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. 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 [read more]. On the other hand a Dynamic Interacting Bubble Simulations (DIBS) is being further developed at ORNL with the eventual aim of real time diagnosis and control of industrial scale fluidized beds [read more].

MFIX (Multiphase Flow with Interphase eXchanges) 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. 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 computational tool through development of a fast, parallel MFIX code, (2) Develop infrastructure for easy collaborative development of the MFIX code and exchange of information between the developers and users and (3) Experimental validation (to insure that the basic physical models in MFIX are correct). Progress has been made in all three fronts during this year. A newly designed website (http://www.mfix.org) is available with tools like open citation index specifically designed to have a common resource for all the multiphase flow literature at one place. The parallel code has been tested for hybrid (mixed DMP/SMP) parallelization and presented at the ACM SAC meeting and a sample result is shown in Fig. 1. Validation of a large-scale (9m high) fluidized bed and also with various experimental configurations is underway.

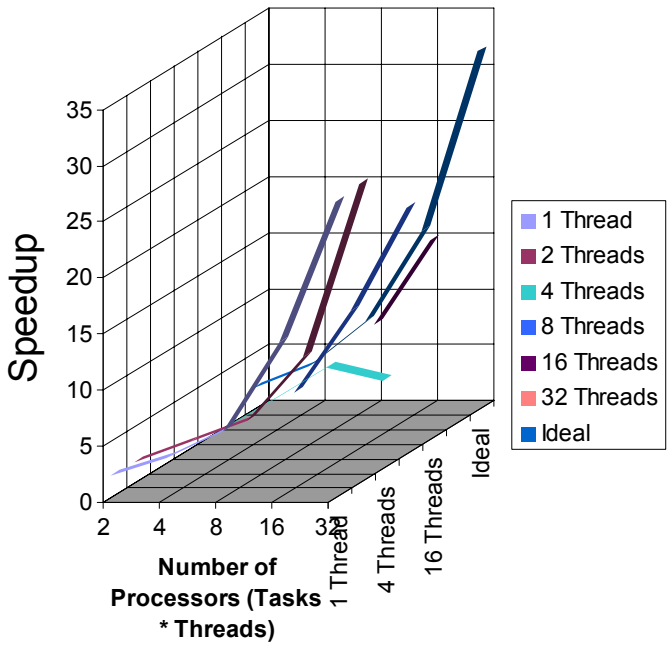

Figure 1: Hybrid Parallel performance with line relaxation as the preconditioner on the ORNL teraflop IBM machine, CHEETAH.

DIBS, a dynamical rules based model for bubble behavior in fluidized beds was developed by Daw and Halow based on experimental observations of bubble interactions. This model has been extended to include chemical reactions and the ozone conversion in a fluidized bed reactor is extensively studied. The model runs real-time and has very good prediction capability as seen in Fig. 2. Currently work is being carried out to directly include the effects of emulsion in the model.

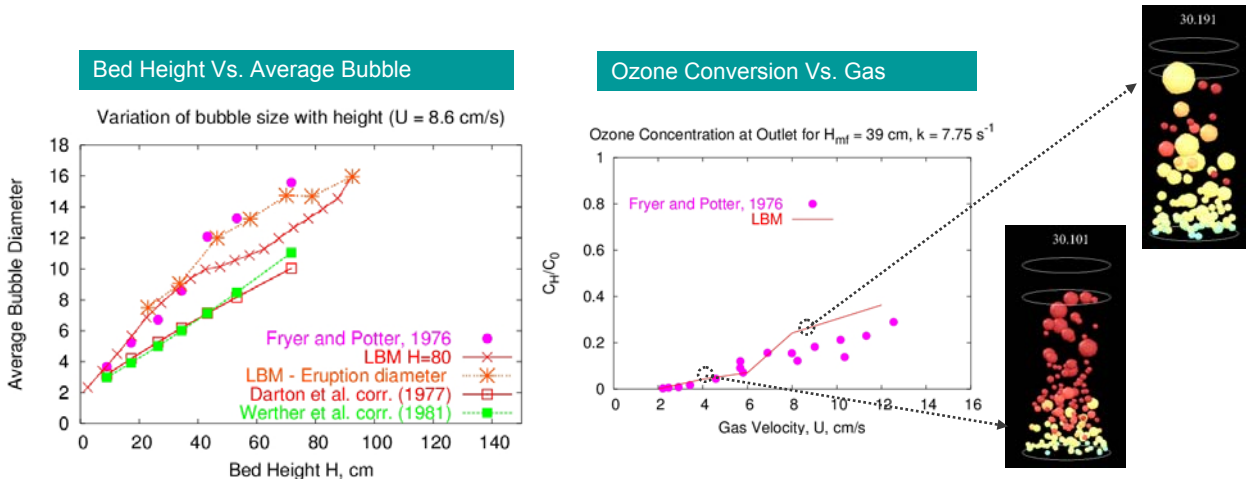

Figure 1: Validation of DIBS model for ozone conversion hydrodynamics and chemistry.