COMPUTATIONAL FLUID DYNAMICS FOR MULTIPHASE FLOW

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INTRODUCTION

Fluidized bed reactors are widely used in the chemical industry and are essential to the production of key commodity and specialty chemicals such as petroleum, polymers, and pigments. Fluidized beds are also going to be widely used in the next generation power plants in aiding conversion of coal to clean gas. However, in spite of their ubiquitous application, understanding of the complex multi-phase flows involved is still very limited. In particular, existing computer simulations are not sufficiently accurate/fast to serve as a primary approach to the design, optimization, and control of industrial-scale fluidized bed reactors. Availability of more sophisticated computer models is expected to result in greatly increased performance and reduced costs associated with fluidized bed implementation and operation. Such improved performance would positively affect U.S. chemical/energy industry competitiveness and increase energy efficiency.

To improve fluidization simulation capabilities, two different projects are undertaken at ORNL with the specific objective of developing improved fluidization computer models. On one hand, a very detailed multiphase computer model (MFIX) is being employed. On the other hand a Dynamic Interacting Bubble Simulation (DIBS) is being further developed at ORNL with the eventual aim of real time diagnosis and control of industrial scale fluidized beds.

MFIX (Multiphase Flow with Interphase eXchanges – http://www.mfix.org) is a general-purpose computer code developed at the National Energy Technology Laboratory (NETL) for describing the hydrodynamics, heat transfer and chemical reactions in fluid-solids systems. It has been used for describing bubbling and circulating fluidized beds, spouted beds and gasifiers. MFIX calculations give transient data on the three-dimensional distribution of pressure, velocity, temperature, and species mass fractions. MFIX code is based on a generally accepted set of multiphase flow equations. However, in order to apply MFIX in an industrial context, key additional improvements are necessary. These key improvements correspond to the two ORNL efforts: (1) To develop an effective and validated computational tool through development of a fast, parallel MFIX code and (2) Develop infrastructure for easy collaborative development of the MFIX code and exchange of information between the developers and users.

DISCUSSION OF CURRENT ACTIVITIES

Over the past several years, ORNL along with its collaborators (NETL, Aeolus, Inc.) has been involved in migration of MFIX to modern high-performance parallel architectures. A hybrid parallel version of MFIX has been developed using MPI communication library and OpenMP compiler directives on shared memory environments. The code has been ported to Linux Beowulf cluster, IBM SP, SGI multiprocessors, and Compaq clusters. Various optimizations and developments are made to improve performance and reduce communication costs for simulations using MFIX. Most of these results have been reported earlier (D'Azevedo et. al. (2001) and Pannala et. al. (2003 a & b)). In this report, we present results from the ongoing validation of a square cross-section circulating fluidized bed, 2D bed and a flower bed. Here is the brief overview of the results with appropriate references.

SQUARE CFB:

As part of the validation effort, we used the simulation of a circulating fluidized bed with a square cross-section, corresponding to the experiments conducted by Zhou et al. [1994 a & b]. The bed has a square cross-section, 14.6 cm wide, and is 9.14 m in height. The schematic of this setup is shown in Fig. 1. The solids inlet and outlet are of circular cross-section in the experiments but for geometric simplicity, we have represented them by square cross-section. The area of the square openings and the mass flow rate corresponds to that of the experiments. At a gas velocity of 550 cm/s the drag force on the particles is large enough to blow the particles to the top of the bed and make the bed flow like a fluid or fluidized bed. The particles strike the top wall and some of them exit through the outlet while the rest fall down to encounter the upcoming stream of solids and gases. The square cross-section makes it easy for subgrid model development by providing uniform computational cells. This problem also is of industrial importance as the size of the configuration corresponds to typical pilot-scale plants used in the industry.

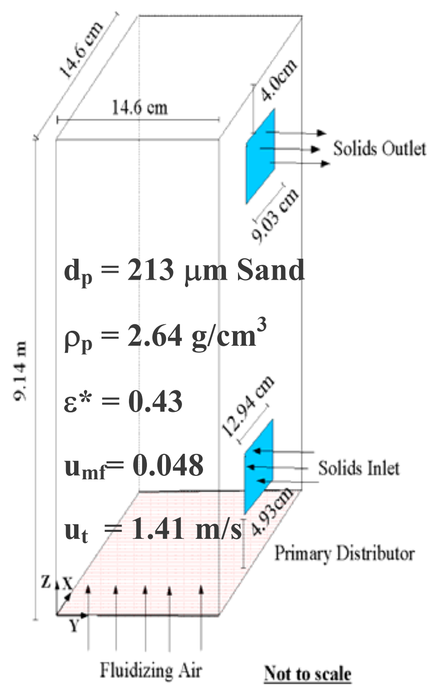


Figure 1: Schematic of the simulated CFB.

