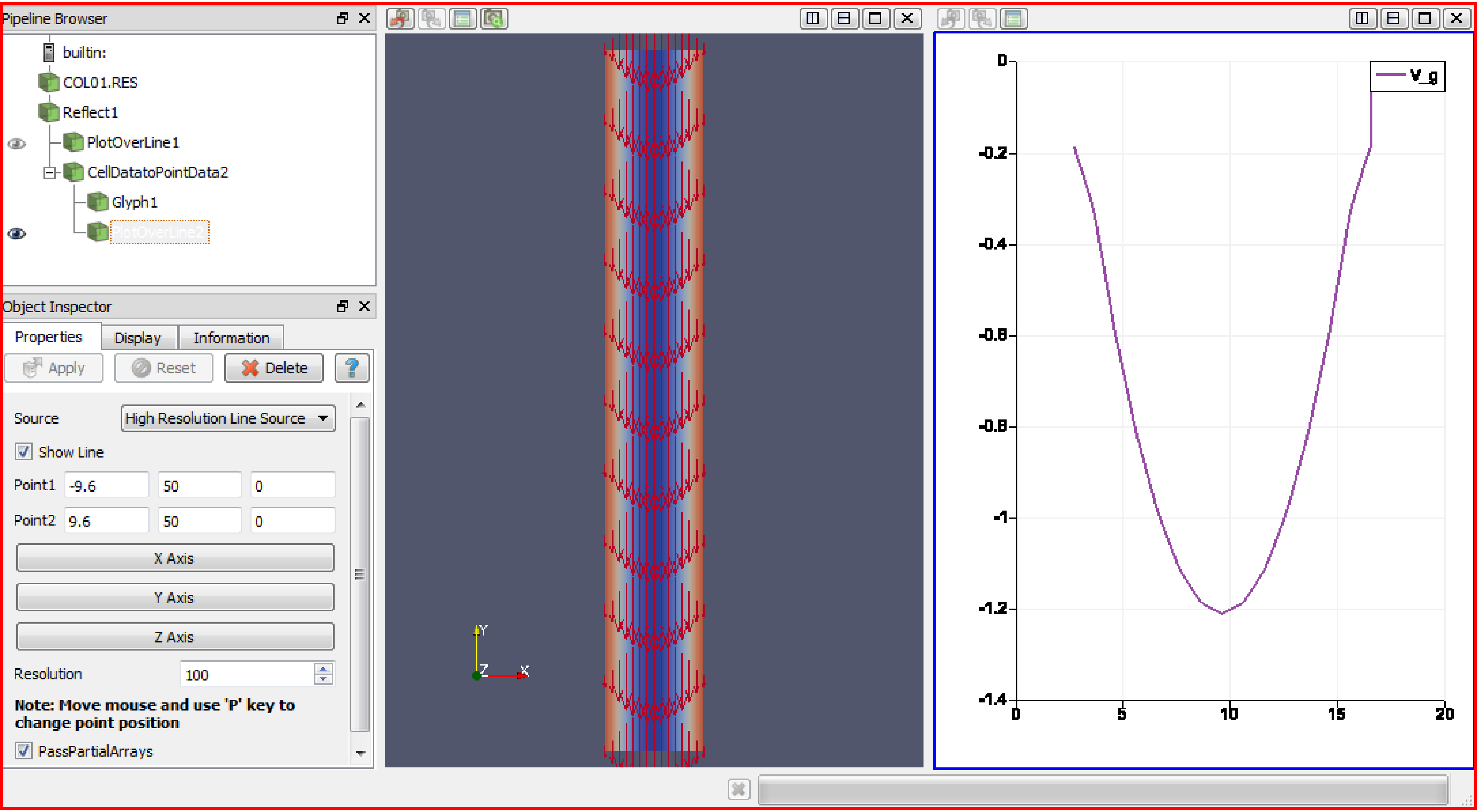
- **Launch paraview from desktop shortcut or from program menu and select the *.RES file**



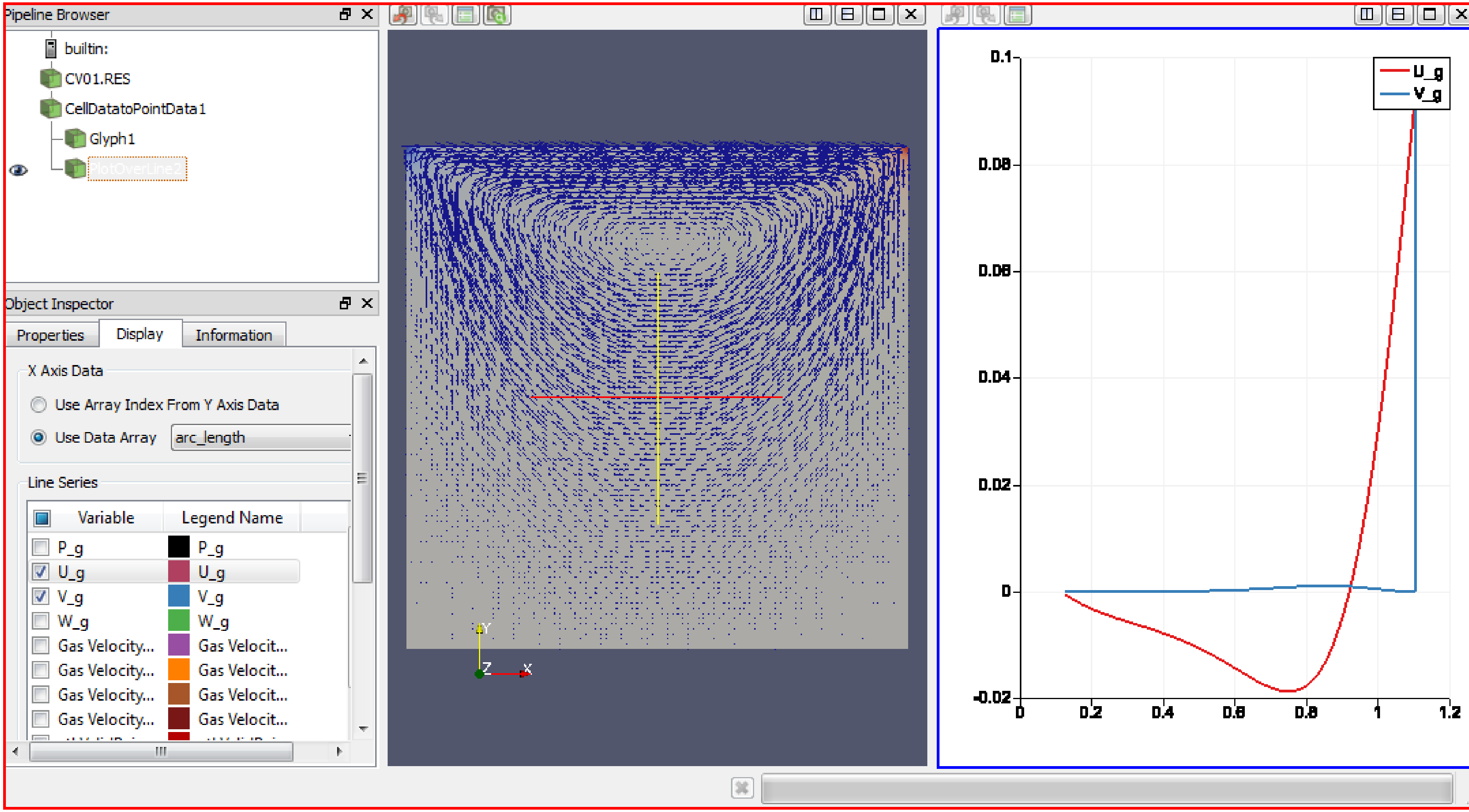
Select the data you need – safe to select all and press apply button



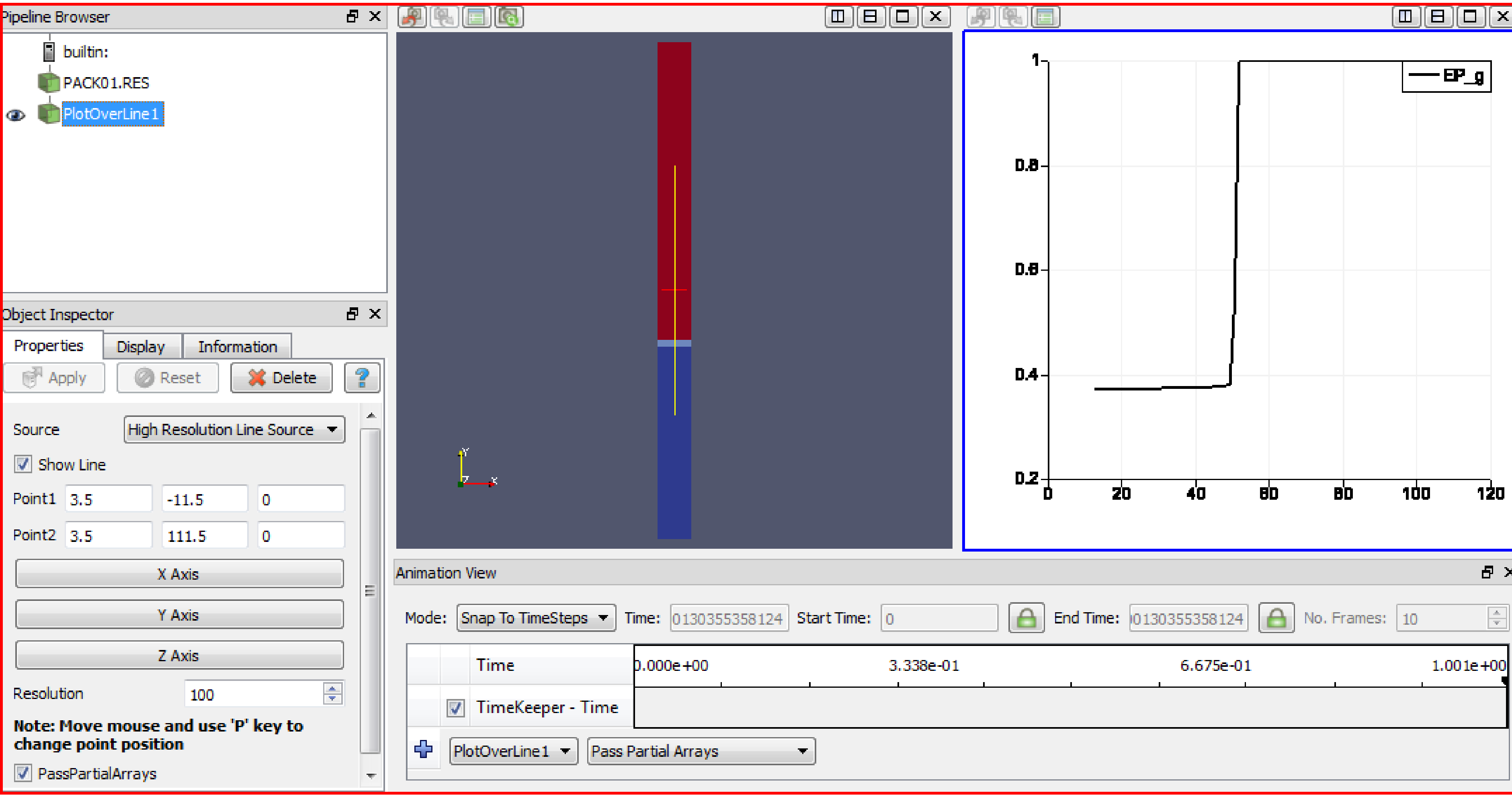
Some results



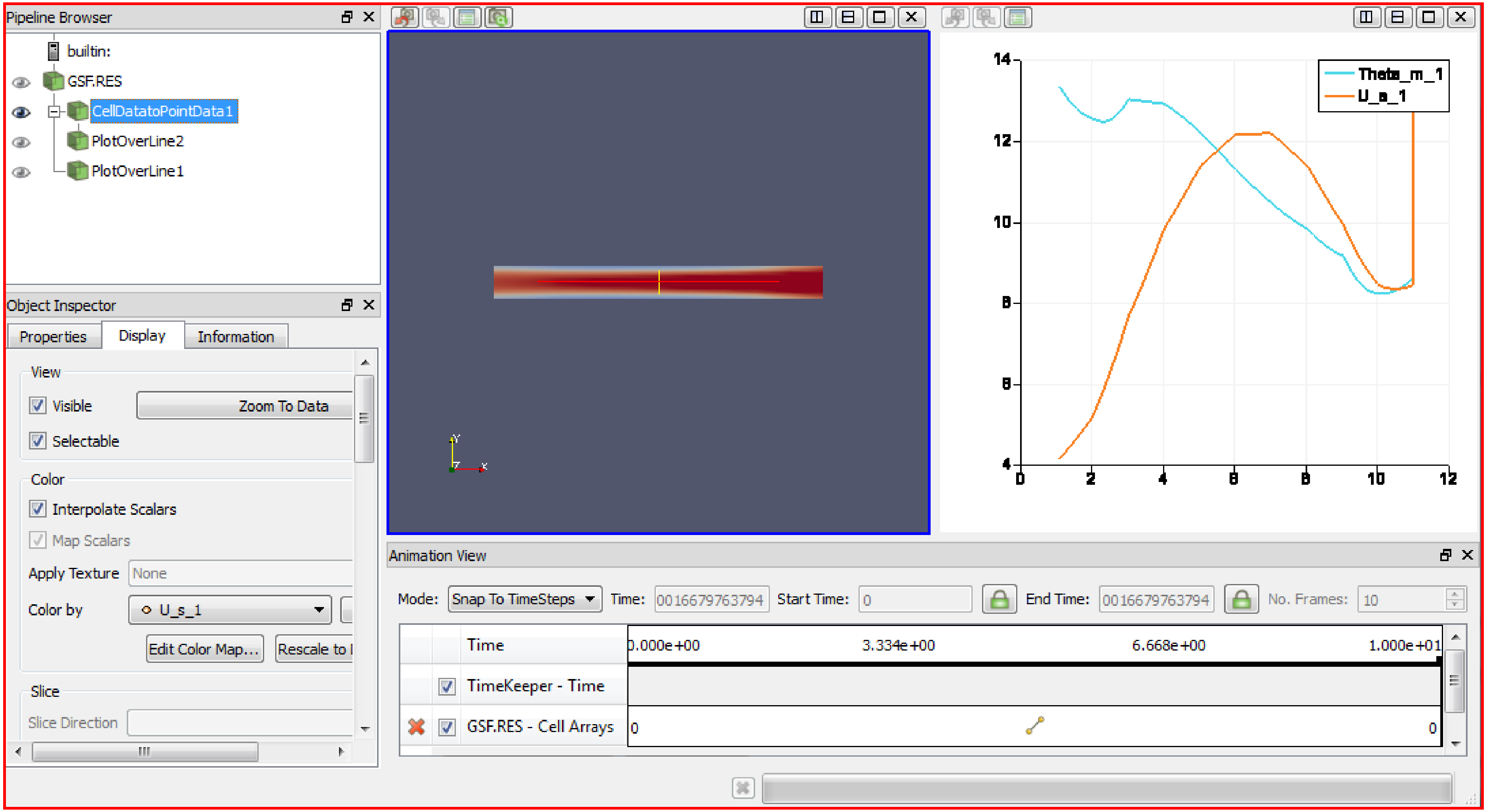
Driven Cavity



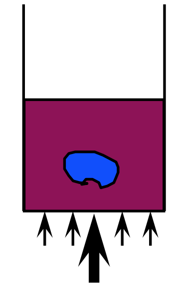
Steady Packed Bed

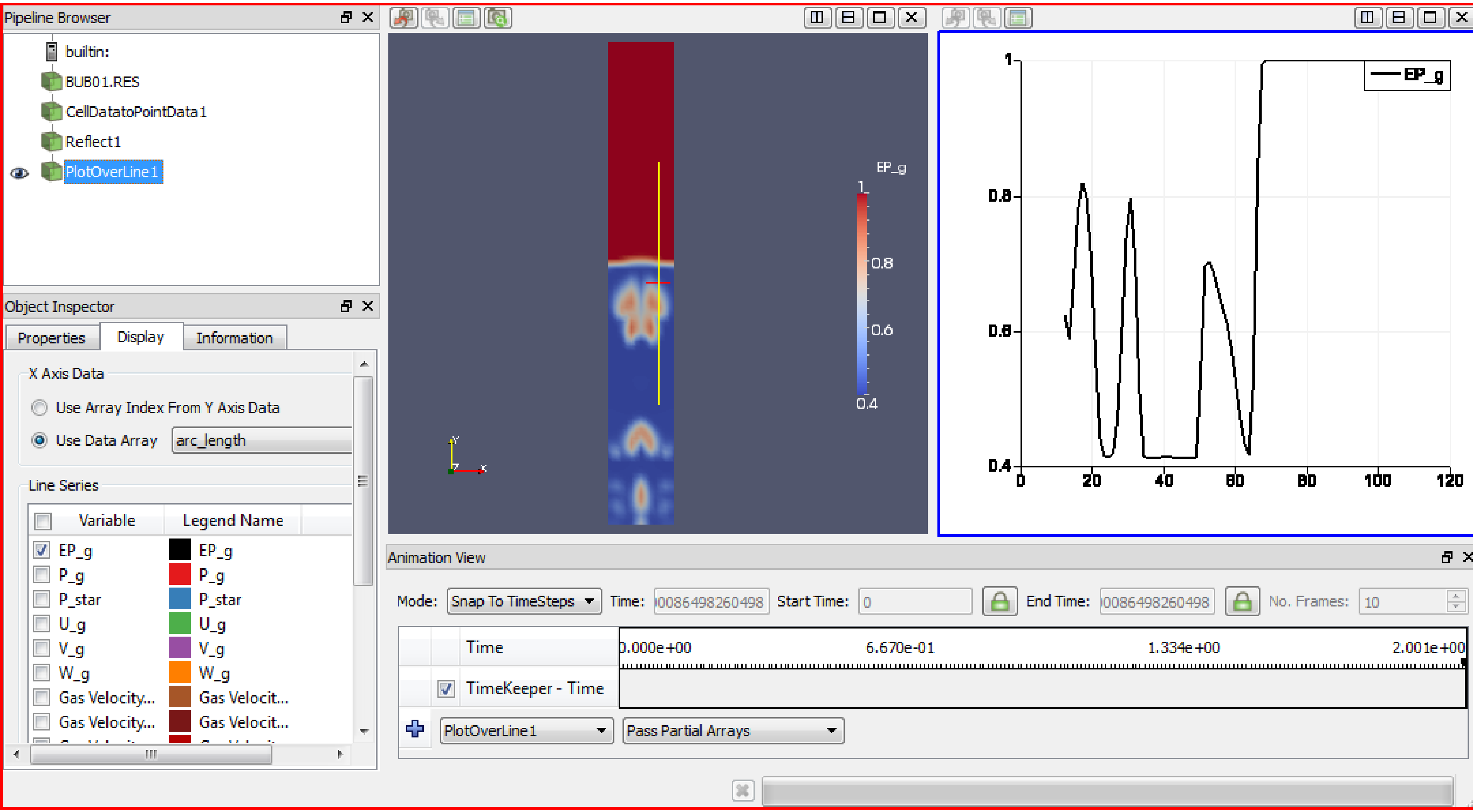


Granular Shear



Fluidized Bed with Jet





Continuity Equation

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

$$\sum_{m=1}^{N} \varepsilon_m = 1$$

index.html

solve_continuity_8f.html

Momentum Equation

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

Interaction within the phase → stresses

–collisions, sliding or rolling friction

–electrostatic, van der Waals, capillary

solve__vel__star_8f.html

Momentum Equation

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

Interaction between phases → interphase forces

Momentum Equation

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

Interactions with rest of the universe → body forces

Day 3: Getting more out of MFIX

Sreekanth Pannala
Senior Research Staff Member
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pannalas@ornl.gov

presented at

Coal Gasification Short Course

Criciúma, Santa Catarina, Brazil
May 10-14, 2010

Much thanks to Drs. Thomas O'Brien and Jeff Dietiker

Outline

- **Day 1**
  - **Install Cygwin, MFIX, Paraview**
  - **Reacting multiphase flows**
  - **Volume averaged equations, closures, code walk through**
- **Day 2**
  - **Hands-on training: Hydrodynamics cases**
- **Day 3**
  - **Hands-on training: Study the effect of grid resolution, numerical schemes etc.**
  - **Hands-on training: Cartesian grid**
- **Day 4**
  - **Hands-on training: Add heat and mass transfer, chemical reactions**
- **Day 5**
  - **Hands-on training: Put all the things learned to a case with hydrodynamics, heat and mass transfer and chemical reactions**
  - **Close with future pointers**

