M3TC: Selected Projects in Mathematical Modeling of Industrial Processing in the Minerals, Metals and Materials Sector

The following list of projects is for illustrative purposes to demonstrate the capability in computational modeling of processes of industrial interest. The objectives of the Mathematical Modeling Group of M3TC headed by Professor A.S. Mujumdar (ESP/ME, NUS) is being formed to help improve the efficiency and cost-effectiveness of industrial processing. Such models ,once validated, can be used for optimization as well as model-based control of processes. Also they can be used to intensify innovation, evaluate totally new concepts, improve energy efficiency, safety of operation and reduce environmental impact. All this can be achieved at considerably reduced cost and in a shorter timeframe.

Current Projects:

1. CFD model of a lost foam casting process

- The application of Lost Foam Casting (LFC) is increasing worldwide as it can make complex shaped castings in one step and requires no sand binders resulting in cost savings and less environmental problems. However, LFC casting is a much more complicated process in both physical and chemical aspects than traditional investment and sand mold casting. Many physical processes, such as heat and mass transfer, fluid flow, chemical reaction, solidification, etc are involved in this casting technique. In this investigation, a computational fluid dynamics model was developed to simulated the fluid flow of liquid metal and heat transfer involved at the melt/foam interface (Gap) resulting from foam degradation during mould filling in the LFC process. A parametric study will be also carried out to study the influence of the operation conditions such as metal species, liquid metal temperature, filling pressure, EPS foam properties etc on the quality of the casting product and energy savings. Such investigation contributes to a better understanding the mould filling process and an optimal process parameter design.

2. A computational study of No_x and noise production in a pulse combustor

- NO_x emission from a premixed Hemolthz type pulse combustors is investigated numerically. Computed NO_x concentrations are compared with published experimental measurements. Generation and propagation of sound waves in the combustor will be simulated using the Broadband Noise Source models. Gas pressure oscillation in the combustion chamber is monitored and analyzed using the Fast Fourier Transform (FFT) to obtain the overall sound pressure level and power spectra. Noise sources are identified and possible noise reduction methods are discussed. Parametric studies were also carried out for a range of pulse frequencies and fuel/air ratios.

3. Multiphysics Model to Microwave Sintering of Metals

- Microwave heating and sintering of various materials has been widely studied and applied in different industrial applications. Compared to conventional furnaces where heating is via convection, a microwave furnace provides more rapid and efficient way of heating volumetrically and sintering. Furthermore, rapid heating limits grain growth during sintering and thus helps improve the microstructure and mechanical properties of the sintered products. However, there has been little study of microwave sintering of metals and alloys considering that the metallic materials reflect microwave. Furthermore, the mechanism is still not well understood, especially regarding the effects of the magnetic field of the electromagnetic wave. In this study, a multi-physics model was tested to simulate the sintering process of metals by adding the magnetic and electric field contributions into the heating source. Results show that the magnetic field plays important role in the sintering, especially for ferromagnetic materials. Comparison between our simulation and the published experimental data will be conducted as well. It should be possible to use magnetic fields to control the sintering process.

Industry and academic institutions are invited to contact Professor Mujumdar at mpeasm@nus.edu.sg for details.

Potential Projects:

1. Simulation of Post combustion in the electrical Arc furnace

- In the state-of-the-art electric arc furnace (EAF) - flat-rolled steelmaking plant, about 1.5 kmol of CO is generated per ton of steel, which if combusted to CO2, represents 425 MJ of energy recovery. The potential use of this energy and the corresponding increase in productivity is the economic driving force behind post combustion (PC) technologies. The current work is carried out to develop a comprehensive model for the PC process in the EAF. The model includes fluid flow, combustion reactions, de-combustion reactions, as well as radiative and convective heat transfer. A 3D CFD model for PC will provide a tool to examine how and where the combustion takes place and how much and to where the heat is transferred. The parameters for the PC process, such as the location of the PC injector, injection angle, and oxygen rate, can be easily changed in the numerical model. It is expected to provide important information for the optimization of a PC process.