In this problem, a three-dimensional Cartesian coordinates system was used. The spanwise directions were discretized into 15 cells (~1 cm, I & K-dimensions) and the axial, streamwise direction into 200 cells (~4.3 cm, J-dimension). Three-dimensional domain decomposition was performed using 8 processors. Several other high-resolution simulations were also carried out and were reported earlier (Pannala, 2003 a & b). Fig. 2 gives a snapshot from such high-resolution simulations indicating the core-annulus structure and the solids buildup at the corners.

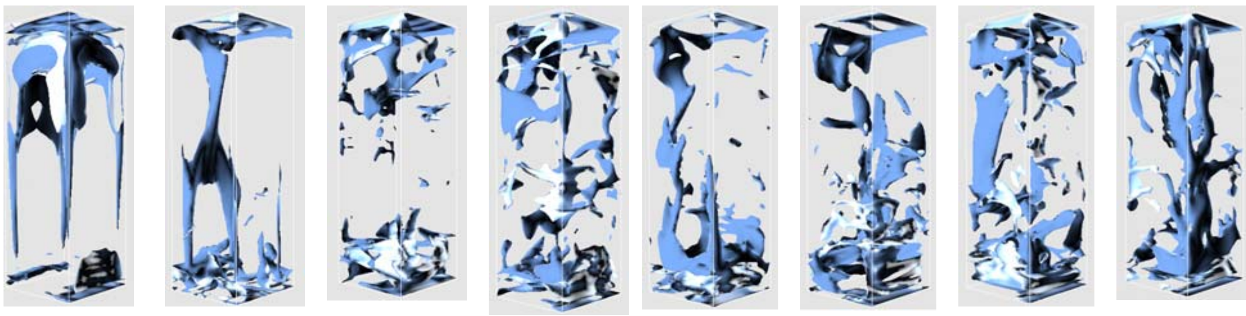


Figure 2: Instantaneous snapshots of voidage surface (=0.85). Indicates the core-annulus flow and the solids flowing down at the walls (used MAVIS for visualization).

Fig. 3 describes the procedure to develop the subgrid model for the MFIX coarse-grid simulation. A representative cell of the coarse grid is simulated using 64x64 grid and the data is collected for various solids fractions. This information is then used to fit expressions for solids viscosity and pressure. These expressions for solids viscosity and pressure were later used in the coarse-grid simulations instead of kinetic theory.

