Project Title: EPIC - Modeling of Multiphase Flows

HPC machine: SuperMike2

SU's being requested: 250,000

1 Technical Merit

1.1 Background, problem statements, methodology

My research group in the Department of Chemical Engineering consists of 6 PhD students and 2 Post-doctoral fellows. The research group members are as follows:

PhD students	Postdocs
Omitted	

The research area is "Multiphase Computational Fluid Dynamics". The applications are strongly applied to chemical and energy industry. We call our effort EPIC- Enabling Process Innovation through Computation. We develop our own algorithms (CFD-DEM – Discrete Element Modelling and IBM-Immersed Boundary Method) as well as use commercially available software (STAR CCM+, FLUENT, COMSOL) and open source software (OpenFOAM) for fluid dynamics modelling. Our computational needs to understand and improve the multiphase flow models in service of design innovations in process industries are significant. Process modelling is important to the State of Louisiana since there are over 300 chemical plant, processing fuels and chemicals. Four specific projects are described below in this proposal.

Our research group engages in computational research dealing with understanding multiphase flows and through which to enable process innovation in the chemical manufacturing industry. Currently we have 12 different projects being studied by members of group some times in collaboration with international research groups in India and China. Here we describe the technical merits of four project ideas in some detail.

Conventional flow distributors using pressure-based or trough type designs are confronting challenges as the low outlet densities and poor flow distribution limit their performances. In recent years, fractal distributors have been attracting interests extensively from both academia and industry. The inherent symmetry in their geometries allow fractal distributors to scale to any dimension and have high outlet density and consequently uniform flow distributions.

In our study, we have fabricated fractal distributors of 12"x12" with up to 256 outlets in a fractal configuration and tested their performance based on a filter press-based ion exchangers devices. It is always highly desired in the industry to gain the insight of flow profile inside chemical equipment. While, such data almost impossible to obtain on site, Computational Fluid Dynamics (CFD) can be extremely useful in this scenario. The fractal distributor with 256 outlets have been tested with CFD simulations. From CFD results, we can be able to understand the flow distribution inside resin as the flow passes through it. The resin volume swept by fluid is an important indication the effectiveness of resin usage and our goal is to minimize the "deadspace".