This is tentative and subject to change based on the feedback, pace, etc.,

What we have learned yesterday

- Reviewing few existing cases
  - To understand the different parts of the mfix.dat file
  - This corresponds to setting up the case
- Compiling the code
  - We will make life little bit easier today
  - $ echo alias make_mfix=\"sh ~/mfix/model/make_mfix\" >> ~/.bashrc
- Running the code
  - ./mfix.exe
- Analyzing/Visualizing the output
  - Launch paraview and view/process the results

Good practices

- Review all the tests and tutorial cases
  - If possible run all the cases closest to your desired configuration
  - When in doubt refer to the readme file to get yourself familiar with the keywords in the mfix.dat file
- Setting up the case
  - Pick the mfix.dat closest to your interest
  - Make necessary changes
    - It is important to start with hydrodynamics, add heat and mass transfer and later chemical reactions
  - Have the mfix.dat file extensively commented and well formatted so that it is easy to read
    - Less chances for error
    - There is good error checking but really not fool-proof

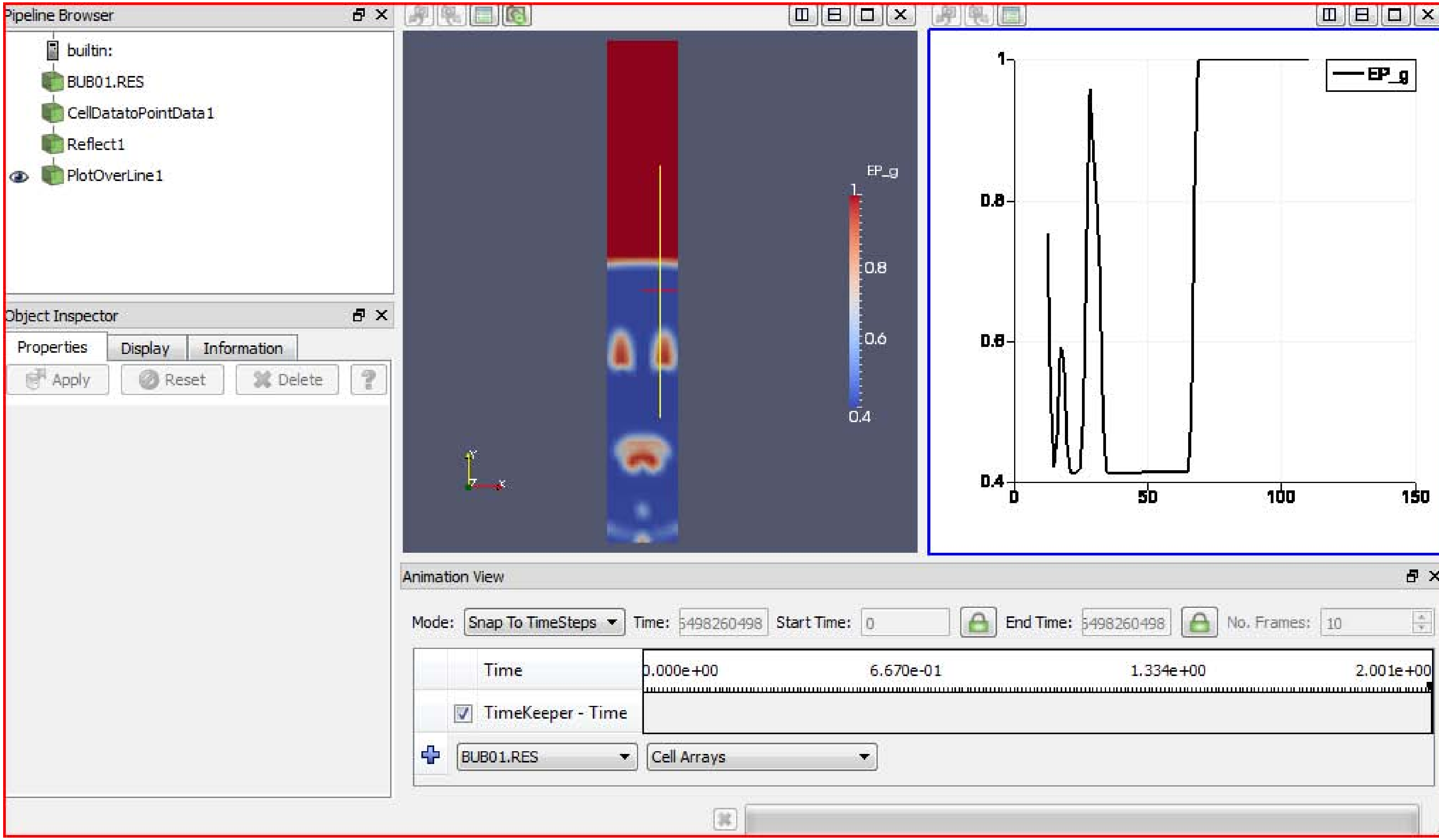
Bad practices

- Editing mfix source files (.f), make_mfix or mfix.dat using windows note pad
  – Cygwin/linux is allergic to windows
  – Always use cygwin/linux based editors such as vi, nedit, emacs….
- Editing source files in the model directory
  – Copy them to your run directory
  – Edit them in your run directory and the make script will automatically pick up your files
  – Always run make_mfix to make sure you have the latest executable

First assignment: effect of high order numerics

- Go to mfix/tutorials directory
- $mkdir fluidBed1_new
- $cd fluidBed1_new
- $cp ../fluidBed1/mfix.dat .
- $nedit mfix.dat
- Add the following line in the run section:
  'DISCRETIZE = 9*2'
- Compile, Run, Visualize

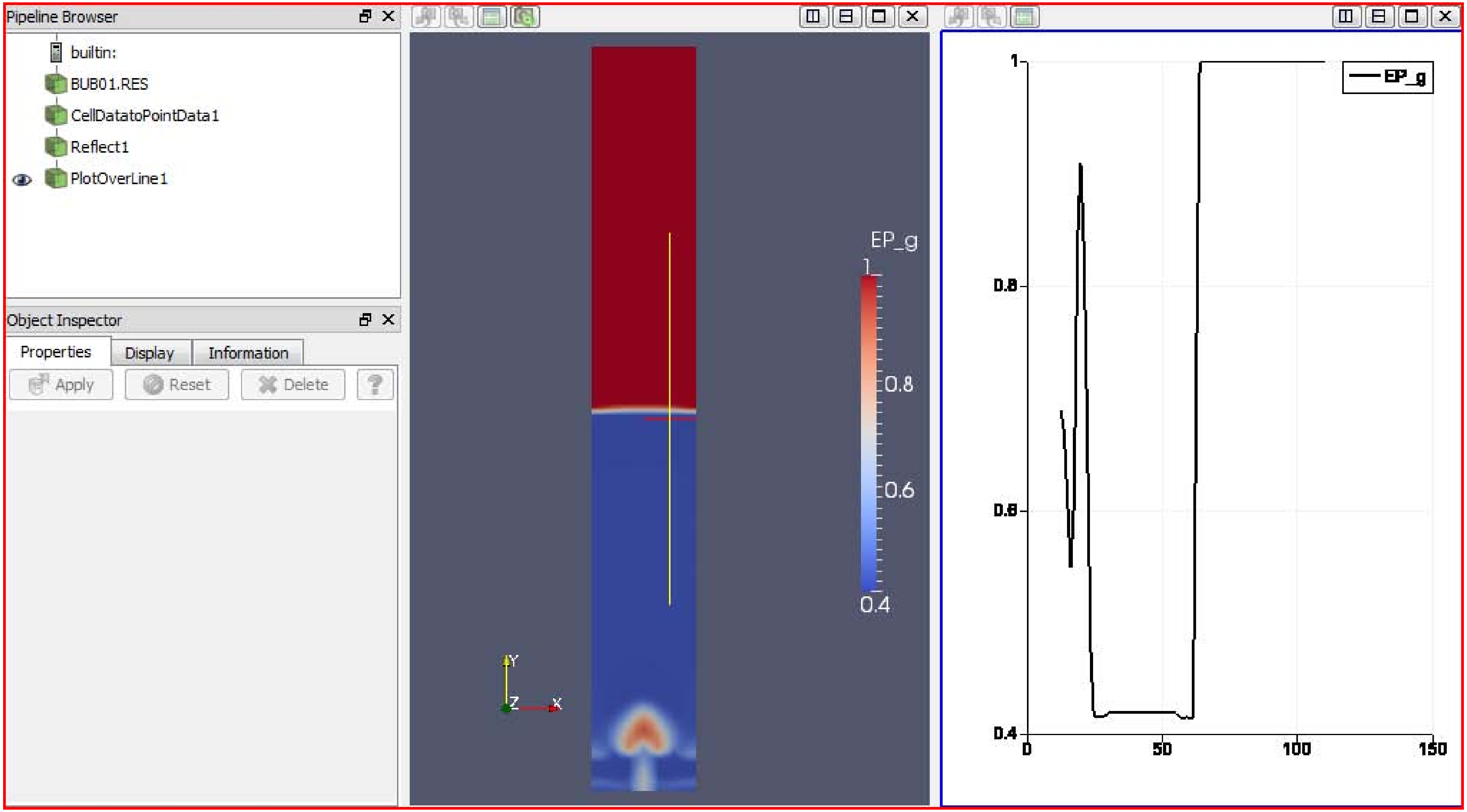
Results


Pipeline Browser
builtin:
BUB01.RES
CellDatatoPointData1
Reflect1
PlotOverLine1
Object Inspector
Properties
Display
Information
Apply
Reset
Delete
EP_g
1
0.8
0.6
0.4
EP_g
1
0.8
0.6
0.4
0
50
100
150
Animation View
Mode: Snap To TimeSteps
Time:
Start Time: 0
End Time:
No. Frames: 10
Time
0.000e+00
6.670e-01
1.334e+00
2.001e+00
TimeKeeper - Time
BUB01.RES
Cell Arrays

Second assignment: effect of higher resolution

- Go to mfix/tutorials directory
- $mkdir fluidBed1_hres
- $cd fluidBed1_hres
- $cp ../fluidBed1/mfix.dat .
- $nedit mfix.dat
- Change JMAX to 200 – doubling the resolution
  - Change TSTOP to 0.2 – 2.0 seconds takes to much time
- Compile, Run, Visualize
  - New twist – good for long runs
  - $nohup.exe .\mfix.exe > out1 &
  - $tail –f out1

Results



Pipeline Browser
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BUB01.RES
CellDatatoPointData1
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PlotOverLine1
Object Inspector
Properties
Display
Information
Apply
Reset
Delete
EP_g
1
0.8
0.6
0.4
Y
Z
X
EP_g
1
0.8
0.6
0.4
0
50
100
150

Take away message

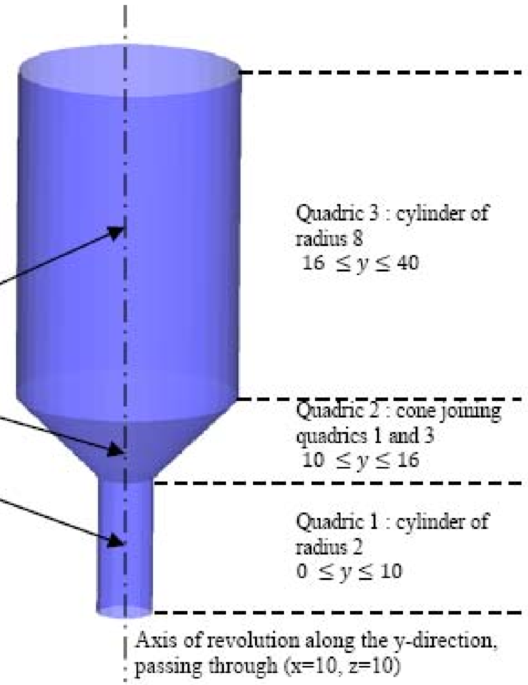
- Changing resolution or order of the scheme can affect convergence
  - Unpredictable computational cost
  - Sometimes non-convergence
- It is recommended to go to a fine enough grid resolution beyond which the changes are not significant
- If you can converge with the high-order schemes – that is the preferred choice

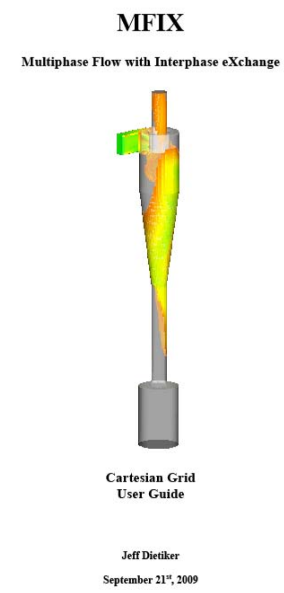
Third assignment: Cartesian grid (Spouted Bed)

- Copy the spoutedbed1.tar.gz to tests directory
- $tar xzvf spoutedbed1.tar.gz
- This case has a user modified routine in cartesian_grid directory
  - A bug I had to fix this morning to get the case working on cygwin with gfortran
  - $diff cartesian_grid/get_cut_cell_flags.f ../../model

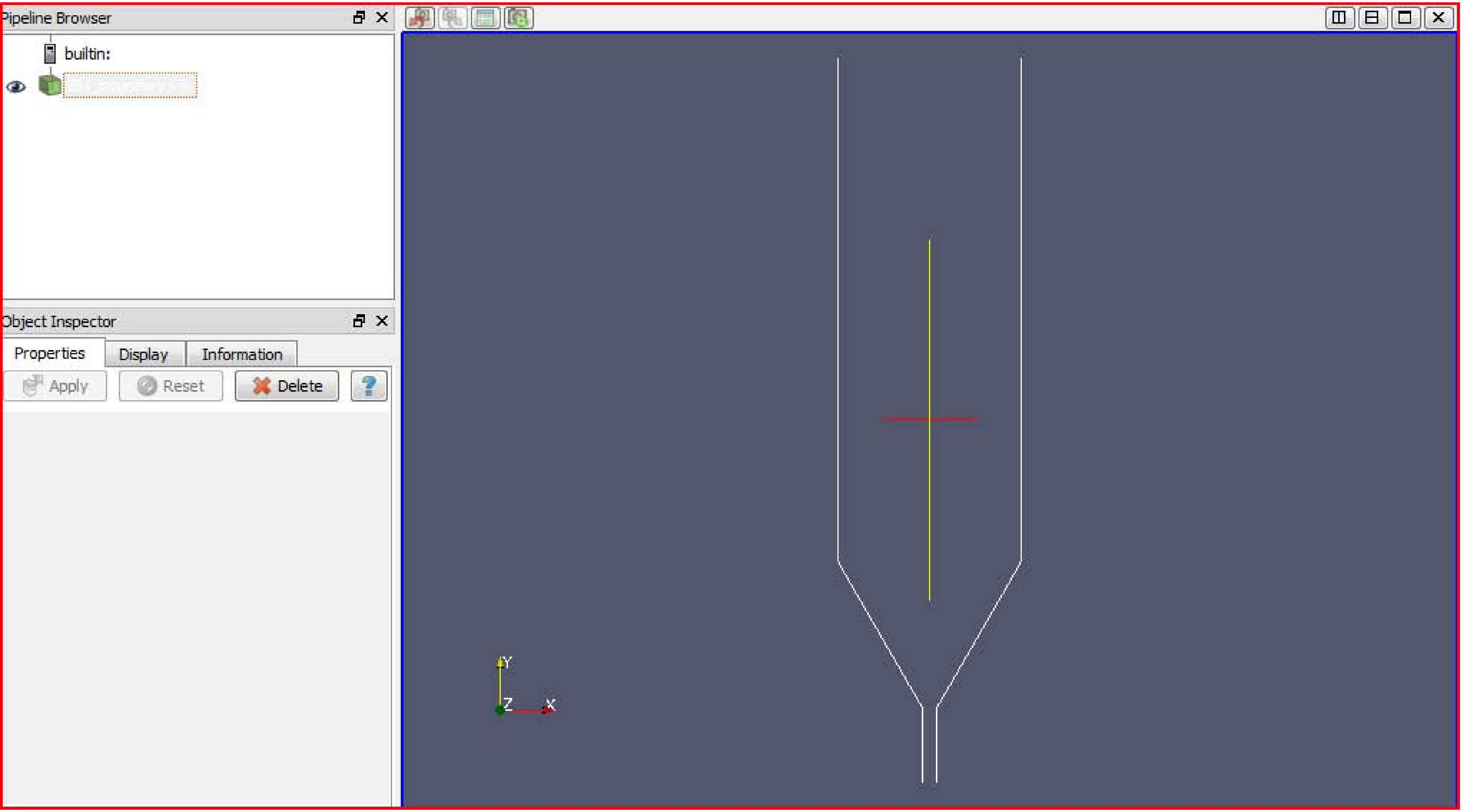
This capability uses quadrics and there intersections to define detailed geometry

```
N_QUADRIC = 3

QUADRIC_FORM(1) = 'Y_CYL_INT'  'Y_CONE'  'Y_CYL_INT'
RADIUS(1)       =     2.0        0.0        8.0
HALF_ANGLE(2)   =                45.0

t_x(1)          =    10.0       10.0       10.0
t_y(1)          =     0.0        8.0        0.0
t_z(1)          =    10.0       10.0       10.0

clip_ymin(1)    =     0.0       10.0       16.0
clip_ymax(1)    =    10.0       16.0       40.0

N_GROUP = 1

GROUP_SIZE(1) = 3
GROUP_Q(1,1)  = 1
GROUP_Q(1,2)  = 2
GROUP_Q(1,3)  = 3

GROUP_RELATION(1) = 'PIECEWISE'
```