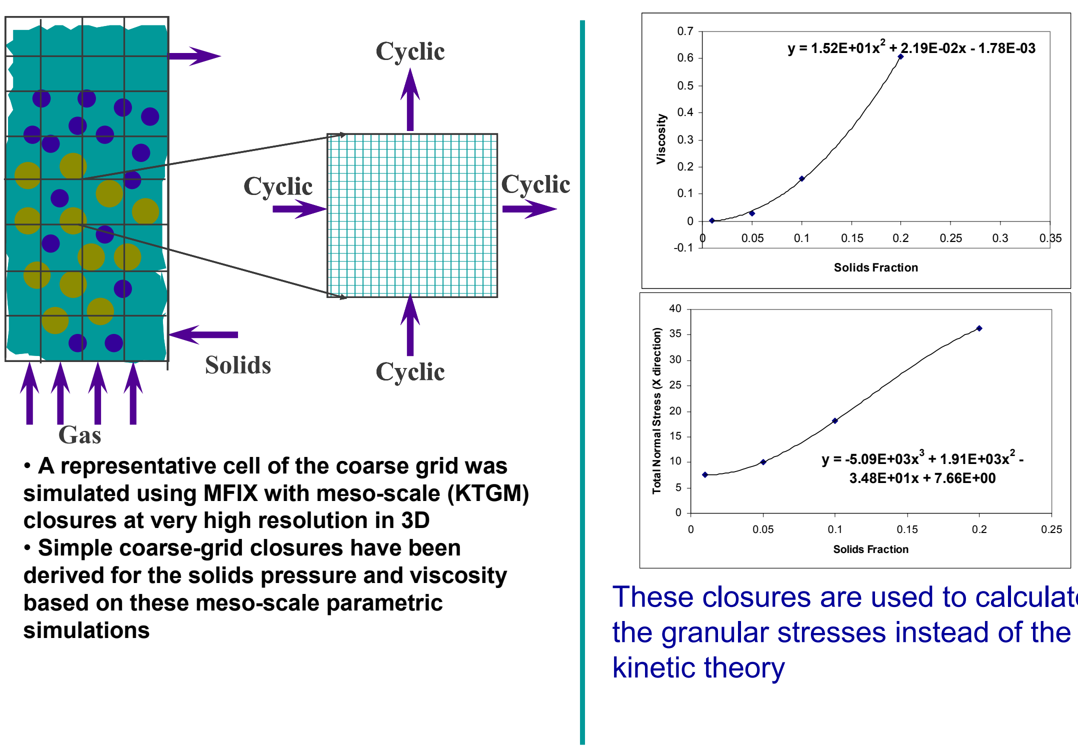


Figure 3: A schematic describing the closure construction based on the high-resolution subgrid simulations

The results of coarse-grid with both the subgrid model and with out the subgrid model are contrasted in Fig. 4. Here the subgrid model agrees reasonably well with the experiments but results at other locations (presented in Pannala et al., 2003c) are not that promising.

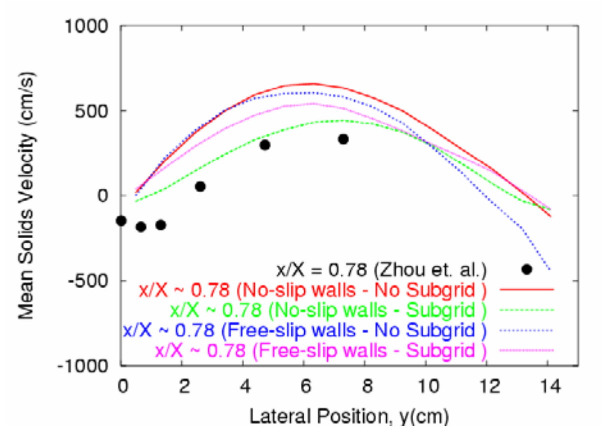


Figure 4: Lateral profiles of time-averaged voidage fraction at z=5.13 with and without subgrid model.

The subgrid model does not account for any anisotropy due to the walls or the inlet/outlet. It is proposed to modify the subgrid model based on the schematic described in Fig. 5 to improve the accuracy of the coarse-grid simulations.

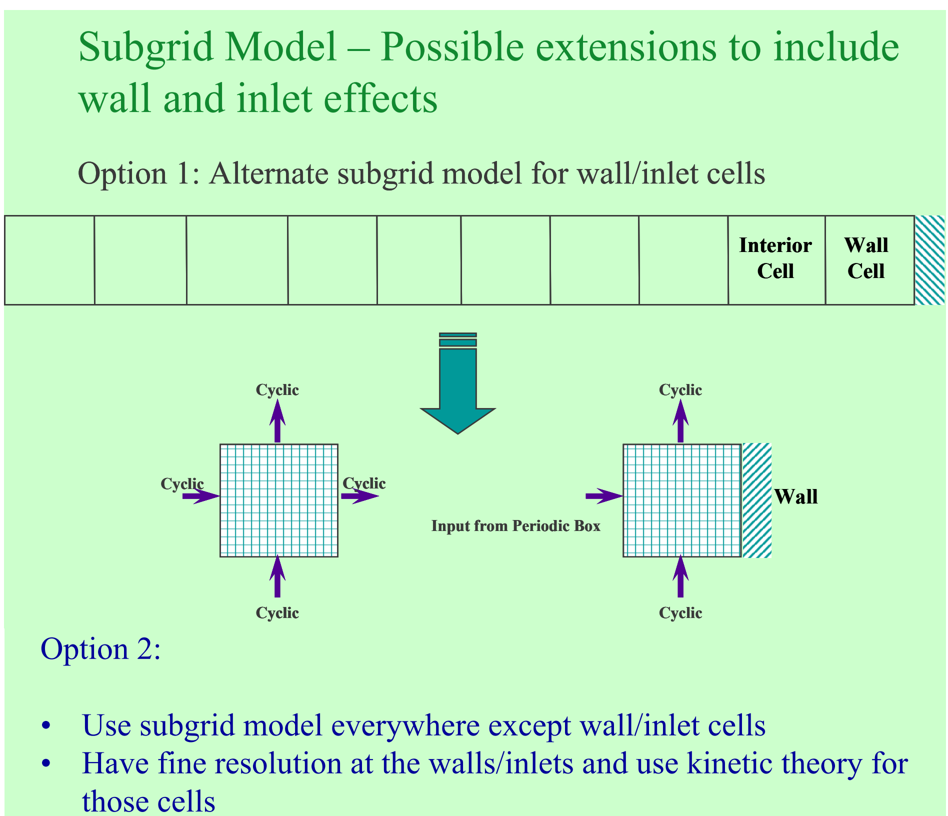


Figure 5: A schematic describing the closure construction for the wall and inlet cells.

