Team of Energy Minimization Multi-Scale Model (The EMMS Group)
Brief Introduction

The research on the Energy Minimization Multi-Scale (EMMS) model for gas-solid fluidization started at almost three decades ago by Prof. Jinghai Li, mentored by Prof. Mooson Kwauk. That gives birth to the Group and its name. To verify its stability condition, The Pseudo-Particle Modeling (PPM) was proposed to investigate the dominant mechanisms inherent in multiphase flow systems. By combining the EMMS drag model and computational fluid dynamics (CFD), the multi-scale CFD method was developed to improve the accuracy and efficiency of the simulation for multiphase systems. Now the EMMS Group is devoted to the study of meso-scale modeling for multiphase complex systems and its applications in process engineering. It has established far-reaching, global links in these fields and is becoming an interdisciplinary research hub.

Research Activities

The researches in the EMMS Group have now covered fundamentals, technological platforms and industrial applications. Thanks to the constant support of NSFC, MOST and CAS etc., the group has been extending and deepening their studies on the EMMS model continuously to new systems including gas-liquid flow, granular flow, emulsion systems etc., all of which are formulated as a Multi-Objective Variational (MOV) problem. Along with these developments, the Group gradually recognized that meso-scales, the scales between the elements and systems on a certain level, are the core of multiscale problems universally encountered in industries and nature. The meso-science is hence proposed due to its universality and importance, which is now the focus of the fundamental research of the EMMS Group. The major NSFC plan on meso-science entitled "Mechanism and manipulation of meso-scales in multi-phase reaction processes", which is also the first program in the world on the meso-science, has been initiated by the EMMS Group.

Along with the theoretical developments, the EMMS model, PPM and CFD capabilities were thus established, leading to the EMMS Paradigm characterized by the structural consistency among the problems, models, software and hardware to achieve high accuracy, capacity and efficiency (ACE) for simulation of multiphase systems. In order to implement the EMMS Paradigm in industrial practice, a multi-scale parallel computing system was developed. This system paved the way to Virtual Process Engineering (VPE) – realtime simulation of industrial multiphase systems with high accuracy and online integration of measurement and control systems.

With these capabilities, the EMMS Group has established close collaborations with world-renowned enterprises including Alstom, Baosteel, BASF, BHPb, BP, EDF, GE, Intel, Lenovo, NVIDIA, PetroChina, Shell, Shenhua, SinoPec, Total, Unilever etc. That benefits the Group in both fundamental studies and technological development.
1. The Mole-8.5 Supercomputing System

Built in April 2010, this GPU-based supercomputing system, boasts a peak performance of 1.1PetaFlops in double precision (DP). It was ever ranked 19th in Top500 and 8th in Green500 lists. Focusing on multi-scale simulation, it is one of the most energy-efficient high performance computing (HPC) systems in the world.

2. Virtual Process Engineering Platform

Constructed in Oct. 2011, the first Virtual Process Engineering platform (VPE1.0) aims to realize multi-scale simulation of chemical reactors in real-time. This platform consists of four subsystems: experiment & measurement, control & data acquisition, HPC, and visualization. VPE 1.0 allows digital control of both real equipment operation and virtual state simulation synchronously, together with real-time and high-precision measurement and 3D visualization of flow and transport processes in multi-phase complex systems.

3. The ETH-IPE CFB Platform

Originally built in ETH Zurich and upgraded by the EMMS Group in 2002, it consists of a CFB riser unit (10800*411mm ID) and a downer unit (326mm ID). Equipped with in-house developed techniques, this platform serves as a powerful tool for the validation of simulation results. The CFB unit is equipped with more than 80 conventional pressure, pressure difference, temperature, flowrate and power measurement sensors and 8 automatic control loops. These facilities have been operated for approximately 8000 hours. With the use of innovative instruments, mostly developed in-house, including laser optical fiber probes, mechanical probes with piezo-electrical pressure sensors, X-ray computed tomography, etc., fundamental and application-oriented studies have been carried out on fluid dynamics, heat and mass transfer in CFB, etc. Culminating in a comprehensive experimental CFB database, it has already in use at several recognized
research groups such as EDF (Paris), IFP (Solaize), ABB Alstom Power (Paris), Lurgi (Frankfurt), Von Roll (Zurich), Swiss Calculation Center (Manno), Los Alamos National Laboratories (Los Alamos, NM) and inside IPE.