Geometry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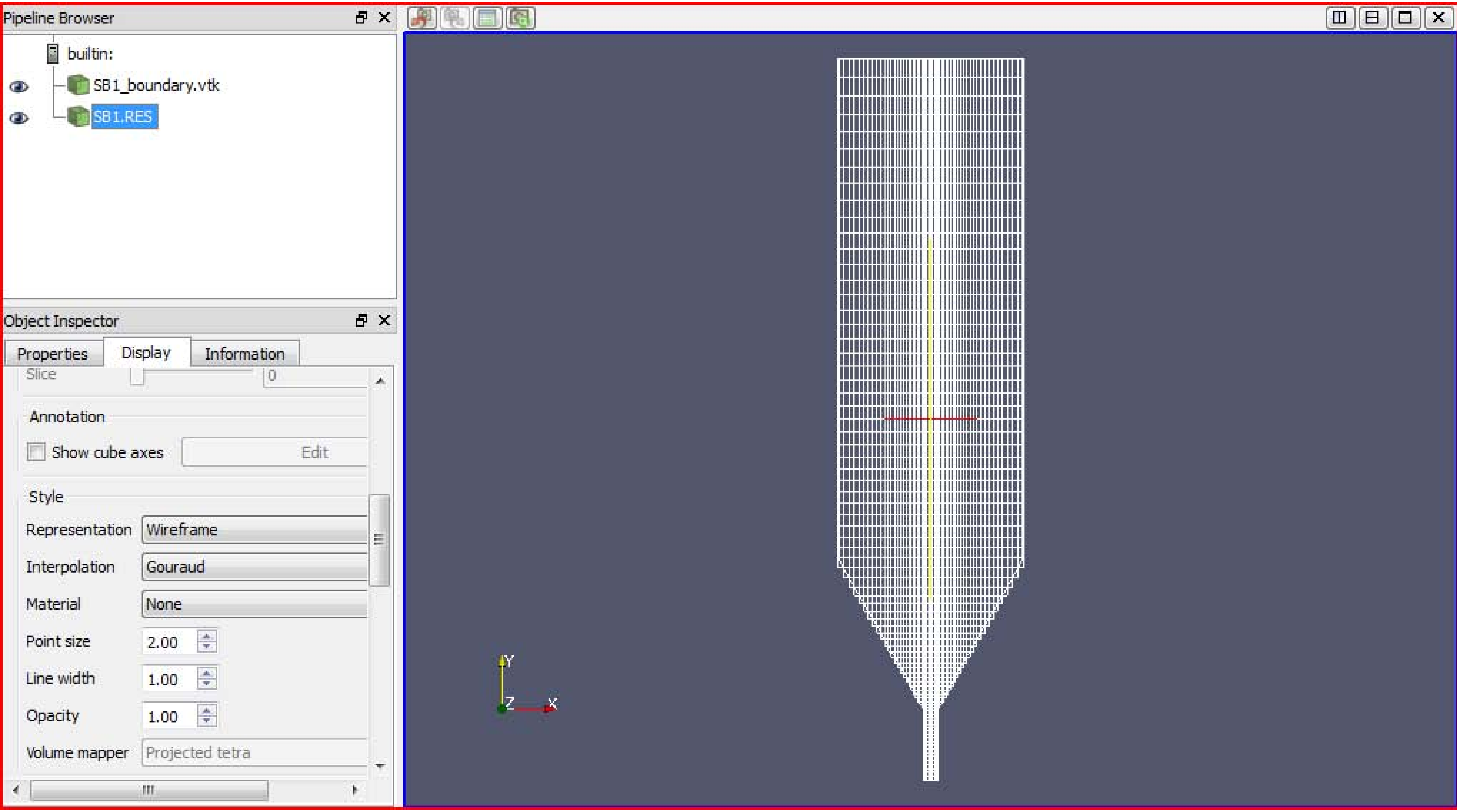
builtin:
Object Inspector
Properties
Display
Information
Apply
Reset
Delete
Y
Z
X

Geometry



Pipeline Browser
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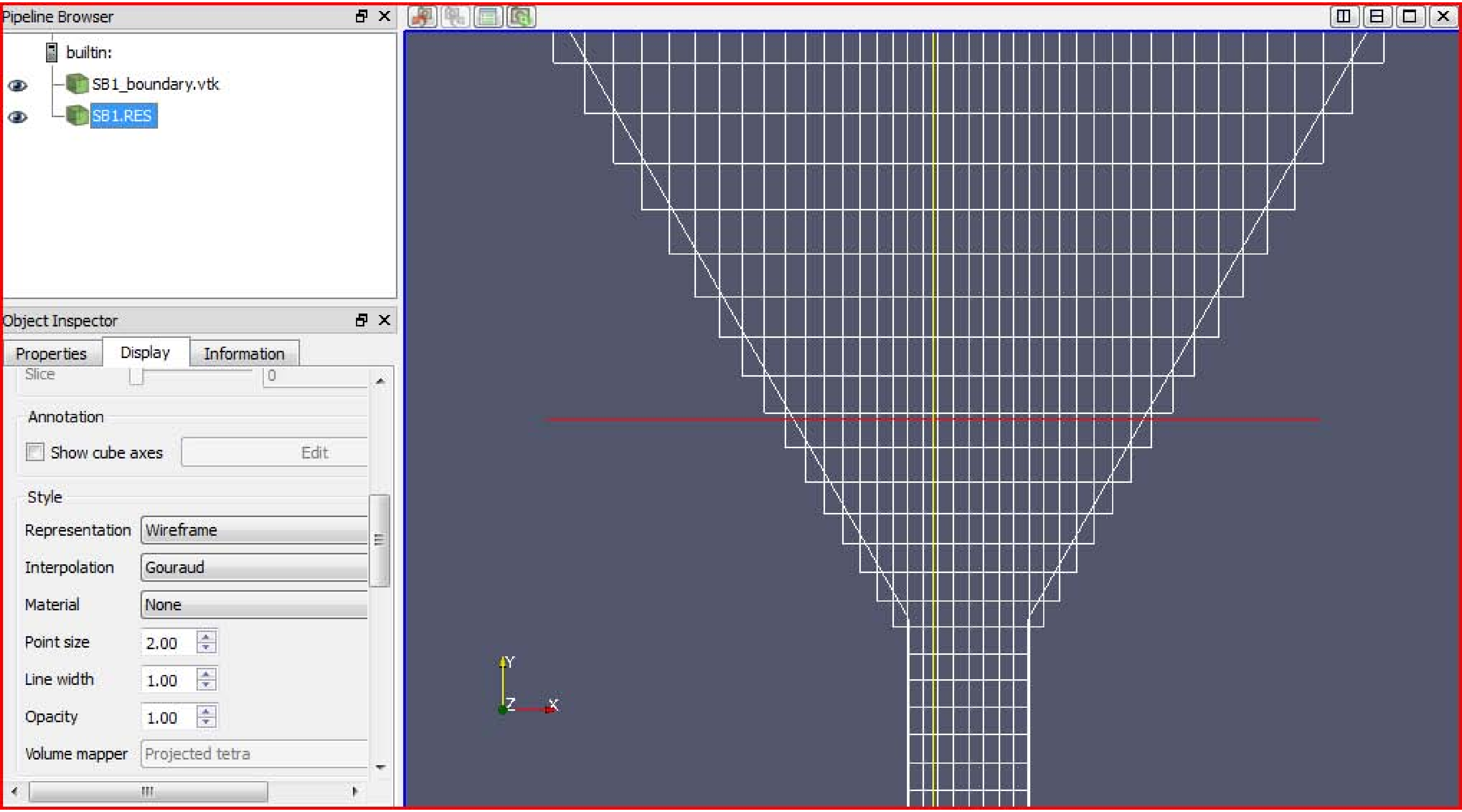
SB1_boundary.vtk
SB1.RES
Object Inspector
Properties
Display
Information
Slice
0
Annotation
Show cube axes
Edit
Style
Representation
Wireframe
Interpolation
Gouraud
Material
None
Point size
2.00
Line width
1.00
Opacity
1.00
Volume mapper
Projected tetra
Y
Z
X

Geometry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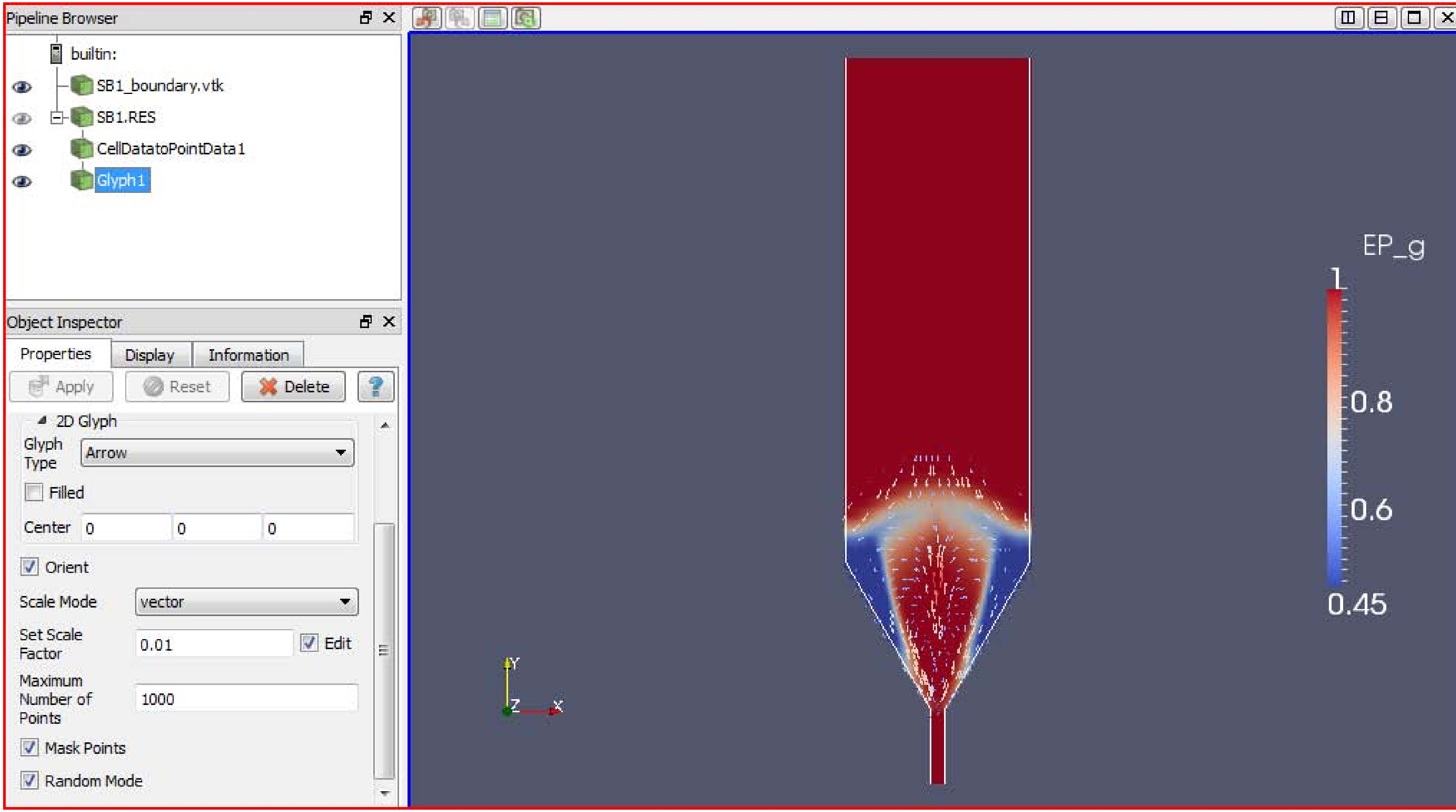
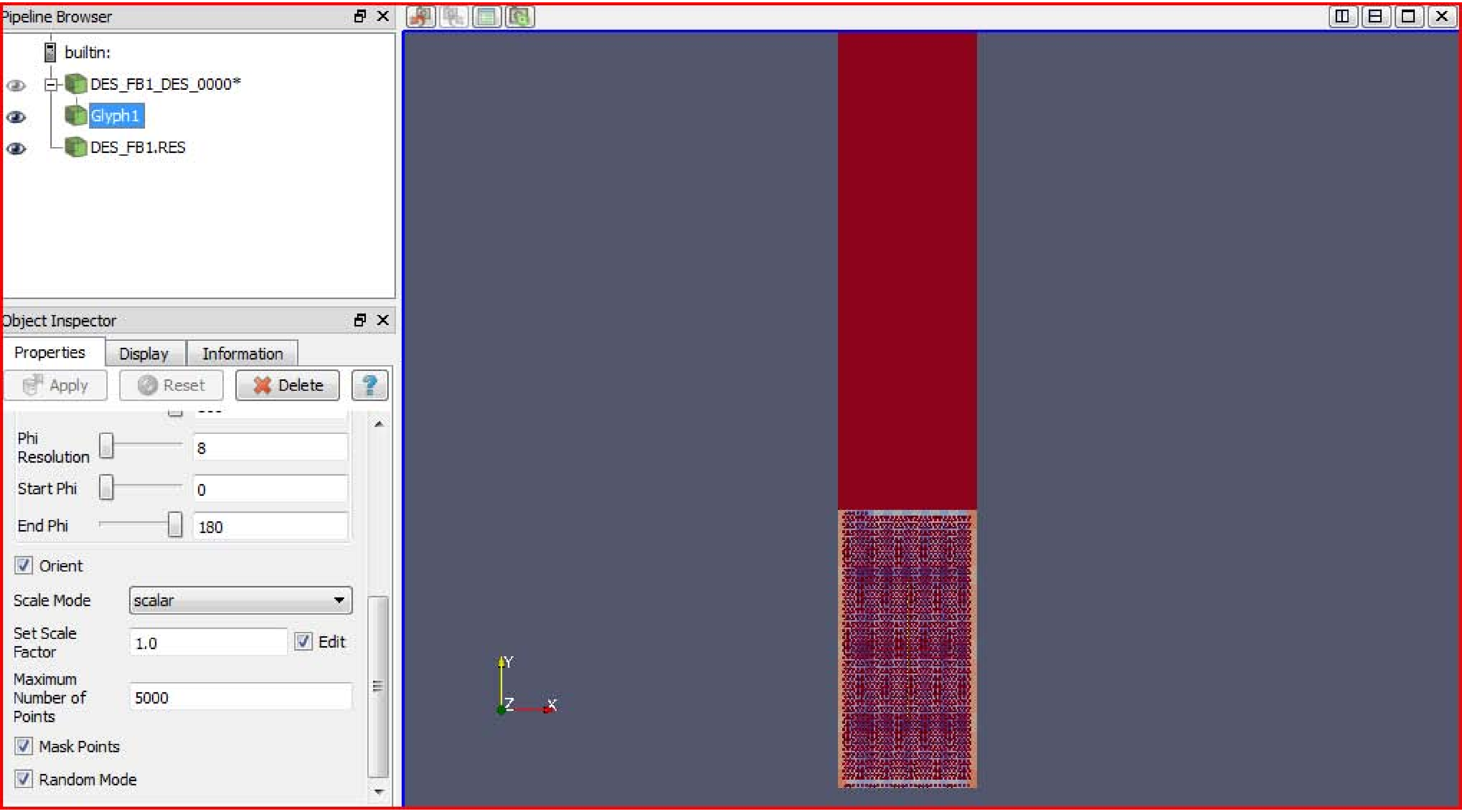
Initial Results