Here are the brief conclusions of the subgrid modeling effort for the square CFB problem:

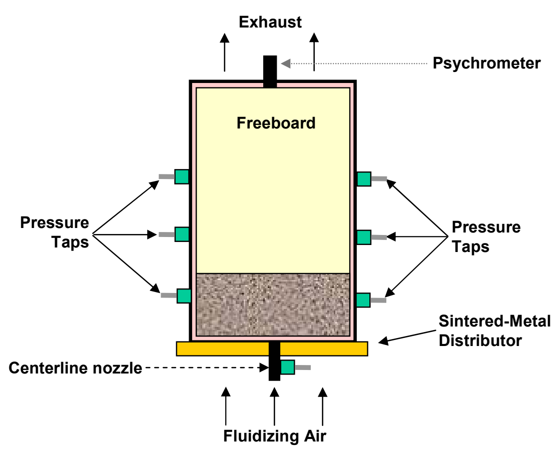
- MFIX with subgrid model seems to be as good or better than kinetic theory away from walls and inlets
- Reasonable qualitative agreement
- Suggests that higher resolution is needed to resolve the inlet/exit sections, the high solids region and high shear region or different subgrid models in these regions
- Require a modified subgrid model which accounts for asymmetries at the walls and inlets/outlets

Future work will include the following to improve the accuracy of the subgrid model:

- Modify the subgrid model to include wall/inlet effects
- Full scale simulation with modified subgrid model
- High resolution simulation with clustered grid around the inlet and outlet
- Role of different numerics, drag rules, kinetic theory formulations on experimental comparisons

2D BED:

In order to validate and fine-tune certain particle properties for MFIX simulations, we are also comparing MFIX results against the 2D bed experiments at UT (University of Tennessee). The schematic of the experimental setup along with relevant parameters is shown in Fig. 6. The 2D bed is a fluidized bed made into thin slab that can be directly viewed to observe the gas and solids flow patterns. The rectangular geometry makes simulation easier by avoiding the center-line problems associated with cylindrical co-ordinate system used for cylindrical beds. Both 2D and 3D simulations studies of this bed with ZrO_2 were carried out and one such result is shown in Fig. 7.



General construction:

- 0.5 cm thick plexiglass
- 25.3 cm wide, 1.9 cm deep, 77.5 cm tall
- High-DP sintered-metal distributor
- Centerline nozzle (5 mm square) with independent flow control
- Flush wall taps (0.318 cm diameter) at 7.5, 18.7, 28.7 cm above distributor
- Heavy steel mounting frame (61 cm tall) on 48 cm square floor plate with leveling screws (adjustable vertical bias)

Recent experiments:

- 0.3mm ZrO_2 (Group B/D)
- 16cm static bed height
- grid flow (~0.15 – 1 U_{mf})
- various nozzle flows (~15 – 45 m/s)
- No HP filtering
- MFIX simulations ongoing

Instrumentation:

- High-speed pressure (200 Hz), HP/LP filtering, 12-bit A/D
- Digital still/video imaging, 720 × 480 pixels, 30 fps; reflected lighting (SS) or transmitted lighting (glass)
- Psychrometer at bed exit

Figure 6: Schematic of the 2D bed with details of construction and instrumentation.

Here is a summary of the results shown in Fig. 7. The instantaneous void fraction and gas pressure surface contours are plotted on the top. The pressure trace in the jet is plotted on the bottom-left and indicates high-frequency fluctuations of around ~ 10 Hz. The image from the experiments is shown on the bottom-right. The observed void fraction results agree qualitatively with the experimental video and the observed frequency matches that of the experiment. Further analysis and simulations of the 2D bed are underway and will possibly result in a publication.