**Research Progress**

1. **EMMS-based continuum model**

According to the EMMS model, all complex systems consist of $n$ states alternately prevailing in the systems with respect to time and space, each of which corresponds to a dominant mechanism. The compromise between these states can be formulated as the compromise between corresponding dominant mechanisms. A “fluid” in continuum model for complex systems can then be defined as the physical realization of one dominant mechanism, and the interaction between “fluids” is constrained by dominant mechanisms and quantified by the EMMS model. This allows the description of each “fluid” and the coupling between “fluids” to be simplified because the underlying mechanisms involved are already considered in defining the “fluid”.

2. **Supercomputing and Virtual Process Engineering in the EMMS Paradigm**

To materialize the EMMS Paradigm, a multi-scale supercomputing system (Mole-8.5) reaching 1.1PetaFlops peak performance was established accordingly (Ge et al., 2011. *Chem. Eng. Sci.* 66:4426-4458; Fig.5), which powers the VPE platform, as shown in Figs. The supercomputing system and VPE platform can serve as a versatile industrial R&D and training facility (Liu et al., 2012. *Chem. Eng. Prog.* 108:28-33) and has already enabled a wide range of fundamental studies and industrial collaborations.

3. **Gas-liquid system**

Bubble columns are considered as favorable reactors in process engineering. Simulation based on Eulerian-Eulerian method, though usually employed in commercial CFD packages, is still not powerful enough to capture real physics due to our limited understanding on the multi-scale flow structure (Fig.6) and hence inadequate development of closure laws.
including drag and turbulence models. The EMMS model developed for gas-liquid flow was used as a closure law for the effective drag coefficient on bubbles in the simulation of gas-liquid flow. In addition to mass and momentum conservation equations, the stability condition reflecting the compromise between two different dominant mechanisms serves as another constraint for the model, and therefore it is expected to offer a more accurate drag closure for CFD simulation. The new model can well predict the radial gas holdup distribution, the total gas holdup as well as the two-phase flow field without the need of adjusting model parameters. The model was also integrated into the two-phase turbulence model and population balance model for bubble breakup and coalescence recently, showing the great potential and advantage in understanding the complex nature of multi-scale structure of gas-liquid flow in bubble column reactors (Yang et al. 2011. Chem. Eng. Sci. 66:3212-3222; Xiao et al. 2013. Chem. Eng. Sci. 100:279-292).

4. Turbulence

Traditional turbulence models still suffer from empirism and hence low accuracy. Recently, an EMMS-based meso-scale turbulence model was proposed. A turbulence stability condition, similar to that in the EMMS model for gas-solid systems, is formulated to close the dynamic equations of turbulence, allowing the inhomogeneous structural parameters of turbulence to be optimized (Zhang et al. 2014. Particuology 16:142–154). The model reproduced successfully the lid-driven cavity flow at $Re=10000$, while the standard $k$ model, assuming the whole fluid in the cavity in turbulent state, fails to predict the tertiary vortices in the lower left and right corners (Fig. 7), as near the walls and corners, the viscosity effect dominates rather than the inertia effect, so the fluid should be close to laminar flow instead of fully turbulent flow. The EMMS-based turbulence model can treat it well since the coexistence of laminar and turbulent flow are assumed anywhere. Future development of the model is expected to describe more complicated turbulent flows.