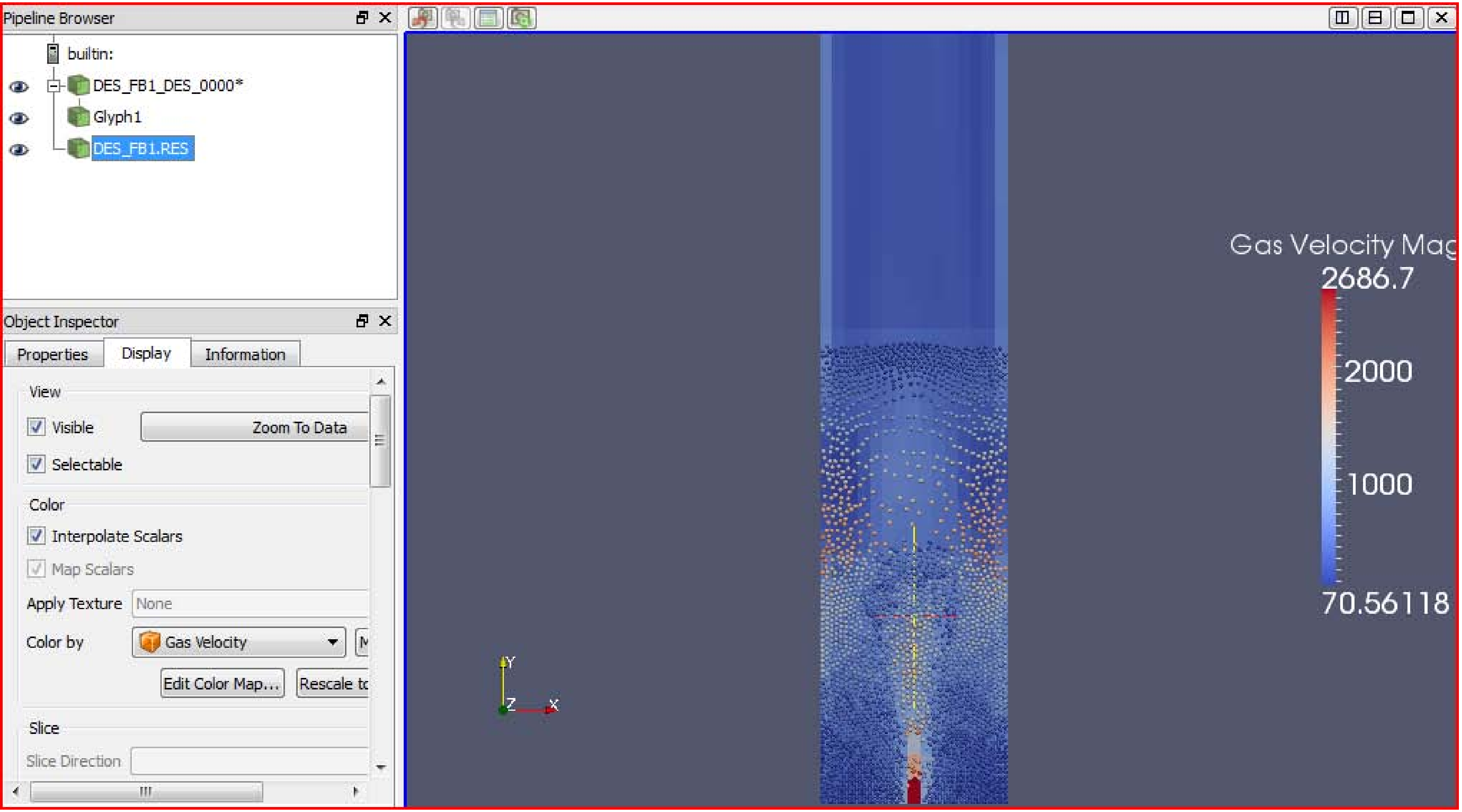
Fourth assignment: discrete element method

- Go to mfix/tutorials directory
- $cd FluidBed_DES
- $nedit mfix.dat
- Change TSTOP to 0.5
- Compile, Run, Visualize
  - $nohup.exe .\mfix.exe > out1 &
  - $tail –f out1
  - Let us look at the particles

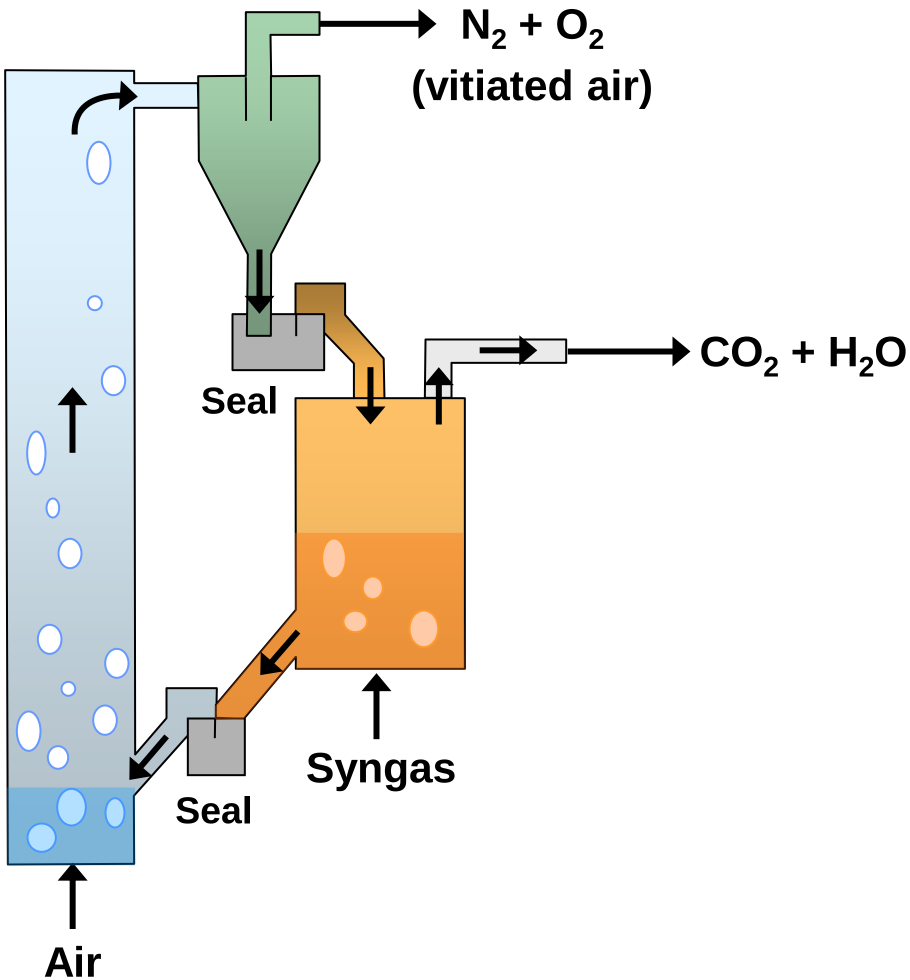
Visualization



More results



Chemical Looping Combustion of Coal (requires ex-situ gasification)

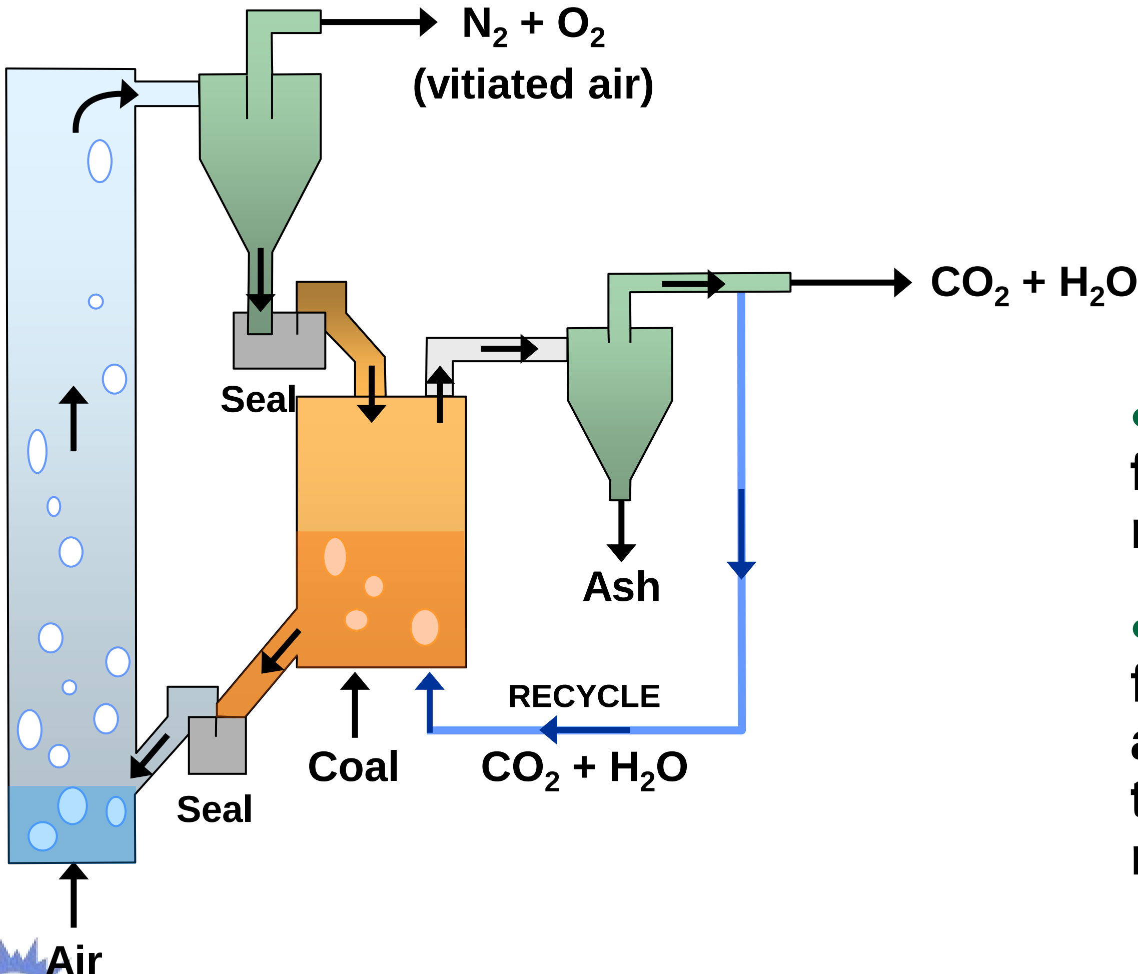


- Syngas is provided by an external oxygen-blown coal gasifier
- Air reactor – carrier is oxidized by air; heat is released
- Cyclone – hot oxidized carrier is sent to fuel reactor; hot vitiated air is used for power generation
- Fuel reactor – carrier oxidizes fuel to CO_2 and H_2O (usually endothermic); reduced carrier is returned to the air reactor (without any fuel).

NETL Lewis and Gilliland (1954);Knoche und Richter (1968); Ishida (1994); Lyngfelt, et al., 2001

Oak Ridge National Laboratory

Chemical Looping Combustion of Coal (involves *in-situ* gasification)



- **Recycle gas must:**
  1) help to fluidize the fuel reactor

     (there is extensive self fluidization due to reactions)
  2) gasify (burn out) the char.
- **Char must be stripped from the FR → AR solids return.**
- **Ash may be elutriated from the fuel reactor and/or separated from the FR → AR solids return.**

Lewis and Gilliland (1954); Andrus et al. (2005), Scott et al. (2006), Cao and Pan (2006), Fan et al. (2007), Leion, Mattisson and & Lyngfelt (2007); Berguerand, N., and A. Lyngfelt (2008)

Advantages of CLC Technology

1) Produces a separate CO_2/H_2O gas stream

   No cost of separation

   Separation of H_2O on cooling/compression

   CO_2 stream at process pressure

   Could contain CO, H_2, unburned fuel, SO_2, fuel-N, Hg, …

2) No/Low NO_x

   No thermal or prompt NO_x (low T of Air Reactor)

   No "hot-spots" (fluidized bed processes)

   Fuel NO_x … not determined (???)

3) In-bed tar cracking and control

   Metal oxides are currently used to catalyze tar cracking

4) Compatible with S-capture technologies

   S sorbent could be added to the bed.

Advantages of CLC Technology (cont.)

4) **CLC uses well-established boiler technology**

similar to CFB boilers

5) **Hg removal would be facilitated**

smaller volume, more concentrated stream from FR

6) **Heavy metals (including Hg) may stay with the ash at lower T**

7) **Fewer materials concerns**

lower temperatures than conventional combustion

8) **Small vessel sizes/ lower construction costs**

higher volumetric heat release rate than conventional combustion

9) **Higher thermodynamic efficiency**

possible for some systems (decrease irreversibility)

10) **Improved H_2O utilization**

Disadvantages of CLC Technology

1) Carrier circulation

   Solids handling

   Non-mechanical valves

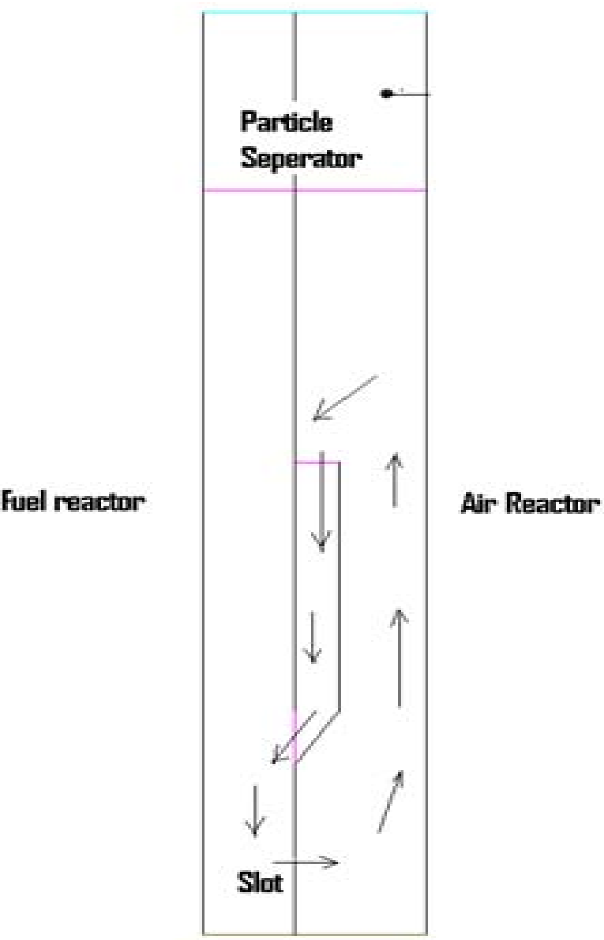
2) Dual reactors

3) Carrier issues: fabrication, durability, poisoning, …

4) Lower exhaust gas temperature (<1000 ºC)/pressure

   Difficult to couple to a gas turbine – loss in efficiency

Fifth assignment: Simple chemical looping setup (Kronberger Experiment)



Air reactor

- High velocity region carries particles upwards
- heat is released in hot flow experiments

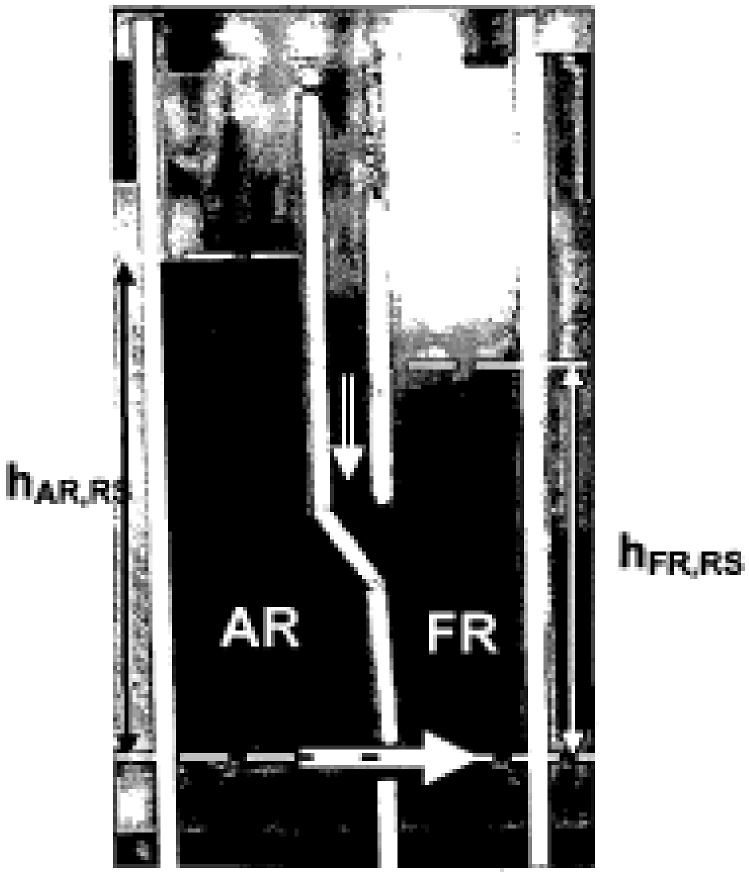
Particle Separator

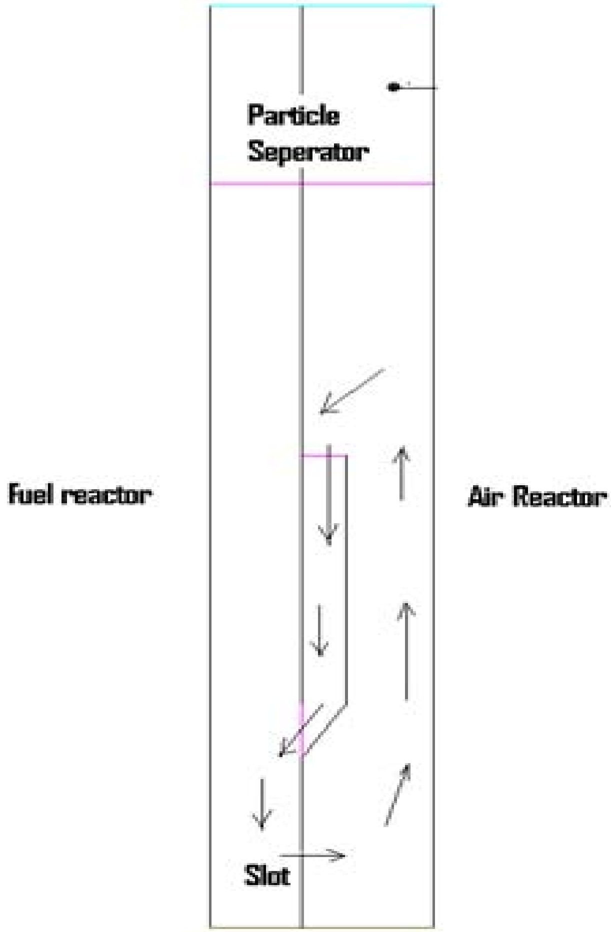
- Expanded cross-sectional area in the depth direction (Perpendicular to plane of paper)
- Decreases gas velocity and prevents particles from leaving the reactor

Fuel reactor

- Low velocity region
- Carrier returned to the air reactor through slot at bottom.