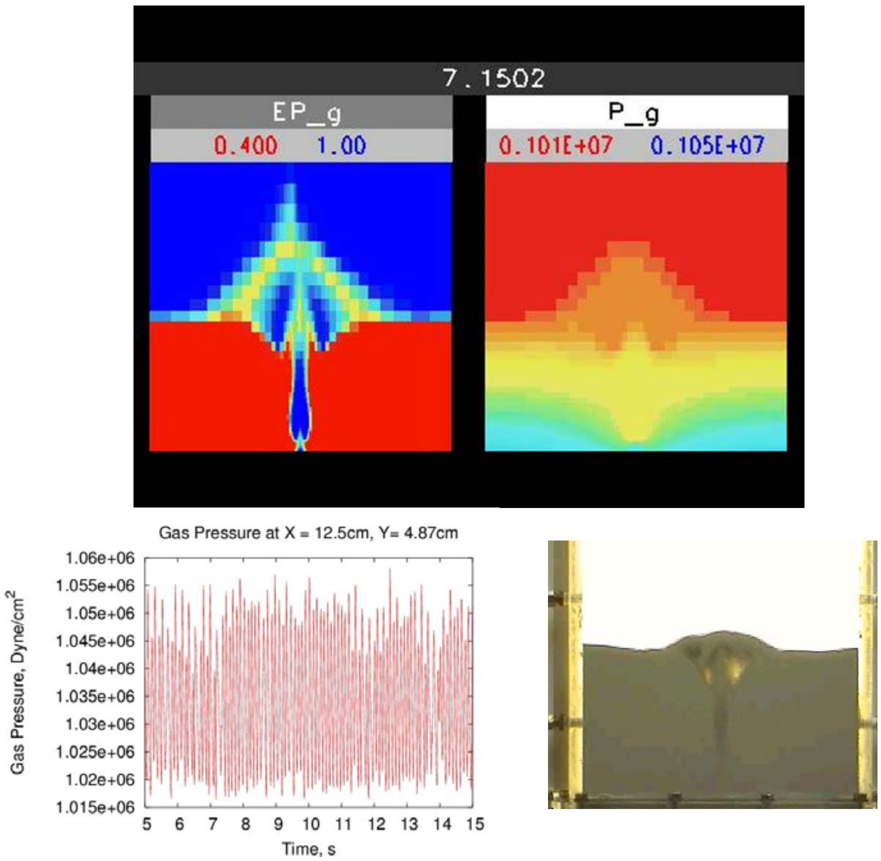
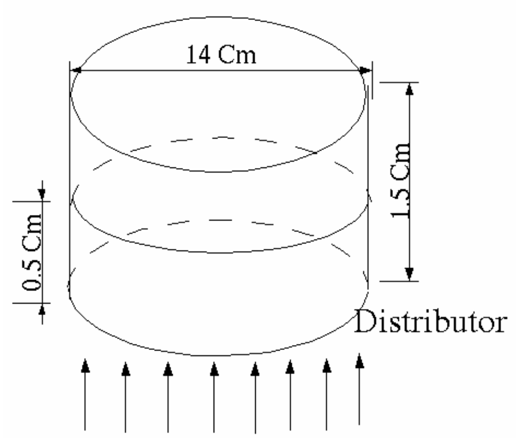


Figure 7: 2D bed results: a) Instantaneous snapshot of gas void fraction and gas pressure surface contours, b) Time trace of the gas pressure at the inlet and c) Snapshot of the spout from the 2D bed experiment.

FLOWER BED:

The flower bed (with interesting surface patterns) experiments performed at Argonne National Laboratory (ANL) serve as another valuable data-set to validate MFIX. The patterns observed in the experiments are very sensitive to the flow and particle parameters. The bed experiences sub-harmonic response at specific forcing frequencies and exhibits stable patterns on the surface. The schematic of the experimental setup along with relevant parameters is shown in Fig. 8. Here the inflow is superimposed with a sinusoidal varying gas flow. The forcing frequency of the imposed flow in the results described below is 14 Hz.



Mean Flow + Sinusoidal Forcing

$$U = U_o + U_f * Sin(2\pi f\ t)$$

Figure 8: Schematic of the ANL's flower bed configuration

In the experiments, the granular material experiences oscillatory behavior due to the imposed modulating flow. This leads to a non-uniform wave propagation of compressed granular material as the bed expands and contracts. In fig. 9, iso-surface of void fraction corresponding to 0.44 (capped with the lower and upper values) of a typical 3D simulation is shown. The colors are made transparent so that solids motion in the bed is visible. From the animation of the results, it is found that the upward propagation is slower than downward sweep as should be expected in these beds. The experiment might be mimicking the one with a vibrating plate but with a non-linear forcing through the drag terms. More details like gas/solid velocities, granular temperature and other quantities will be analyzed in the future.