5. Protein folding and material preparation

We propose a multi-scale simulation method to study protein folding (Fig. 8). First, we use genetic algorithms (GA) to determine the key protein structures from a global view. Then, we employ molecular dynamic (MD) simulations to reveal the local folding pathways, thus providing an integrated landscape of protein folding. Our multi-scale simulations of a peptide RN24 show that the multiple characteristic states of a protein are dominated by multiple mechanisms and the state corresponding to minimum free energy is one of these characteristic states (Xu et al. 2013. J. Biomol. Struct. & Dyn. 31:779-787). The formation of material is a complex process influenced by many factors including temperature, concentration and so on. However, according to the EMMS model and the principle of compromise, these factors are only the superficial parameters and the real players are the...
competition of dominant mechanisms. Diffusion and reaction are identified as such mechanisms, both affected by the superficial factors. By tuning the diffusion and reaction rates of reactive ions, snow-flake-shaped calcium carbonate particles were first obtained in both experiments and simulation (Fig. 9) (Wang et al. 2013. *Cryst. Growth Des.* 13:1820-1825; Wang et al. 2013. *Particuology* 11:301-308), which are believed to be the result of the compromise between the diffusion and reaction. Future discovery and generality of the compromise effect in shaping materials will probably leads to a rational synthesis of materials.

6. Portable Computed Tomography

The newly developed portable Computed Tomography Fig. 10 is powered by lithium polymer battery and controlled via WIFI signal. Equipped with multi-piece translation gantry, the PCT scanner can be easily dismantled into several parts and put into a roller luggage. The portability feature makes this scanner qualified for filed and outdoor measurement. Since the development of PCT, we have offered services to several customers, including BUCT, CUMT, Great Wall Volkswagen and Total.

![Portable computed tomography scanner](image)

**Selected Publications and Achievements**

The Group now has more than 70 members, including 6 full professors, 17 associate professors, 7 assistant professors and 29 graduate students.

**Prof. Jinghai Li (Group Leader),** graduated from the Department of Thermal Engineering of the Harbin Institute of Technology in 1982. He entered a master's degree program at his alma mater in the same year. He obtained his Ph.D. from the CAS Institute of Process Engineering (IPE), in Beijing in 1987. He conducted his post-doctoral research at the City University of New York and the Swiss Federal Institute of Technology. After returning to China in 1990, he served as assistant professor, associate professor, professor, vice director and director of IPE in succession. In February 2004, he was appointed a vice president of CAS.

Prof. Li established the Energy-Minimization Multi-Scale (EMMS) model for gas-solid systems. The model has been extended to many different complex systems, and generalized into the EMMS paradigm of computation featuring the structural similarity between problem, modeling, software and hardware, which has been implemented by constructing a supercomputer with capacity of 1 Pflops and has been used widely in chemical and energy industries. He is also engaged research in clean coal technology. Currently, he is devoted to promoting the concept of mesoscience based on the EMMS principle of compromise in competition as an interdisciplinary science.

He is vice president of International Council for Science (ICSU) for Scientific Planning and Review, the vice chairman of China Association of Science and Technology, the vice president of the Society of Energy Research. He sits on editorial committees or international advisory boards for several international periodicals, such as Powder Technology, Advances in Chemical Engineering, Chemical Engineering Science, Reviews in Chemical Engineering, and Granular Matter. He is editor in chief of *Particuology*. He holds memberships from CAS (Chinese Academy of Sciences), TWAS (The Academy of Sciences for the Developing World) and SATW (Swiss Academy of Engineering), The Royal Academy of Engineering (RAEng), Australian Academy of Technological Sciences and Engineering (ATSE).

He received a variety of prizes and honors, both national and international, including Particle Technology Forum Award from AIChE(2010), Medal Lecture Award from the TWAS (2012), Hongkong Qiushi Young Scientist Prize (1996), two National Natural Science Awards (1989, 1995) and Young Scientist Prize(1996) in China, a Technology Innovation Prize from CAS (2001).
Prof. Li Guo was born in 1966. He graduated from University of Science and Technology of China in 1981 and received his M.S. degree in computer application from IPE, CAS in 1989. He has been a professor of IPE since 1997. He was awarded the 2nd Prize (1994) and 3rd Prize (1992) of Scientific & Technology Advancement, Chinese Academy of Sciences, and the 3rd Prize of Beijing Scientific & Technology (2007). He has published 90 papers, 2 monographs and 1 co-authored monograph. He has held 5 patents and had 12 computer software copyright registrations.