Photographs Kronberger Experiment





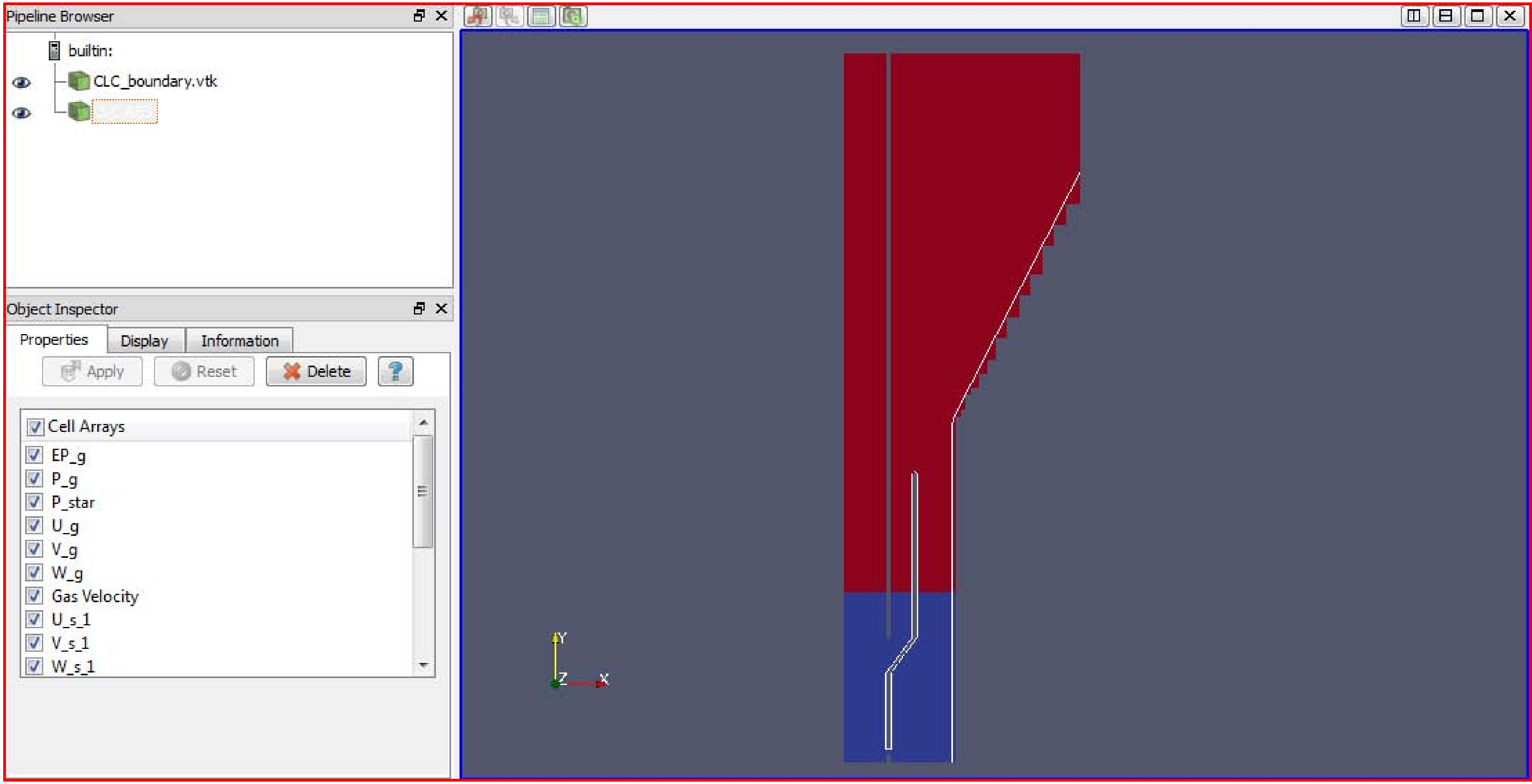
Details of Reactor

Experimental Parameters	
Width of Fuel Reactor	19 mm
Width of Air Reactor	27 mm
Depth of Fuel and Air Reactors	19 mm
Width of Lower Slot	1.5 mm
Width of Downcomer	11 mm
Fluidizing Gas	13/87 vol % N_2/He (~50/50% by Mass)
Fuel Reactor Velocity	0.05 m/s (18*umf)
Air Reactor Velocity	0.172m/s (1.45*u_t)
Temperature	298K
Pressure	1 atm
Solid Particles	70 micron FCC-Geldart A
Solid Inventory	53g
Particle density	1500 kg/m3

Eulerian-Eulerian Model Parameters

Description	Model
Drag coefficient	Gidaspow (1992)
Granular shear viscosity	Gidaspow (1992)
Granular bulk viscosity	Lun *et al. (1984)*
Frictional stress	Schaeffer (Friction Viscosity) Johnson (Friction Pressure)
Solids pressure	Lun *et al. (1984)*
Radial distribution function	Ogawa *et al. (1980)*
Granular temperature	Algebraic equation-balance between production and dissipation.
Granular conductivity	Gidaspow (1992)

Geometry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W_s_1
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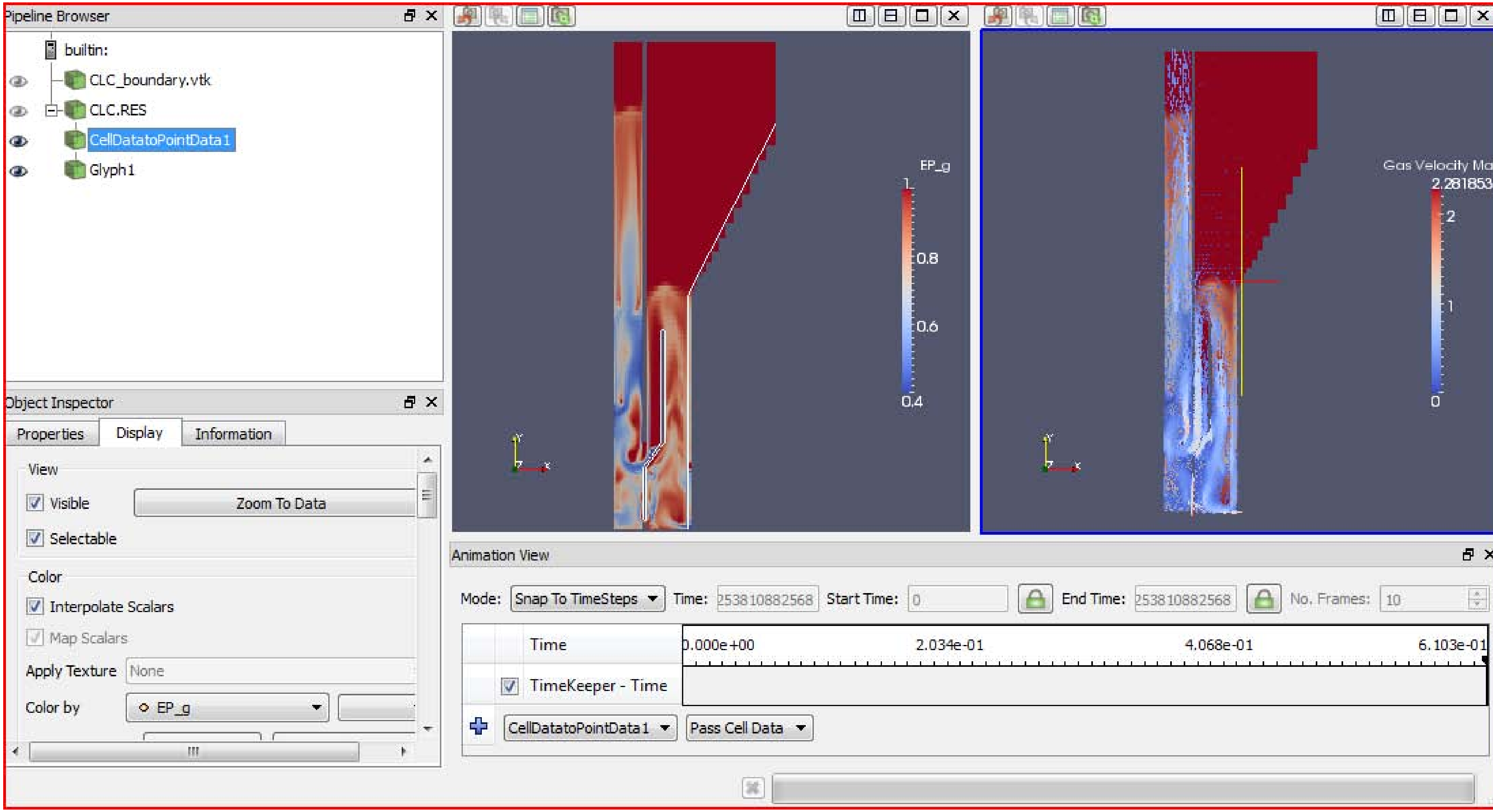
X

Initial results



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Interaction within the phase → stresses

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solve_vel_star_8f.html

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Interaction between phases → interphase forces

Momentum Equation

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Interactions with rest of the universe → body forces

Day 4: Heat & Mass Transfer; Chemical Reactions

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pannalas@ornl.gov

presented at

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  - **Close with future pointers**

This is tentative and subject to change based on the feedback, pace, etc.,

What we have learned yesterday

- Reviewing few existing cases and modify numerics/resolution
  - To become familiar with the mfix.dat file
- Compiling the code
  - make_mfix
- Running the code
  - nohup ./mfix.exe > out1 &
- Analyzing/Visualizing the output
  - Launch paraview and view/process the results
- Advanced numerical techniques and more detailed models

Good practices

- Review all the tests and tutorial cases
  - If possible run all the cases closest to your desired configuration
  - When in doubt refer to the readme file to get yourself familiar with the keywords in the mfix.dat file
- Setting up the case
  - Pick the mfix.dat closest to your interest
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- Editing source files in the model directory
  - Copy them to your run directory
  - Edit them in your run directory and the make script will automatically pick up your files
  - Always run make_mfix to make sure you have the latest executable

What is in mfix directory

- **CHANGES – lists changes from previous versions**
- **Readme.pdf – very important file to get started**
- **doc – various documents, another good resource in addition to the documents online**
- **Tutorials – good cases to run and to get familiar with the code and capabilties**
- **ani_mfix – if you want to use this for visualization – I prefer Paraview and that is what I will show today**
- **model – all the code lies here**
- **tests – good set of cases to go through**
- **cartesian_grid_tutorials – if you are interested in cartesian grid**
- **post_mfix – set of post-processing tools to analyze data – maybe we will get a chance to use this**
- **tools – various tools, e.g. to generate make files if you add new source files in the model directory**

Readme version 2010-1 1

MFiX

Multiphase Flow with Interphase eXchanges
Version MFIX-2010-1 (Date: 02/02/2010)

Notice

Neither the United States Government nor any agency thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed or represents that its use would not infringe privately owned rights.

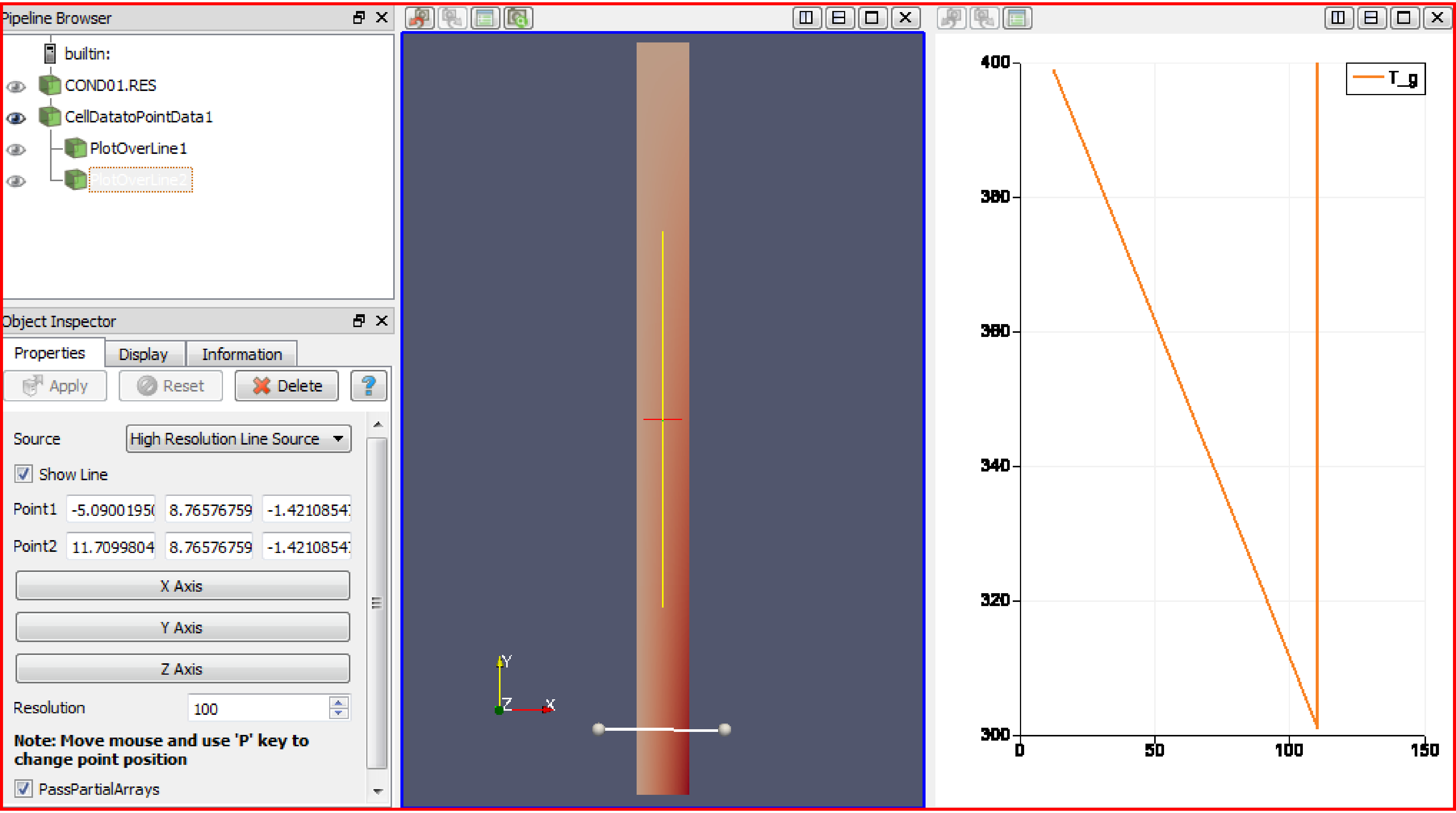
- MFIX is provided without any user support for applications in the user's immediate organization. It should not be redistributed in whole or in part.
- The use of MFIX is to be acknowledged in any published paper based on computations using this software by citing the MFIX theory manual. Some of the submodels are being developed by researchers outside of NETL. The use of such submodels is to be acknowledged by citing the appropriate papers of the developers of the submodels.
- The authors would appreciate receiving any reports of bugs or other difficulties with the software, enhancements to the software, and accounts of practical applications of this software.