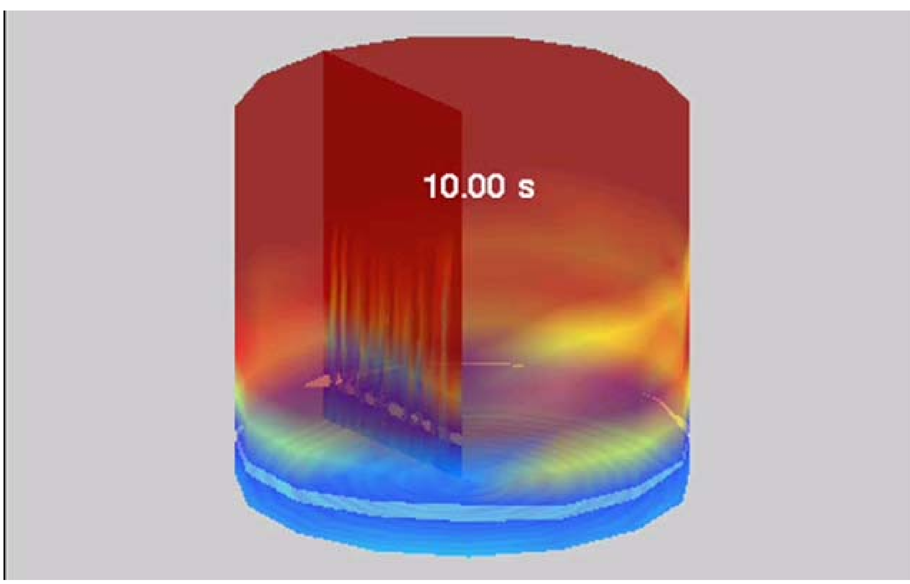


Figure 9: Iso-surface of void fraction (= 0.44) capped with the lower and upper values. The colors are made transparent so that the entire bed is visible.

The 3D simulations performed did not contain the sub-harmonic response necessary to generate the interesting patterns observed in the experiments. There could be many reasons for this:

- The artificial rotation in the 3D simulation due to cylindrical co-ordinates is suppressing the sub-harmonic response.
- The grid resolution is not sufficient to resolve the small spouts observed in the experiments and thus not capturing the self organization of the same.

In order to address the above deficiencies, a simple high-resolution 2D simulation was carried out. This 2D simulation should capture the planar wave-pattern, if this pattern formation is not geometric specific and more universal. In fig. 10, void fraction surface contours at different time instants are plotted showing the expansion and collapse of the solids. These images correspond to plane wave-pattern formation, suggesting that the observed patterns might be more universal than the experimental configuration at ANL.

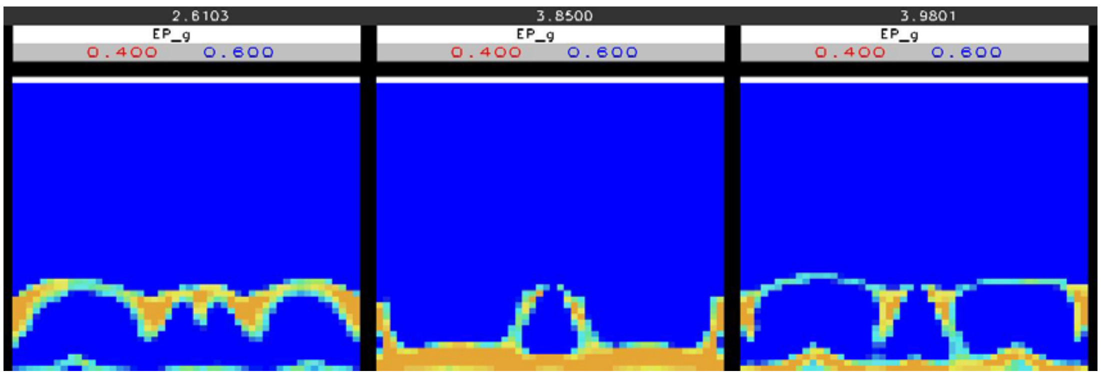


Figure 10: Void fraction surface contours at different time instants showing the expansion and the collapse of the solids.