Research Interests
High performance computing; Virtual process engineering; Computer software development; Chemistry information system; Computer control system.

Prof. Wei Ge got his Ph.D from Harbin Institute of Technology in 1998 and has been professor of chemical engineering at Institute of Process Engineering, CAS since 2006. He is mainly engaged in multi-scale simulation of particle-fluid two-phase systems. He further developed the Energy-Minimization Multi-Scale (EMMS) model proposed by Li and Kwauk (1987) for gas-solid flow and explained the controversial “choking” phenomenon in fluidization as a bi-stable state. He also proposed the so-called pseudo-particle modeling which enables simulation of macro-scale flow phenomena from microscopic physics through large-scale parallel computation. With this approach he studied statistical properties of gas-solid flow and verified the stability condition employed in the EMMS model. As project leader, he developed the multi-scale supercomputing system, Mole-8.5, to bridge simulation of molecular details to reactor performance.

He is author of over 130 journal papers and 5 monographs. He won the Excellent Doctor Dissertation Award of Harbin Institute of Technology in 2001, the Outstanding Youth in Basic Science Award of Zhou Guangzhao Foundation in 2008, the P&G Outstanding Youth Award in Particuology of Chinese Society of Particuology in 2011 and the National Science Fund for Distinguished Young Scholars in 2012.

Affiliation
Associate editor, Chemical Engineering Science (2012–)
Council member of the Chinese Society of Particuology (2002–)
Editorial board member of Particuology (2005–)
Principal investigator, CUDA Center of Excellence, NVIDIA (2009–)

Research Interests
Particle methods for the simulation of multiphase systems; Multi-scale analysis and non-equilibrium statistical mechanics of complex flows in chemical engineering; Software platform and system architecture for massive parallel processing of discrete dynamics systems.
Prof. Wei Wang was born in 1973 and received his Ph.D. degree in Chemical Engineering from Institute of Process Engineering (IPE), Chinese Academy of Sciences in 2001. He has been a professor of IPE since 2008. He was awarded the Chemical Engineering Science Most Cited Authors Award (2012), MIC-Particuology Excellent Article Award (2012) and Lu Jia-xi Young Scholar Award (2008). He has published over 40 papers, 1 co-authored monograph and 5 book chapters and held 6 patents.

Affiliation
International Advisory Board, the International Conferences on Fluidized Bed Technology (2014–)
Youth council member of the Chinese Society of Particuology (2012–)
Member of Youth Innovation Promotion Association, CAS (2011–)

Research Interests
Multiphase flow, mass transfer and reaction; Multiscale CFD modeling; Industrial reactor simulation; CT technology.

Prof. Xiaoxia Li was born in 1964. She received her B.S. of chemical engineering from Tsinghua University in 1985 and M.S. of computer chemistry from Chinese Academy of Sciences in 1988. She joined Institute of Process Engineering (IPE, formerly Institute of Chemical Metallurgy), Chinese Academy of Sciences since 1988. She was an associate professor of IPE in 1996 - 2005 and has been a professor of IPE since 2006. She was awarded the 1st and 3rd Prize of Scientific & Technology Advancement, Chinese Academy of Sciences, and the 3rd Prize of Beijing Scientific & Technology. She has published over 60 scientific papers and authored a book of 'The Chemical Resources on Internet' in 2000 by Science Press, Beijing and reprinted in 2002 for its popularity, also coauthored another three books and one book chapter, and has 7 computer software copyright registered.