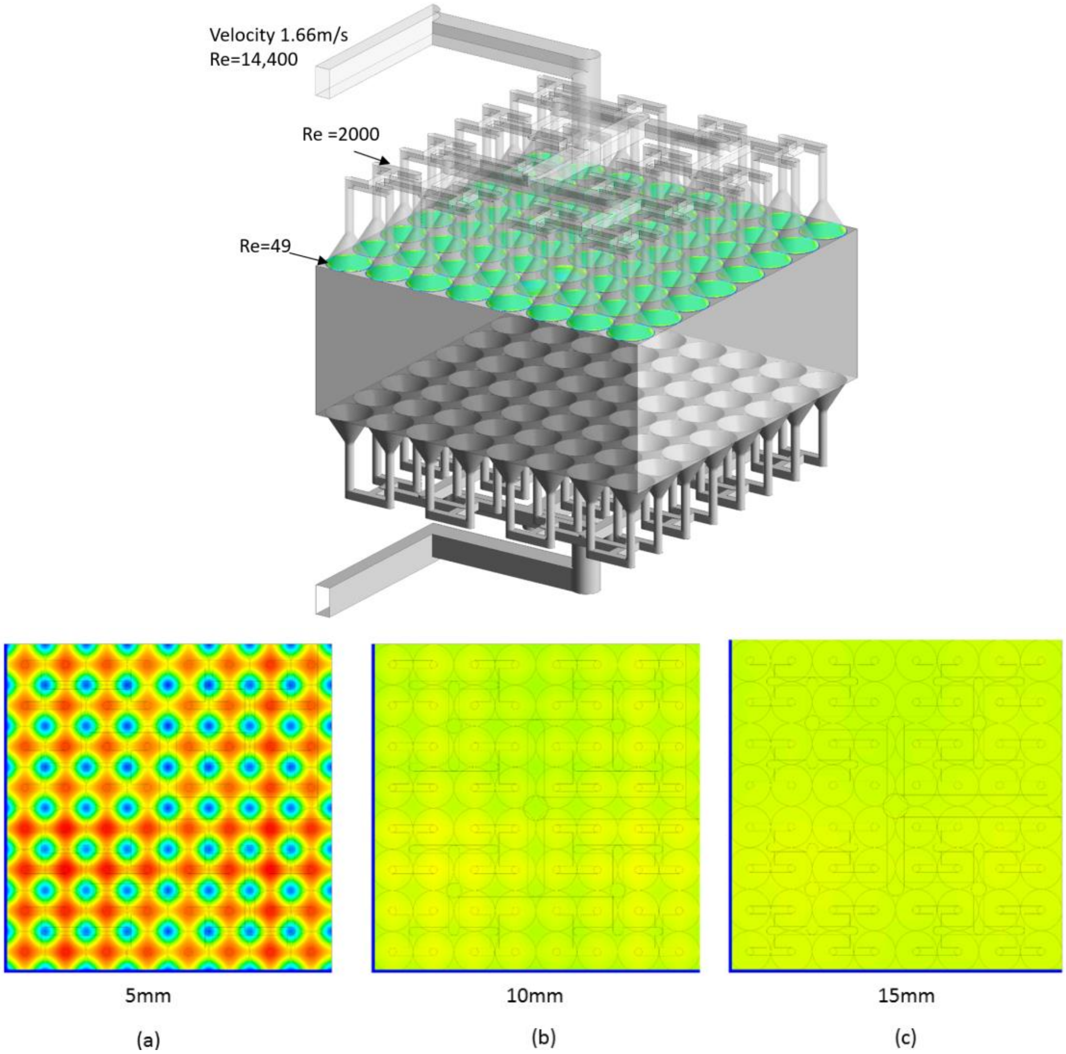

Figure 1 shows the pattern of vertical velocity plot inside resin at 5, 10 and 15 mm plane respectively.

For fluid flow, K-epsilon equations have been used

$$\rho \frac{\partial}{\partial x_j} k u_j = \frac{\partial}{\partial x_j}\left[\left(\mu + \frac{\mu_t}{\sigma_k}\right)\frac{\partial}{\partial x_j} k\right] + G_k + G_b - \rho\varepsilon$$

$$\rho \frac{\partial}{\partial x_j} \varepsilon u_j = \frac{\partial}{\partial x_j}\left[\left(\mu + \frac{\mu_t}{\sigma_\varepsilon}\right)\frac{\partial}{\partial x_j} \varepsilon\right] + \rho C_1 S\varepsilon - \rho C_2 \frac{\varepsilon^2}{k+\sqrt{v\varepsilon}} + C_{1\varepsilon}\frac{\varepsilon}{k} C_{3\varepsilon} G_b$$

and the turbulent viscosity μ_t is computed by

$$\mu_t = \rho C_\mu k^2/\varepsilon$$

In order to quantify the malfunctioning operations, the volumetric percentages of the dead space and channeling zones were estimated based on the modelling results The dead space is defined as the region where the velocity magnitude of the process stream is 2.5% below the superficial velocity. In contrast, "channeling" refers to the phenomenon that fluid passes through bed prematurely with a much shorter residence time. A zone with the fluid velocity that is 2.5% over the superficial one is defined as "channeling" zones. The degree of heterogeneity is defined as the sum of dead space percentage and channeling zone percentage.

1.2 Immersed Boundary with Heat Transfer - in house IBM Code

Our first goal is to reproduce the granular jet experiment numerically. In the figure below, A and B are void collapse experiment. The goal is to check the dependence of system behavior—like how much it is fluidized by the bubble motion—on particle size. C and D remove the void and introduce the large object (it is not visible as shown are volume fraction of small particles). The object size determines the amount of energy it imparts into the small particles and this would vary the system qualitatively. We will test with different object size, impact velocity, physical parameters of the small particles, and different fluid density/viscosity.