Table of Contents

First assignment: Heat conduction (heat transport)

- Go to mfix/tests directory
- $cd conduction
- $nedit mfix.dat and review the file
  - Find the differences as compared to the hydrodynamic cases
- Compile, Run, Visualize

Results



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COND01.RES
CellDatatoPointData1
PlotOverLine1
PlotOverLine2
Object Inspector
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Display
Information
Apply
Reset
Delete
Source
High Resolution Line Source
Show Line
Point1
-5.0900195(
8.76576759
-1.4210854
Point2
11.7099804
8.76576759
-1.4210854
X Axis
Y Axis
Z Axis
Resolution
100
Note: Move mouse and use 'P' key to change point position
PassPartialArrays
Y
Z
X
T_g
400
380
360
340
320
300
0
50
100
150

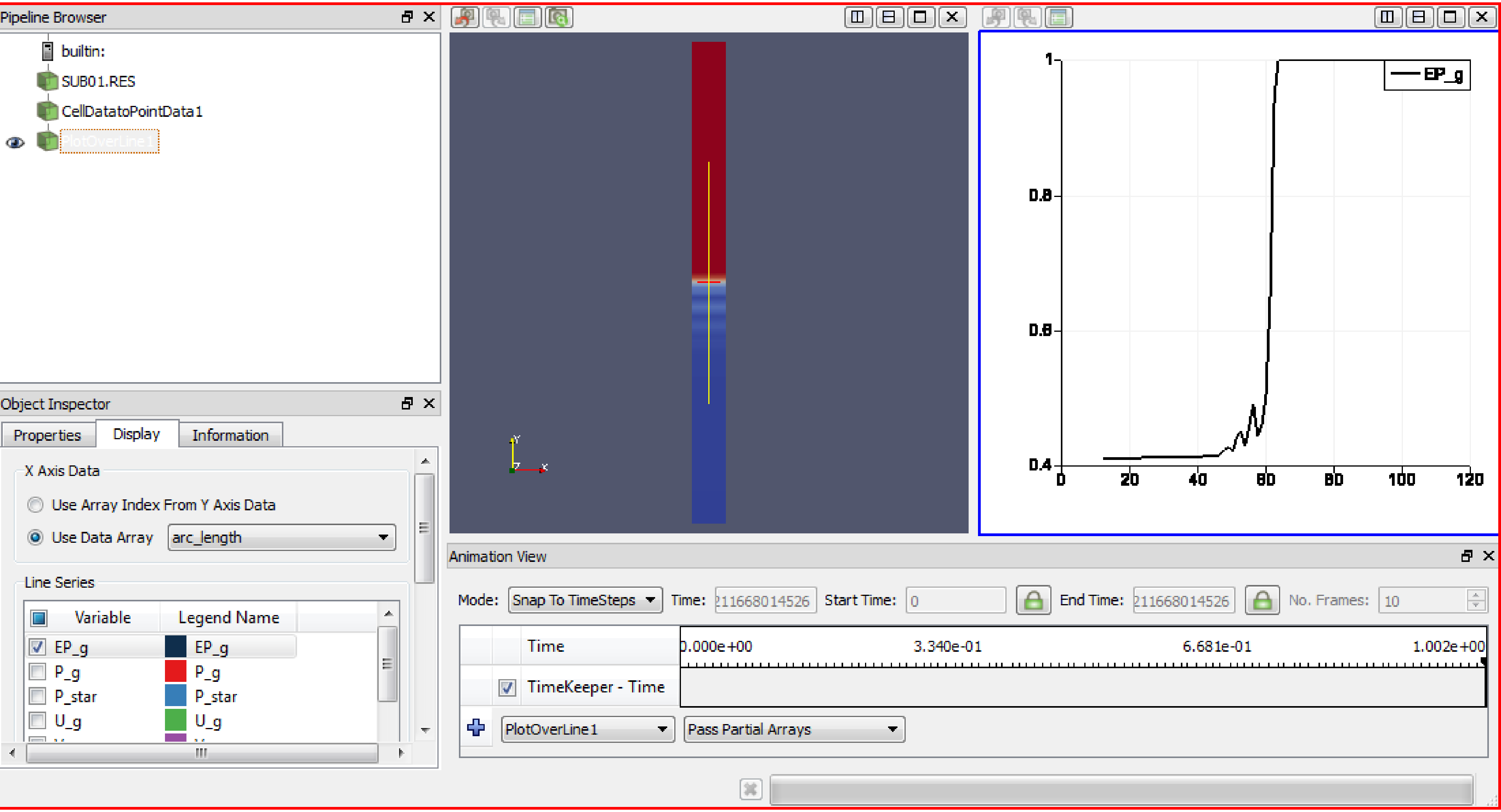
Second assignment: Drying (mass transfer)

- Go to mfix/tests directory
- $cd drying
- $ls and review the files
- $nedit mfix.dat and review the file
- Do the same for rrates.f, usr3.f and calc_h.f
- Compile, Run, Visualize
  - $nohup.exe .\mfix.exe > out1 &
  - $tail –f out1

Third assignment: Phase change (mass transfer)

- Go to mfix/tests directory
- $cd drying
- $ls and review the files
- $nedit mfix.dat and review the file
- Do the same for rrates.f
- Compile, Run, Visualize
  - $nohup.exe .\mfix.exe > out1 &
  - $tail –f out1
- Now change c(1) in mfix.dat and see the changes in self fluidization behavior

Results



Pipeline Browser
builtin:
SUB01.RES
CellDatatoPointData1
PlotOverLine1
Object Inspector
Properties
Display
Information
X Axis Data
Use Array Index From Y Axis Data
Use Data Array
arc_length
Line Series
Variable
Legend Name
EP_g
EP_g
P_g
P_g
P_star
P_star
U_g
U_g
EP_g
1
0.8
0.6
0.4
0
20
40
60
80
100
120
Animation View
Mode:
Snap To TimeSteps
Time:
211668014526
Start Time:
0
End Time:
211668014526
No. Frames:
10
Time
0.000e+00
3.340e-01
6.681e-01
1.002e+00
TimeKeeper - Time
PlotOverLine1
Pass Partial Arrays

Fourth assignment: Adiabatic flame temperature

- Go to mfix/tests directory
- $cd adiabaticFlame
- $ls and review the files
- $nedit mfix.dat and review the file
- Do the same for rrates.f, usr3.f and species_indices.inc
- Compile, Run, Visualize
  - $nohup.exe .\mfix.exe > out1 &
  - $tail –f out1

Results

```
$ more POST_Aflame.dat

Adiabatic Flame Temperature =  0.207E+04
P_g =  0.700E+07
CH4= 0.230E-12 O2= 0.375E-01
CO2= 0.127     H2O= 0.104
N2 = 0.732
```

Fourth assignment: Simple plug-flow reactor

- **Go to mfix/tutorials directory**
- **$cd reactor1b**
- **$ls and review the files**
- **$nedit mfix.dat and review the file**
- **Do the same for rrates.f and usr3.f**
- **Compile, Run, Visualize**
  - **$nohup.exe .\mfix.exe > out1 &**
  - **$tail –f out1**

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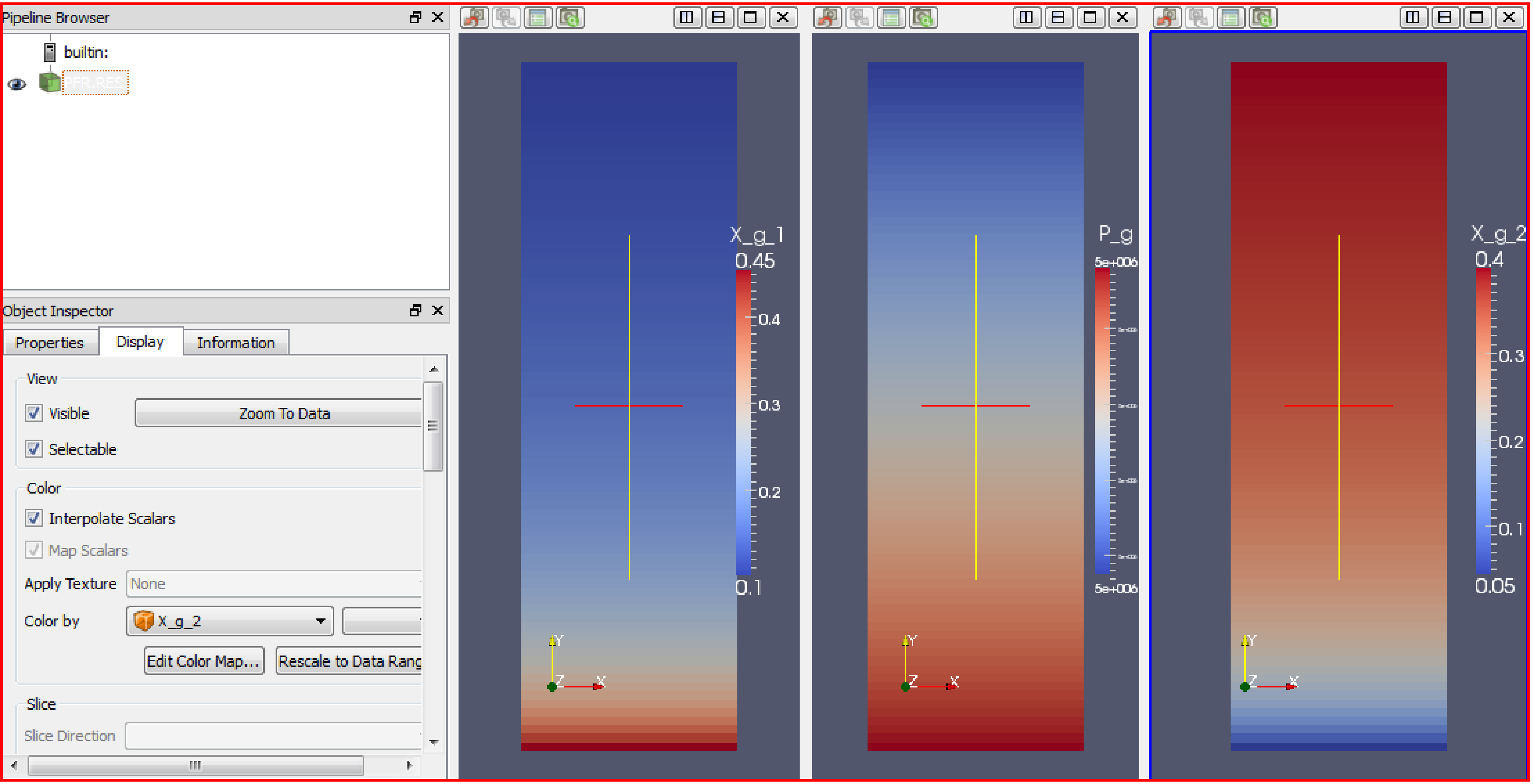
OAK RIDGE National Laboratory

Results



Pipeline Browser
builtin:
Object Inspector
Properties
Display
Information
View
Visible
Zoom To Data
Selectable
Color
Interpolate Scalars
Map Scalars
Apply Texture
None
Color by
X_g_2
Edit Color Map...
Rescale to Data Rang
Slice
Slice Direction
X_g_1
0.45
0.4
0.3
0.2
0.1
P_g
5e+006
5e+006
X_g_2
0.4
0.3
0.2
0.1
0.05
Y
Z
X

Take away message

- **Heat & Mass transfer and Chemical reaction rates are little bit more involved**
  - **One needs to edit source files**
- **Use the examples as much as possible to get familiarized with the way MFIX expects information**
- **If you have convergence issues, it is possible to start with lower reaction/transfer rates and ramp-up with time**

Continuity Equation

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

$$\sum_{m=1}^{N} \varepsilon_m = 1$$

index.html

solve__continuity_8f.html

Energy Balance

solve_energy_eq_8f.html

originates from a work term for ε changes

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

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

Energy Balance

Viscous dissipation

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

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

Energy Balance

Energy sources; e.g.., radiation

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

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

Energy Balance

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

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

heat conduction

Energy Balance

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

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

Interphase heat transfer

Energy Balance

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

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

Energy transfer with mass transfer

Energy Balance – In Terms of Temperature

Energy balance equations for solids phases m = 1, M

$$\varepsilon_m \rho_m C_{pm}\left[\frac{\partial T_m}{\partial t} + U_{mj}\frac{\partial T_m}{\partial x_j}\right] = -\frac{\partial q_{mi}}{\partial x_i} - \gamma_{gm}\left(T_m - T_g\right) - \Delta H_m + \gamma_{Rm}\left(T_{Rm}^4 - T_m^4\right)$$

Energy balance equation for gas phase g:

$$\varepsilon_g \rho_g C_{pg}\left[\frac{\partial T_g}{\partial t} + U_{gj}\frac{\partial T_g}{\partial x_j}\right] = -\frac{\partial q_{gi}}{\partial x_i} + \sum_{m=1}^{M}\gamma_{gm}\left(T_m - T_g\right) - \Delta H_g + \gamma_{Rg}\left(T_{Rg}^4 - T_g^4\right)$$

Heats of Reaction

$$-\Delta H_m = \sum_n \left[\left(H_{m,ref}\right)_n + \int_{T_{ref}}^{T_s} C_{pmn}(T)dT \right] \varepsilon_g \rho_g \left(\frac{\partial X_{gn}}{\partial t} + U_{gi} \frac{\partial X_{gn}}{\partial x_i} \right)$$

$$\approx \sum_n \left[\left(H_{m,ref}\right)_n + \int_{T_{ref}}^{T_s} C_{pmn}(T)dT \right] \left(R_{mn} - \sum_{n=1}^{N_m} R_{mn} X_{mn} \right)$$

$$-\Delta H_g \approx \sum_n \left[\left(H_{g,ref}\right)_n + \int_{T_{ref}}^{T_g} C_{pgn}(T)dT \right] \left(R_{gn} - \sum_{n=1}^{N_g} R_{gn} X_{gn} \right)$$

Fluid-Particle Heat Transfer

The interphase heat transfer coefficient

$$\gamma_{fm} = \frac{6\kappa_f \varepsilon_m Nu_m}{d_{pm}^2}$$

where the Nusselt number is calculated using Gunn (1978) correlation

$$Nu_m = (7 - 10\varepsilon_f + 5\varepsilon_f^2)(1 + 0.7\,\mathrm{Re}_m^{0.2}\,\mathrm{Pr}^{1/3}) + (1.33 - 2.4\varepsilon_f + 1.2\varepsilon_f^2)\,\mathrm{Re}_m^{0.7}\,\mathrm{Pr}^{1/3}$$

1. Gunn (1978)

Fluid-Particle Heat Transfer

- **To predict heat transfer to immersed tubes (with coarse numerical grid), the model will need a wall heat transfer coefficient[1]**

1. Syamlal and Gidaspow (1985), Kuipers et al. (1992), Witt and Perry (1996)

Heat Conduction

- **Fourier's law form assumed**

$$\vec{q}_m = -\varepsilon_m k_m \nabla T_m$$

- ***k_m* is obtained from packed bed conductivity formula**[1]

- **In packed bed combustion, *k_m* also accounts for interparticle radiation; *e.g.*[2],** $k_p = 2\sigma d_p T_p^3$

1. MFIX manual, p.20; 2. Gort(1993)

Species Mass Balance

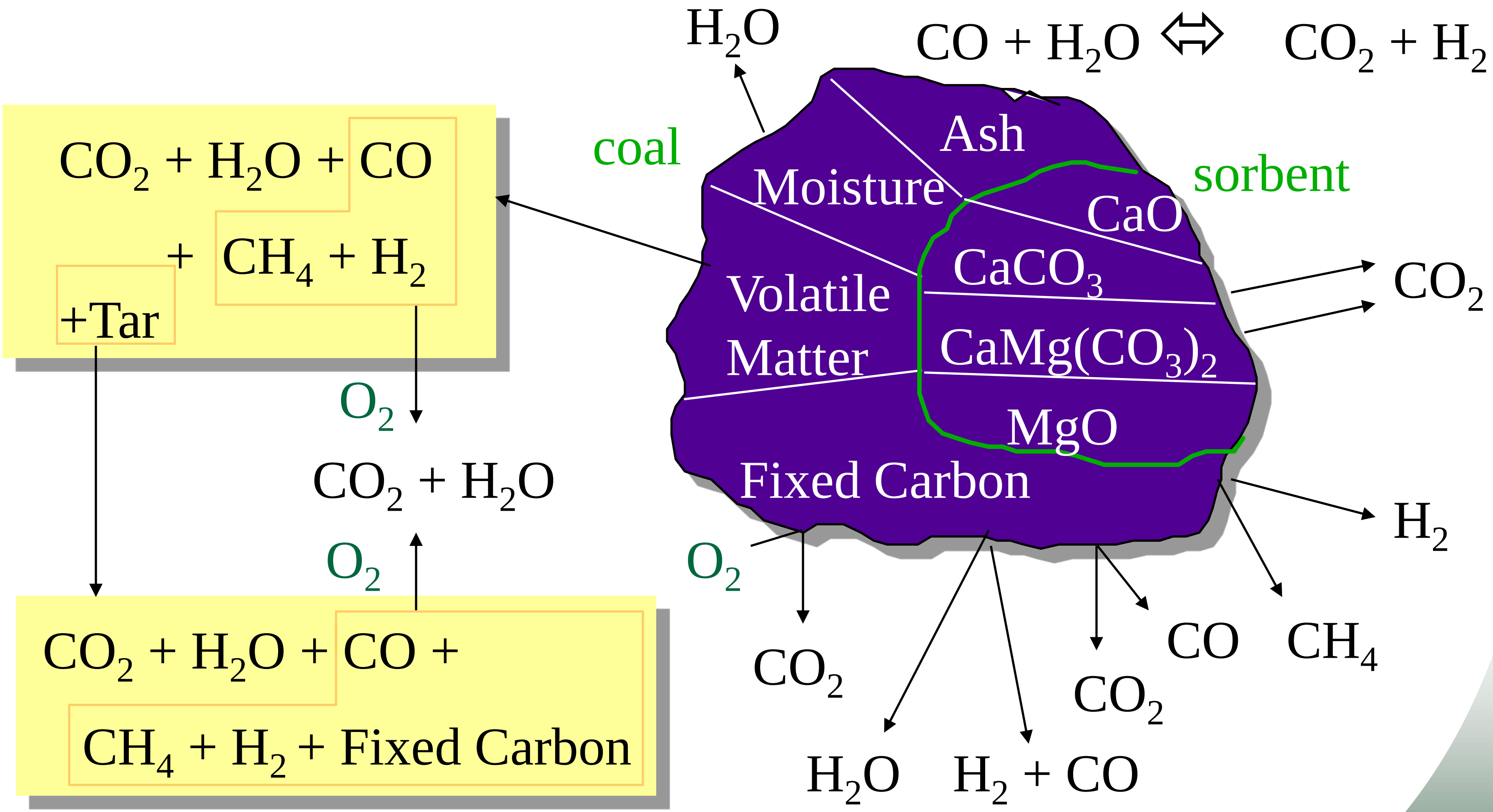
- **Multiphase chemical reactions are described by tracking chemical species in each of the phases**

$$\frac{\partial}{\partial t}(\varepsilon_m \rho_m X_{mn}) + \nabla \cdot (\varepsilon_m \rho_m X_{mn} \vec{u}_m) = \nabla \cdot (\varepsilon_m \rho_m D_{mn} \nabla X_{mn}) + R_{mn}$$

solve__species__eq_8f.html

rrates_8f.html

Reaction Model: Coal Gasification



Homogeneous Reaction

- **Kinetics equation[1] for $CO + {}_2O_2 \rightarrow CO_2$**

$$r_a = 3.98 \cdot 10^{14} \exp\left(\frac{-40{,}000}{1.987 T_f}\right)\left(\frac{\rho_f X_{fO2}}{32}\right)^{0.25}\left(\frac{\rho_f X_{fCO}}{28}\right)$$

$$\left(\frac{\rho_f X_{fH2O}}{18}\right)^{0.5} \varepsilon_f \; (g-mole/cm^3 \cdot s)$$

- **In multiphase formulation the rate expression is multiplied by ε_f**

1. Westbrook and Dryer (1981)

Heterogeneous Reaction

- **Kinetics eq[1] for C + CO_2 ←→ 2CO**

$$r_b = 930\exp\left(\frac{-45{,}000}{1.987 T_{fp}}\right)\left(\frac{\varepsilon_p \rho_p X_{pFC}}{12}\right)\left(p_{CO2} - p_{CO}^2 / K\right)$$