In order to confirm the sub-harmonic response, we plotted the power spectra of the void-fraction in the bed in fig. 11. This clearly shows a sub-harmonic response at the ½ the frequency of the forced frequency.

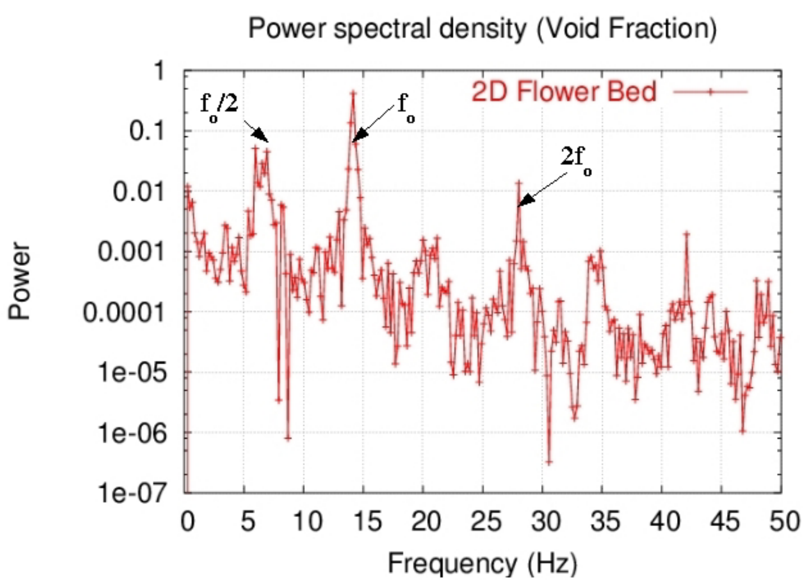


Figure 11: Power spectra of the pressure in the bed showing the sub-harmonic response typically observed in the experiments corresponding to the pattern formation.

More simulations have to be performed to confirm this behavior and all these will feed into validation of MFIX for the ANL flower bed setup.

MFIX DEVELOPMENT AND COLLABORATION UPDATE:

CVS (concurrent version system) has been used for seamless integration of the various components of the development work. Web/Java based tools have been used to make this process easier and facilitate the virtual collaboration between these diverse set of developers and researchers. In addition, a website (www.mfix.org) has been started to help free exchange of information between the developers, researchers and users. Over 350 researchers have downloaded MFIX and some of them are active participants in various discussions through the mailing lists. These researchers are from National Labs, Universities, Industry, and Research Labs around the world (see Table 1).

Aeolus Research	Ecole des Mines de Douai	Iowa State University	P&K Associates	Univ. of Alberta
2B3	Edinburgh University	IPN, Mexico	Pittsburgh Supercomputing Center	Universidad Politécnica de Madrid
Almidones Mexicanos SA de CV	EniTecnologie	ISR	Politecnico di Milano	Universite de Rennes1
American Air Liquide	EPM-Madylam	Italian University	Princeton University	University of Alaska Fairbanks
Anco Maritime Activities	EWRE ltd	KAPL/Lockheed Martin	Reaction Engineering	University of Bergen - Norway
Andrews & Kurth	ExxonMobil Research & Engineering	KBC Advance Technologies	Regional Engineering College Durgapur	University of Bristol
Argonne National Laboratory	FC-TECH	KFUPM	Reliant Resources	University of Calabria - Italy
ATK Elkton	Federal University of Santa Catarina	Korea Atomic Eergy Research Institute	Research Technologies	University of Calgary
Atomic Energy Authority, Egypt	FLUENT Inc.	Laboratoire Magmas et Volcans	RMIT university	University of California, San Diego
Barnes and Click, Inc.	Foster Wheeler Development Corp.	LANL	Saint Cloud State University	University of Colorado - Boulder
BBWI/INEEL	Hatch Associates, Ltd.	L'ecole Polytechnique de Montreal	San Diego State University	University of Milan
Carnegie Mellon University	Helwan University	Lehigh University	Sasol Ltd. - South Africa	University of New South Wales
CFDRC	Heriot-Watt University	LSG2M	Savannah River Site	University of Nottingham
Chemical Engineering Dept, NUS	Heriot-Watt University	LSTM	Schlumberger	University of Pavia
Chemical Engineering Dept. UCL	Hidro Energía S.A.	M.S. University of Baroda	Simultec AG	University of Pennsylvania
Chinese Academy of Sciences	HIsmelt Corporation	Michigan Technological University	SINTEF Materials Technology	University of São Paulo
Chulalongkorn University - Bangkok	Hitachi-Metals	MillenuimChemicals	St. Mary's University	University of Saskatchewan
CIMAV, Mexico	Hydril	Multiphase flow LAB	STAE	University of Stuttgart
Coal Chemistry Institute, China	ICT Prague	National Academy of Sciences of Belarus	Stanford	University of Washington
Coanda Research and Development Corporation	Idaho National Engineering & Environmental Laboratory	National Chemical Laboratory	Stress Engineering Services	UOP
Colorado School of Mines	Idemitu Petrochemical Co. LTD - Japan	National Environmental Engineering Research Institute	Tata Research Development	US Steel
Comarray Corporation	Imperial College London	National Institute of Technology Durgapur	Telemark University College	UWS
Computational Dynamics Limited	Indian Aluminium Company	National Research Council of Canada	Texas A&M University	VSB - TU Ostrava
Consiglio Nazionale delle Ricerche	Indian Institute of Technology, Bombay	NCL	TFL	West Virginia University
Dalhousie University - Canada	Indian Institute of Technology, Delhi	NERC	The Energy Institute, PSU	Western Kentucky University
DCCC	Indian Institute of Technology, Delhi	NETL	The University of Akron	Westinghouse Savannah River Tech. Center
Delft University of Technology	Indian Institute of Technology, Guwahati	North Carolina State University	The University of Hong Kong	Widener University, PA
DMT	Indian Institute of Technology, Kharagpur	NOVA Chemicals	The University of Tennessee	Wroclaw University of Technology
Dow Chemical	Inst of Engg Thermo.	ORISE/Princeton	TSNIGRI, Russia	Zhejiang University
East China Univ of Sci & Tech	Instituto de Investigaciones Electricas	ORNL	Tulane University	Zurich University of Applied Sciences
Ecole Central De Lyon	Instituto Mexicano del Petroleo	Osaka University	UFSCar	