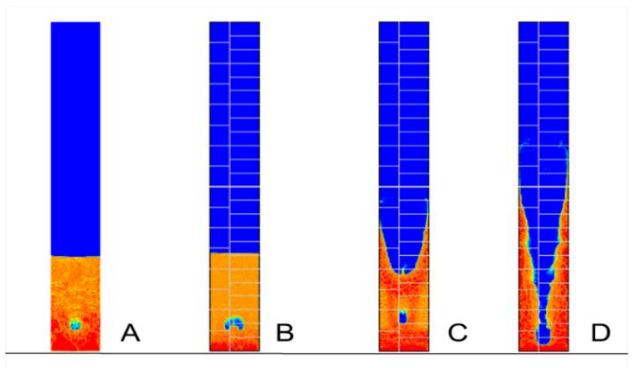

Figure 2 Volume fraction field of quasi-two dimensional IBM-DPM simulations. A and B are void collapse experiment to check the dependence of system dynamics on particle size. C and D are snapshots sometime after a static particle pile is impacted.

1.3 Software scaling

Majority of our simulations are of engineering research in nature done under the EPIC umbrella to explore Enabling Process Innovation through Computations. A subset of our work using OpenFOAM focuses on code development to implement new features such as immersed boundary methods and Discrete Particle Modelling. Even in this case, the base code is an open source code that has been validated for its parallelization capabilities. The other codes such as COMSOL, FLUENT are commercial codes that are well parallelized. Through experience, we have learned how to optimize the use of resources for maximum impact. Depending on the size of the problem (a large scale reactor with 20 million grids for example) we have used as many as 400 processors over several months to study the slugging phenomena in polymer loop reactor, which the company supporting the work finds insightful as they do not have such facility to carry out detailed simulations.

As an example of the scalability of our applications we show results in Figure 3. The case involves simulation of a bubble column diameter of 150 mm and total height 1000 mm. Superficial gas velocity is ~20 mm/s. The flow time is 47.5 seconds assuming final dispersion height of 950 mm. The average mesh cell size is 3 mm. The total number of cells is 520,908. Very satisfactory scale up is obtained using our applications.

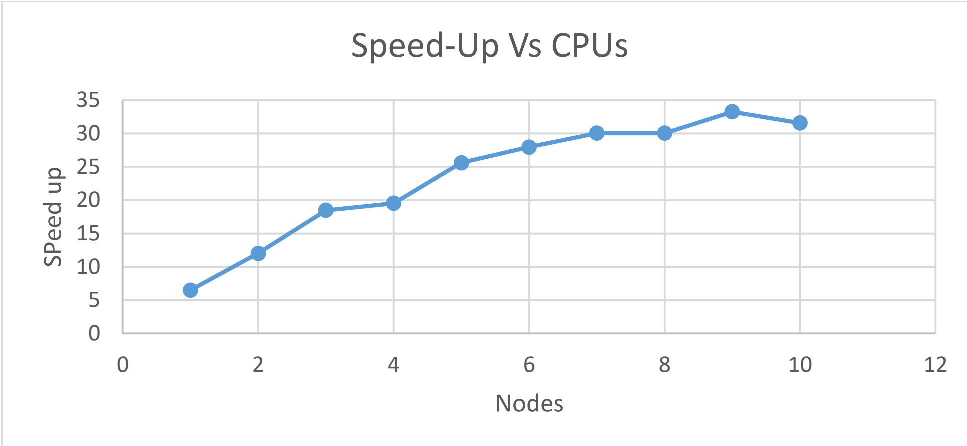

Figure 3 Scale-up of bubble column simulation

1.4 Research schedule

The detailed estimates of SU need for the calendar year (**Jan 2018–Dec 2018**) on SuperMike2 is shown in below. Number of planned simulation per month are listed for each of the four projects.

Simulation Cases per month	**Jan – Dec 2018**
Immersed Boundary simulations (each simulation runs for 7 days on 32 nodes)	2 simulations/month @32 nodes 7days/simulation*24 SU's = 10752 SU/month
Study of granular self-organization in an orbital driven cylinder (each simulation runs for 2 days on 16 nodes).	10 simulations/month @16 nodes 2days/simulation*24 SU's = 7680 SU/month
SU's expected to consumed per month	18, 432 SU per month

Total SU's requested on mike 2 for a total of four projects described here for calendar year Jan-Dec 2018 are 18, 432 x 12 = 221, 184 SUs.