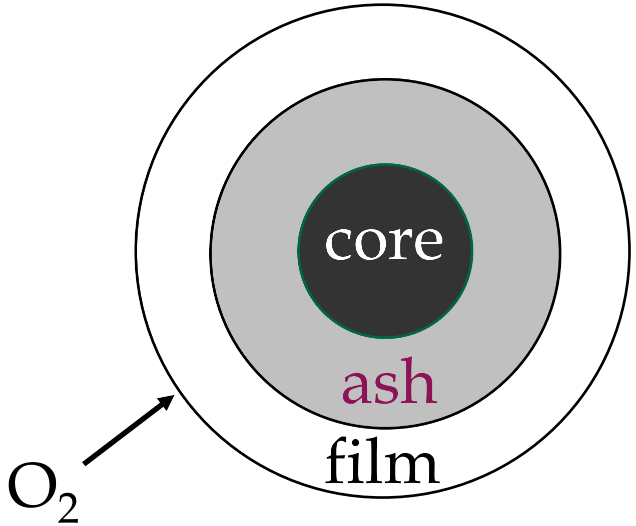
- **Need a reaction temperature; e.g., $T_{fp} = (T_f + T_p)/2$**
- **Need a volume fraction, which depends upon the volumetric basis of the original rate expression**

1. Syamlal and Bissett (1992), Wen et al. (1982)

Heterogeneous Reaction

- **Kinetics equation[1] for 2C + O_2 → 2CO**

$$r_c = \frac{3\varepsilon_m p_{O2}}{16 d_{pm}\left(\frac{1}{k_{fm}} + \frac{1}{k_{am}} + \frac{1}{k_{rm}}\right)}$$



- **Mass transfer coefficient from Gunn equation[2]**

1. MFIX manual p.22

Heat of Reaction

- **In heterogeneous rxns ΔH for each phase could change depending upon the representation of reactions**
  - **Averaging erases info on reaction front**
  - **e.g., in coal combustion the flame may reside at the core surface, in the ash layer, or in surrounding film[1]**
  - **e.g., ΔH for coal combustion[2]:**
    - **$C + 2O_2 \rightarrow CO$ (solids); $CO + 2O_2 \rightarrow CO_2$(gas)**

1. Arri and Amundson (1978); 2. Syamlal and Bissett (1992)

Species Mass Production

- **Based on above three rates the species mass production and mass transfer are**

$$R_{fCO} = 28(2r_b + 2r_c - r_a)$$

$$R_{fO_2} = -32\left(\frac{r_a}{2} + r_c\right)$$

$$R_{fCO_2} = 44(r_a - r_b)$$

$$R_{pFC} = -12(r_b + 2r_c)$$

$$R_{pf} = 12(r_b + 2r_c)$$

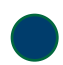
Effects of Mass Transfer

- **On heat transfer**
  - **transfer coefficient needs to be modified**[1]
  - **add an extra heat transfer term**

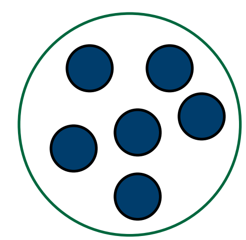
$$R_{ml} h_{ml}$$

- **Group combustion**[2]

single particle combustion



group combustion



1. MFIX manual p.18, 2. Annamalai et al. (1993, 1994)

Day 5: Putting everything together

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presented at

Coal Gasification Short Course

Criciúma, Santa Catarina, Brazil
May 10-14, 2010

Outline

- **Day 1**
  - Install Cygwin, MFIX, Paraview
  - Reacting multiphase flows
  - Volume averaged equations, closures, code walk through
- **Day 2**
  - Hands-on training: Hydrodynamics cases
- **Day 3**
  - Hands-on training: Study the effect of grid resolution, numerical schemes etc.
  - Hands-on training: Cartesian grid
- **Day 4**
  - Hands-on training: Add heat and mass transfer, chemical reactions
- **Day 5**
  - Hands-on training: Put all the things learned to a case with hydrodynamics, heat and mass transfer and chemical reactions
  - Close with future pointers

What we have learned yesterday

- Reviewing few existing cases related to heat & mass transfer, chemical reactions
  - To understand the different parts of the mfix.dat file
  - This corresponds to setting up the case
- Some background on user files needed to heat & mass transfer and chemistry
- Compiling the code
- Running the code
  - ./mfix.exe
- Analyzing/Visualizing the output
  - Launch paraview and view/process the results

Good practices

- Review all the tests and tutorial cases
  - If possible run all the cases closest to your desired configuration
  - When in doubt refer to the readme file to get yourself familiar with the keywords in the mfix.dat file
- Setting up the case
  - Pick the mfix.dat closest to your interest
  - Make necessary changes
    - It is important to start with hydrodynamics, add heat and mass transfer and later chemical reactions
  - Have the mfix.dat file extensively commented and well formatted so that it is easy to read
    - Less chances for error
    - There is good error checking but really not fool-proof

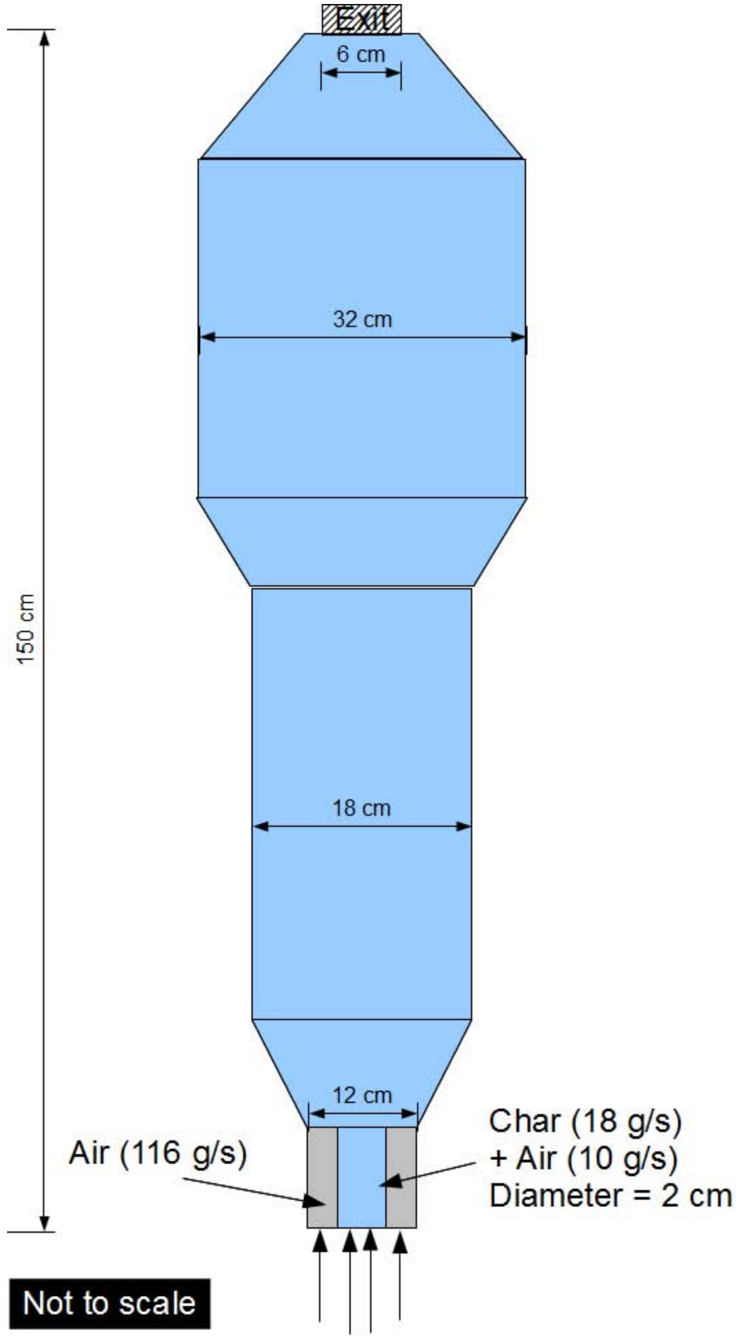
Bad practice

- Editing mfix source files (.f), make_mfix or mfix.dat using windows note pad
  - Cygwin/linux is allergic to windows
  - Always use cygwin/linux based editors such as vi, nedit, emacs….
- Editing source files in the model directory
  - Copy them to your run directory
  - Edit them in your run directory and the make script will automatically pick up your files
  - Always run make_mfix to make sure you have the latest executable

Final assignment: Spouted bed combustor

- Go to mfix/tutorials directory
- $cd SpoutedBedCombustor
- $nedit mfix.dat
- Reduce the TSTOP
- Compile, Run, Visualize

Setup

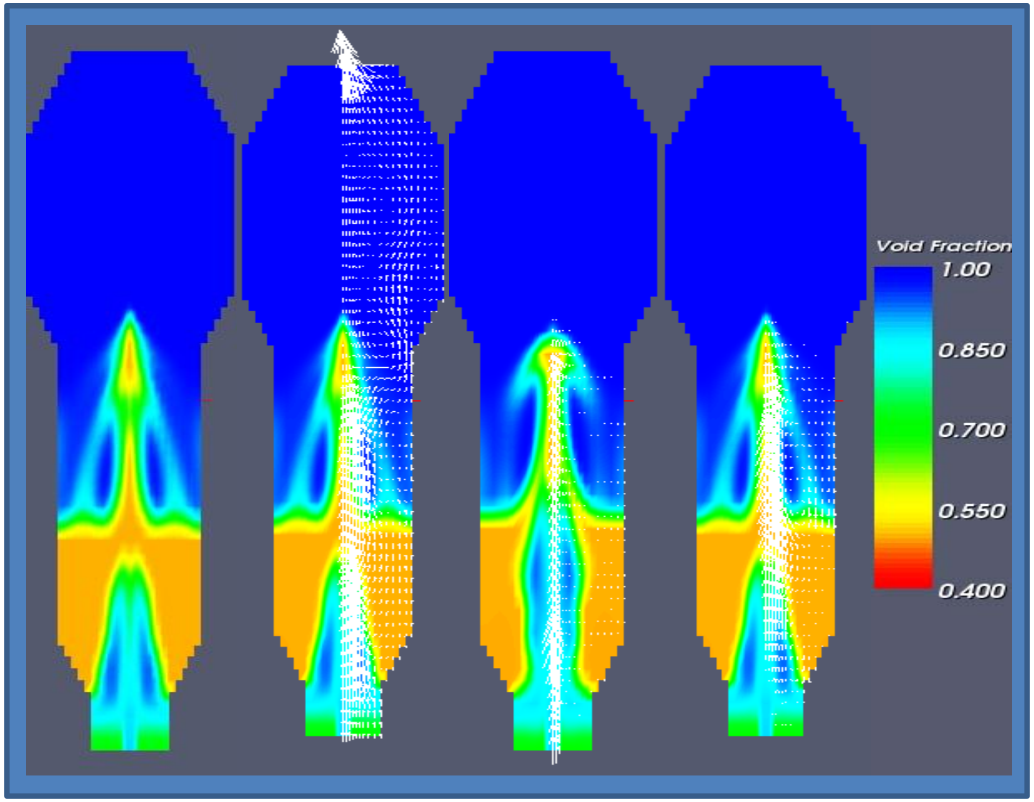


Exit
6 cm
32 cm
150 cm
18 cm
12 cm
Air (116 g/s)
Char (18 g/s)
+ Air (10 g/s)
Diameter = 2 cm
Not to scale

Some salient features

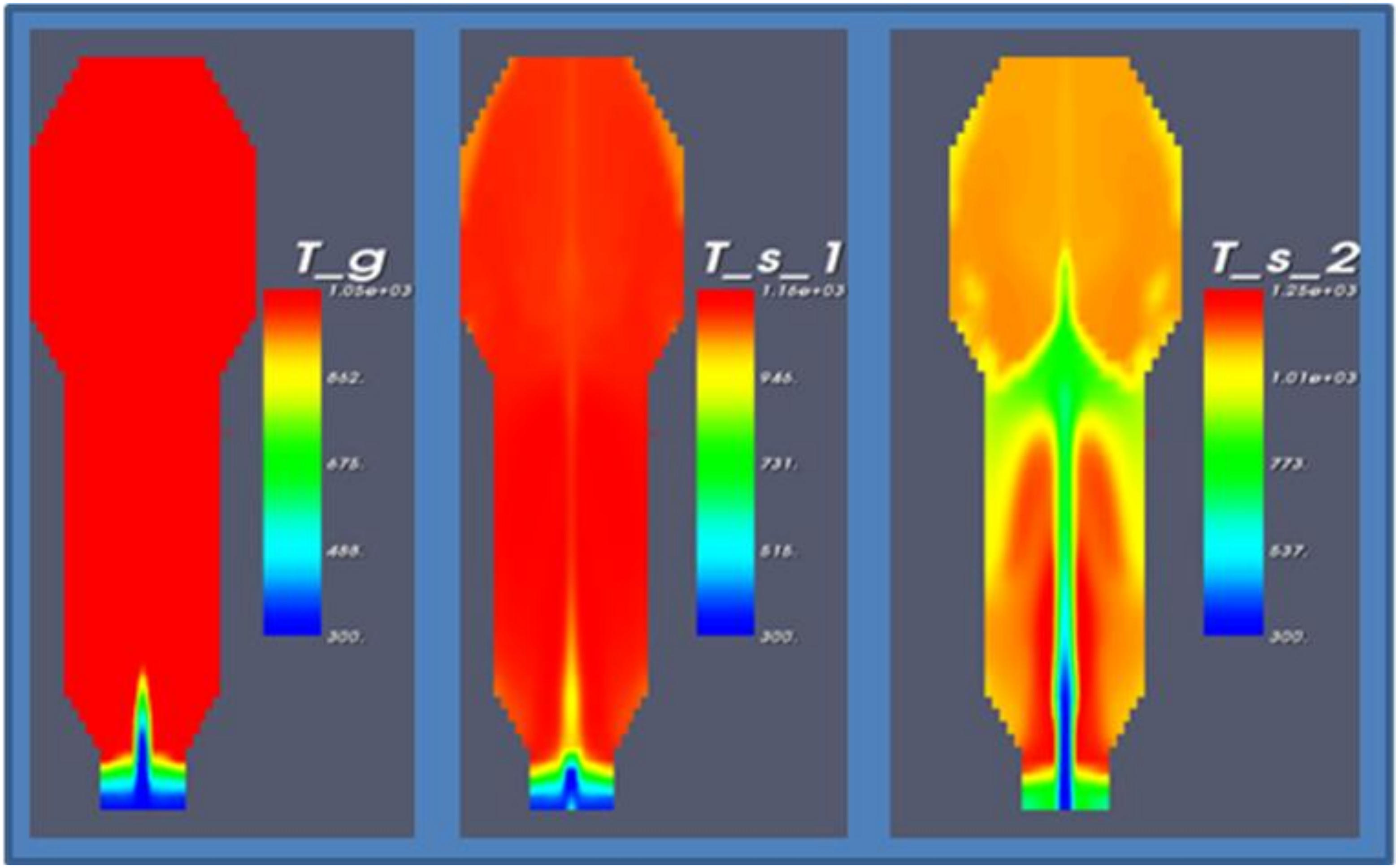
- Char (18 g/s) and air (10 g/s) are fed into the combustor through a central tube.
- A second stream of fluidizing air (116 g/s) enters the annular region surrounding the tube.
- Partial combustion of the char occurs in the combustor.
- The product gases exit from the top of the combustor.
- The char density is 1 g/cm^3 and the particle diameter is 1000 μm.
- Incoming char is at a low temperature and it is critical to consider char heat-up, the incoming char will be treated as a second solids phase called "cold-char."
  - The char already in the combustor will be called "hot-char."
  - When the ash fraction in the cold chare exceeds a certain specified value, say 0.9, it is assumed to convert into hot-char.
  - A fast pseudo-reaction is specified to convert the cold-char at temperatures above that value to hot-char.
  - These ash fraction threshold and rate constant are specified in mfix.dat as constants C(1) and C(2), which are used in the subroutine rrates.