Affiliation
Trustee, Chemical Structure Association Trust (2003–)
Project Director, Asian Chemical Information Network, Federation of Asian Chemical Societies (1999–)
Vice Chairman, Committee of Computer Chemistry, Chinese Chemical Society (2000–)
EXCO member, Chinese National Council for CODATA (2008–)
Member, Women Chemist Council, Chinese Chemical Society (2013–)

Research Interests
Reactive molecular dynamics; Coal pyrolysis mechanisms; Chemical structure processing; Chemistry Web search engines; Chemical databases; High performance computing in chemoinformatics.
Prof. Ning Yang graduated in 1996 with a B.S. degree at Taiyuan University of Science and Technology and a M.S. degree in mineral processing in 1999 at China University of Mining and Technology, and then acquired a Ph.D at CAS Institute of Process Engineering in 2003, developing the EMMS drag model to improve the CFD simulation of fluidization. He worked in the Institute of Fluid Mechanics of Toulouse in France (CNRS/IMFT) as a postdoctoral fellow (2004.10-2006.2), and Oak Ridge National Laboratory (US-DOE) as an advanced visiting scholar (2013.12-2014.3). He obtained the Excellent Young Scientist Fund from National Natural Science Foundation of China (NSFC) in 2012 and Qiushi Outstanding Youth Award for Science and Technology Achievements Transformation (China Association for Science and Technology).

Affiliation
Member of Youth Council of China Society of Particuology (CSP) (2012.3–)
Member of American Institute of Chemical Engineers (2012.1–)
Scientific Advising Committee member, International Conference on Gas-liquid and Gas-liquid–solid Reactor Engineering

Research Interests
Multiscale computational fluid dynamic simulation and its industrial application; Meso-structures in gas-liquid and gas-liquid-solid multiphase reactor systems.

Prof. Yongsheng Han studied chemistry for 7 years from 1993 to 2000 in Changchun University and Science and Technology and Jilin University, respectively, for his bachelor and master degrees. After that, he moved to Tsinghua University where he was conferred doctor degree in the field of materials science and engineering in 2004 under the supervision of Prof. Jianbao Li. Immediately after his graduation, he went to Japan, Nagoya Institute of Technology and worked there as a postdoctoral researcher for more than 3 years under the supervision and collaboration with Prof. Minoru Takahashi and Prof. Masayoshi Fuji. In 2007, he was awarded Alexander von Humboldt fellowship and went to Germany, Max Planck Institute of Colloids and Interfaces, Golm where he worked with Prof. Helmhut Möhwald and Dr. Dmitry Shchukin. In 2011, he succeeded in the application of Hundreds Talent Program from Chinese Academy of Science (CAS) and joined in the Institute of Process Engineering, CAS in the group of EMMS. He has published 61 peer-reviewed papers and 4 patents. His papers have been positively cited nearly 500 times by other researchers. Besides, he is serving as Editorial Board of Journal of Encapsulation and Adsorption Sciences, Materials Science, Journal of Materials Science and Chemical Engineering, and Journal of Nanotechnology and Smart Materials.

Affiliation
Editorial Board of Journal of Encapsulation and Adsorption Sciences (2011–)
Editorial Board of Materials Science (2011 –)
Editorial Board of Journal of Materials Science and Chemical Engineering (2013–)
Editorial Board of Journal of Nanotechnology and Smart Materials(2014–)

Research Interests
The controlled synthesis of functional materials via diffusion and reaction.
Prof. Junwu Wang, obtained his Bachelor's degree, Master's degree and Ph.D, all in Chemical Engineering, from Zhejiang University of Technology (2000), Tianjin University (2003) and IPE, CAS (2008), respectively. From Feb, 2008 to July, 2010, he was a postdoctoral fellow working with Prof. J.A.M Kuipers at the University of Twente, The Netherlands. He was a recipient of the “Hundred Talents Program” awarded by IPE, CAS (2010) and member of Youth Innovation Promotion Association, CAS (2011). He has authored more than 50 publications and patents.

Affiliation
Editorial board of *Mathematical Problems in Engineering* (2014–)
Editorial board of *Advance in Mechanical Engineering* (2013–)
Editorial Board of *International Journal of Chemical Engineering* (2014 –)
Editorial Board of *International Journal of Mechanics* (2013–)
Editorial Board of *Journal of Powder Technology* (2012–)

Research Interests
Fluidization technology; Multiphase flow; Computational fluid dynamics; Continuum mechanics and mesoscience.