Table 1: Affiliations of researchers who have downloaded MFIX code from http://www.mfix.org.

In addition, the website is highly visited with average hits of around 5000 page visits every month as shown in the Fig. 12.

Figure 12: Page visit statistics of MFIX website at http://www.mfix.org.

A new version of MFIX (2004-3) has also been tested and released with the following changes:

Changes from MFIX2003-3 to MFIX2004-3 (Date: 07/08/03)

- k-ε turbulence model for gas-phase (check the turbulent_pipe_flow case in tests).
- Capability to specify fluid mass-flux for periodic cases (check the periodic-flow-fixed-mass-flux case in tests).
- Discrete element simulation (DES) capability; i.e, track particle motion and collisions instead treating particles as a continuum - currently works only in the serial mode (check fluidbed_des in tutorials and Driven_Cavity_DES & kink_DES under tests).
- Chi-scheme for ensuring that the species mass fractions add up to one when flux limiters are used.
- More accurate formulas for D_0 and D_s have been implemented by S. Dartevelle from LANL (Model A and Model B.)
- Updated animate-mfix (to handle new changes and also plot k & eps) is available to download from the MFIX website. Previous versions are archived.
- A new and improved version 1.4 of MAVIS (3D Visualization tool for MFIX) is available and can be downloaded from http://www.psc.edu/~eschenbe.
- A new converter to translate MFIX data to VTK is available from the download site (thanks mainly to Jim Canon at WVU and Brian Dotson at NETL).
- Benchmarked and documented MFIX for all the tests and tutorials on Linux (Look at tests/MFIX_Tests_Benchmarking.html & tutorials/MFIX_Tutorials_Benchmarking.html).
- Many bug-fixes - visit http://www.mfix.org/cgi-bin/cvsweb.cgi/mfix/model/?sortby=date#dirlist.
- Added/modified some test cases and tutorial cases.
- Updated Readme's in the pdf and html formats in root directory.
- Makefile modified to support Intel's ifort 8.0 compiler.
- Scripts and changes to aid easy compilation with windows visual fortran compiler.

The above efforts will be continued into next year. In addition, implementation of various SciDAC (DOE Office of Science's Scientific Discovery through Advanced Computing) developed tools for improved efficiency of MFIX would be explored.

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Zhou, J., J. R. Grace, S. Qin, C. J. Lim and C. M. H. Brereton, Particle velocity profiles in a circulating fluidized bed riser of square cross-section, Chem. Engg. Science, 49, pp. 3217-3226, 1994b.