Hydrodynamic results



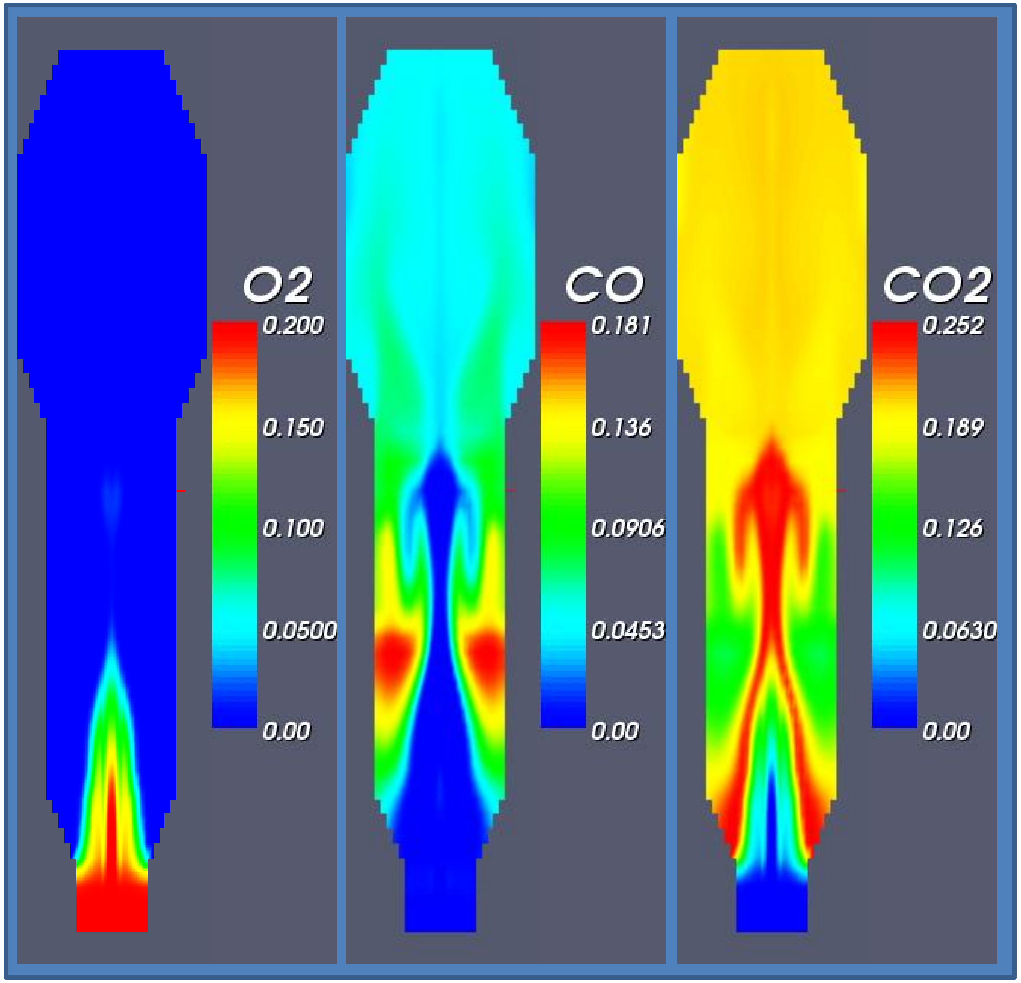
- **Hydrodynamics features of the spouted bed at 10s: a) Void fraction distribution in the spouted bed, b) Void fraction imposed by gas velocity vectors, c) Void fraction imposed by solids 1 velocity vectors, and d) void fraction imposed by solids 2 velocity vectors**

Temperature



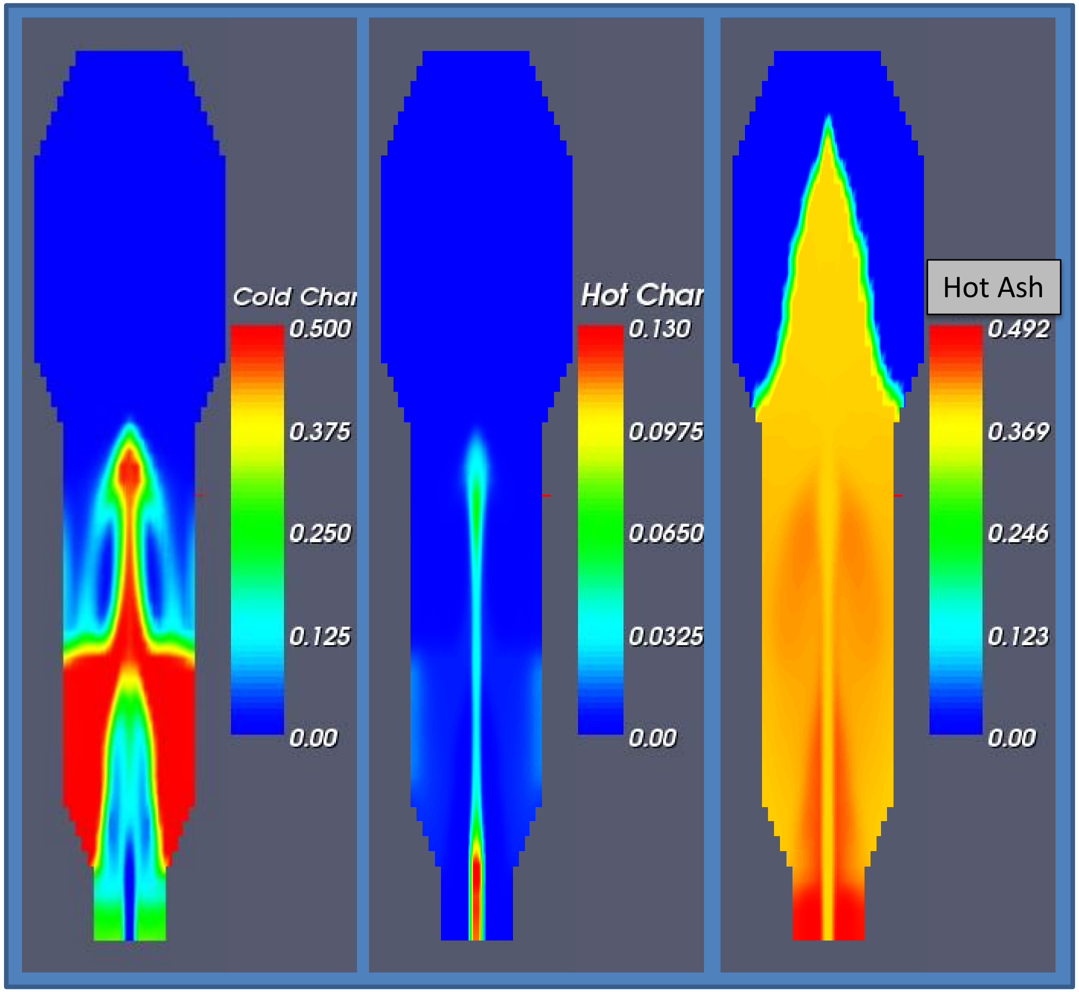
Temperature distribution in the bed a) Gas temperature, b) Solids 1 temperature, and c) Solids 2 temperature

Gas-phase species



Gas phase species distribution in the spouted bed at 10s: a) mass fraction of O_2, b) mass fraction of CO, and c) mass fraction of CO_2

Solids-phase species



Solids phase species distribution in the spouted bed at 10s: a) total cold char (g/cm³), b) total hot char (g/cm³), and c) mass fraction of hot ash

Take away message

- Changing resolution or order of the scheme can affect convergence
  - Unpredictable computational cost
  - Sometimes non-convergence
- It is recommended to go to a fine enough grid resolution beyond which the changes are not significant
- If you can converge with the high-order schemes – that is the preferred choice

Continuity Equation

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

$$\sum_{m=1}^{N} \varepsilon_m = 1$$

index.html

solve_continuity_8f.html

Momentum Equation

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

Interaction within the phase → stresses

–collisions, sliding or rolling friction

–electrostatic, van der Waals, capillary

solve__vel__star_8f.html

Momentum Equation

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

Interaction between phases → interphase forces

Momentum Equation

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

Interactions with rest of the universe → body forces

Energy Balance

solve_energy_eq_8f.html

originates from a work term for ε changes

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

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

Energy Balance

Viscous dissipation

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

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

Energy Balance

Energy sources; e.g.., radiation

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

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

Energy Balance

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

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

heat conduction

Energy Balance

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

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

Interphase heat transfer

Energy Balance

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

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

Energy transfer with mass transfer

Energy Balance – In Terms of Temperature

Energy balance equations for solids phases m = 1, M

$$\varepsilon_m \rho_m C_{pm}\left[\frac{\partial T_m}{\partial t} + U_{mj}\frac{\partial T_m}{\partial x_j}\right] = -\frac{\partial q_{mi}}{\partial x_i} - \gamma_{gm}\left(T_m - T_g\right) - \Delta H_m + \gamma_{Rm}\left(T_{Rm}^4 - T_m^4\right)$$

Energy balance equation for gas phase g:

$$\varepsilon_g \rho_g C_{pg}\left[\frac{\partial T_g}{\partial t} + U_{gj}\frac{\partial T_g}{\partial x_j}\right] = -\frac{\partial q_{gi}}{\partial x_i} + \sum_{m=1}^{M}\gamma_{gm}\left(T_m - T_g\right) - \Delta H_g + \gamma_{Rg}\left(T_{Rg}^4 - T_g^4\right)$$

Heats of Reaction

$$-\Delta H_m = \sum_n \left[\left(H_{m,ref} \right)_n + \int_{T_{ref}}^{T_s} C_{pmn}(T)\,dT \right] \varepsilon_g \rho_g \left(\frac{\partial X_{gn}}{\partial t} + U_{gi} \frac{\partial X_{gn}}{\partial x_i} \right)$$

$$\approx \sum_n \left[\left(H_{m,ref} \right)_n + \int_{T_{ref}}^{T_s} C_{pmn}(T)\,dT \right] \left(R_{mn} - \sum_{n=1}^{N_m} R_{mn} X_{mn} \right)$$

$$-\Delta H_g \approx \sum_n \left[\left(H_{g,ref} \right)_n + \int_{T_{ref}}^{T_g} C_{pgn}(T)\,dT \right] \left(R_{gn} - \sum_{n=1}^{N_g} R_{gn} X_{gn} \right)$$

Fluid-Particle Heat Transfer

The interphase heat transfer coefficient

$$\gamma_{fm} = \frac{6\kappa_f \varepsilon_m Nu_m}{d_{pm}^2}$$

where the Nusselt number is calculated using Gunn (1978) correlation

$$Nu_m = (7 - 10\varepsilon_f + 5\varepsilon_f^2)(1 + 0.7\,\mathrm{Re}_m^{0.2}\,\mathrm{Pr}^{1/3})$$
$$+ (1.33 - 2.4\varepsilon_f + 1.2\varepsilon_f^2)\,\mathrm{Re}_m^{0.7}\,\mathrm{Pr}^{1/3}$$

1. Gunn (1978)

Fluid-Particle Heat Transfer

- To predict heat transfer to immersed tubes (with coarse numerical grid), the model will need a wall heat transfer coefficient[1]

1. Syamlal and Gidaspow (1985), Kuipers et al. (1992), Witt and Perry (1996)

Heat Conduction

- **Fourier's law form assumed**

$$\vec{q}_m = -\varepsilon_m k_m \nabla T_m$$

- **k_m is obtained from packed bed conductivity formula[1]**

- **In packed bed combustion, k_m also accounts for interparticle radiation; *e.g.*[2], $k_p = 2\sigma d_p T_p^3$**

1. MFIX manual, p.20; 2. Gort(1993)

Species Mass Balance

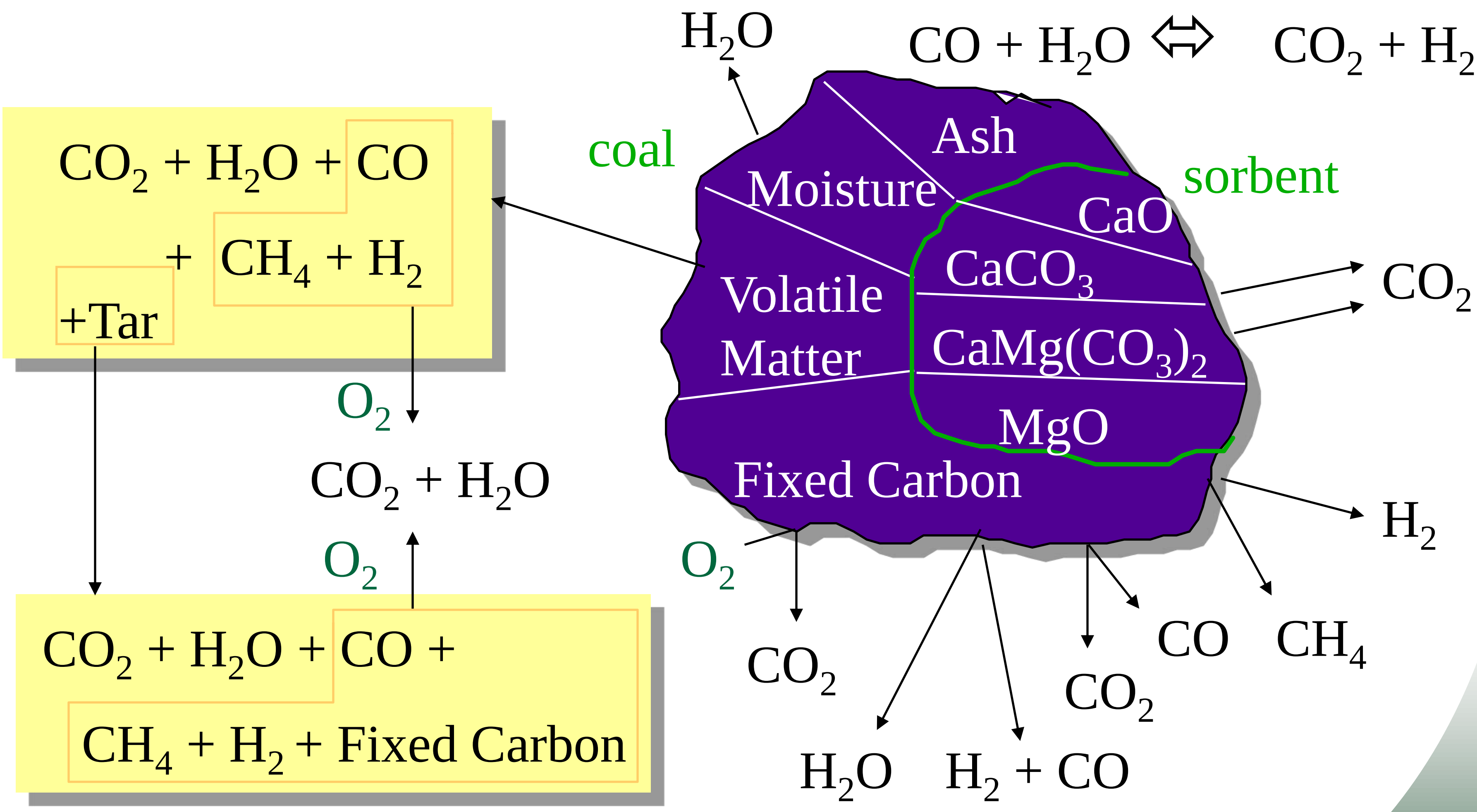
- **Multiphase chemical reactions are described by tracking chemical species in each of the phases**

$$\frac{\partial}{\partial t}(\varepsilon_m \rho_m X_{mn}) + \nabla \cdot (\varepsilon_m \rho_m X_{mn} \vec{u}_m) = \nabla \cdot (\varepsilon_m \rho_m D_{mn} \nabla X_{mn}) + R_{mn}$$

solve__species__eq_8f.html

rrates_8f.html

Reaction Model: Coal Gasification



Homogeneous Reaction

- **Kinetics equation[1] for $CO + {}_2O_2 \rightarrow CO_2$**

$$r_a = 3.98 \cdot 10^{14} \exp\left(\frac{-40{,}000}{1.987 T_f}\right)\left(\frac{\rho_f X_{fO2}}{32}\right)^{0.25}\left(\frac{\rho_f X_{fCO}}{28}\right)\left(\frac{\rho_f X_{fH2O}}{18}\right)^{0.5} \varepsilon_f \quad (g-mole/cm^3 \cdot s)$$

- **In multiphase formulation the rate expression is multiplied by ε_f**

1. Westbrook and Dryer (1981)

Heterogeneous Reaction

- **Kinetics eq[1] for C + CO_2 ←→ 2CO**

$$r_b = 930 \exp\left(\frac{-45{,}000}{1.987 T_{fp}}\right)\left(\frac{\varepsilon_p \rho_p X_{pFC}}{12}\right)\left(p_{CO2} - p_{CO}^2 / K\right)$$

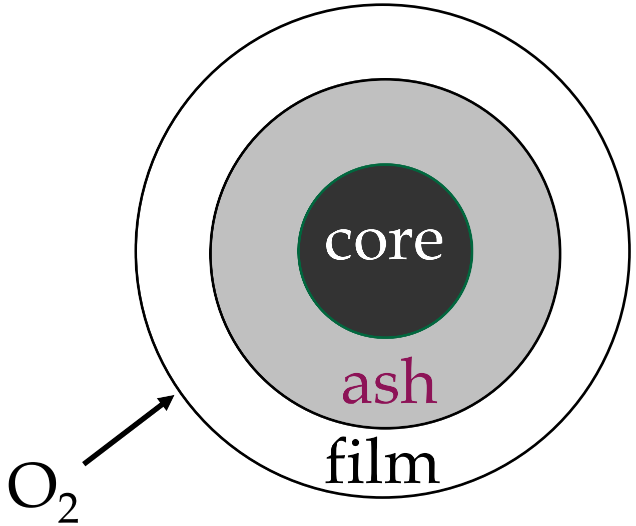
- **Need a reaction temperature; e.g., $T_{fp} = (T_f + T_p)/2$**
- **Need a volume fraction, which depends upon the volumetric basis of the original rate expression**

1. Syamlal and Bissett (1992), Wen et al. (1982)

Heterogeneous Reaction

- **Kinetics equation[1] for $2C + O_2 \rightarrow 2CO$**

$$r_c = \frac{3\varepsilon_m p_{O2}}{16 d_{pm}\left(\frac{1}{k_{fm}} + \frac{1}{k_{am}} + \frac{1}{k_{rm}}\right)}$$



- **Mass transfer coefficient from Gunn equation[2]**

1. MFIX manual p.22

Heat of Reaction

- In heterogeneous rxns ΔH for each phase could change depending upon the representation of reactions
  - Averaging erases info on reaction front
  - e.g., in coal combustion the flame may reside at the core surface, in the ash layer, or in surrounding film[1]
  - e.g., ΔH for coal combustion[2]:
    - $C + 2O_2 \rightarrow CO$ (solids); $CO + 2O_2 \rightarrow CO_2$(gas)

1. Arri and Amundson (1978); 2. Syamlal and Bissett (1992)

Species Mass Production

- **Based on above three rates the species mass production and mass transfer are**

$$R_{fCO} = 28(2r_b + 2r_c - r_a)$$

$$R_{fO_2} = -32\left(\frac{r_a}{2} + r_c\right)$$

$$R_{fCO_2} = 44(r_a - r_b)$$

$$R_{pFC} = -12(r_b + 2r_c)$$

$$R_{pf} = 12(r_b + 2r_c)$$

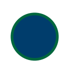
Effects of Mass Transfer

- **On heat transfer**
  - **transfer coefficient needs to be modified[1]**
  - **add an extra heat transfer term**

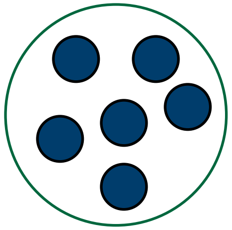
$$R_{ml}h_{ml}$$

- **Group combustion[2]**

single particle combustion



group combustion



1. MFIX manual p.18, 2. Annamalai et al. (1993, 1994)

Final thoughts

- **Readme**
- **Documents in the mfix directories**
- **Tutorial/test cases**
- **Systematic setup and testing**
  - **Hydrodynamics**
  - **Heat and Mass transfer**
  - **Chemical reactions**
- **Use MFIX website (http://mfix.netl.doe.gov) and mailing lists (mfix-help@mfix.netl.doe.gov)**
- **This is an open-source project – you can participate by testing, contributing cases, developing methods/models – the possibilities are infinite with any other constraints**