2. Production mechanism of fine titanium powder using pulse combustion

- Traditional production methods of metal powder, such as direct crushing, thermal spray, the hydrogenative dewatering and rotary electrode method, and electrolysis, do not seem to produce metal grains of satisfactory shape and size uniformity nor do they resolve other problems such as economy, by-products, etc. A novel original method for producing powder titanium offering improved shape uniformity is proposed in this research project. Pulse combustors generate a high temperature, high velocity pulsating combustion gas stream, which can melt elemental metal instantly and then directly convert it into fine powder form, thus producing metal powder of uniform granule size. Thus, this project relates to a novel method and apparatus for producing, in an economical and environment-friendly manner, super-fine metal powder offering high purity and uniform granular shape and size. Beside necessary experiments, lots of numerical works are required to understand the process mechanism and obtain optimal process parameters.

3. CFD optimization on steel casting with magnetohydrodynamics (MHD)

- With the re-structuring and consolidation of the steel manufacturers, issues such as efficiency and energy-saving have become more important and urgent. Numerical simulation is seen as a cost-effective way of developing improved steel technology, especially during the ideas stage. Considering the complex phenomena occurring during steelmaking in different stages such as in tundishes, casting molds, furnaces, and so on, our CFD modeling will initially focus on the effect of magnetohydrodynamics on the steel casting process. Furthermore, we will try to optimize some important parameters such as design of submerged entry nozzle, mold powder performance, electro-magnetic stirring (EMS), and design of spray cooling zone, and so on.

4. Study on Hydrocyclones to remove particulates from liquids/gases

- Hydrocyclones are widely used in many industries, particularly in mineral and chemical processing due to its simple design, high capacity, low maintenance cost, and the small physical size of the device. It is generally known that the operational and geometrical parameters determine the performance of hydrocyclones. Many previous empirical equations and numerical models are quite limited to describe hydrocyclone performance considering the complicated multiphase phenomena and strong vortex motion involved in hydrocyclones. Hence, in this study, a three dimension LES model is proposed to investigate the transport phenomena in hydrocyclones. Some key factors, such as vortex finer and cut size, will be studied thoroughly to improve performance of the process. The simulation results should serve well to the related industrial applications.

5. Furnace optimization of coal combustion

- Coal combustion is a particularly challenging application of CFD. Besides the need to represent the processes directly linked with coal combustion, it is necessary to use a Lagrangian approach to track the coal particles, and the main gas phase solution is turbulent, variable density reacting flow. Furthermore, radiation is an important heat transfer mechanism. In this study, we will focus on the optimization of furnace geometry and other parameters using 3D numerical simulation. The potential of CFD on coal combustion phenomena, furnace and fuel selection would guide us in real applications.

6. Modeling the jet characteristics and cutting performance of abrasive water-jet

- Computational fluid dynamics (CFD) models are developed for ultrahigh velocity water jets and abrasive waterjets (AWJs). Jet dynamic characteristics for the flow downstream from a very fine nozzle are simulated using the under steady state, turbulent, multi-phase flow model. Water and particle velocities in a jet are obtained under different input and boundary conditions to provide an insight into the jet characteristics and a fundamental understanding of the cutting process of water jet.

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Potential Projects:

7. Computer-aided Drying Schedules for Refractory to avoid Explosive Spalling

- *Dr.Z-X. Gong (USA) and Prof. A.S. Mujumdar*
- It is estimated that industry suffers lost revenues in the order of tens of millions of dollars per annum because of defects and failures, such as cracks and explosive spalling , caused by the final drying process of refractory lining. Current practice of purely empirical selection of drying schedules is obsolete and exorbitantly expensive. Based on many years of research on the heat and mass transfer mechanisms in refractory, now computer simulations can be developed to predict the drying schedules for both on-site monolithic furnace linings drying and kiln drying of prefabricated refractory castings with different geometries and permeability. The computer simulated schedules not only can prevent defects such as cracks and explosive spalling, but also shortens the drying time so as to reduce the total cost of the drying process. M3TC can work with interested companies to develop simulations and computer-aided design of drying schedules for specific applications. Dr. Z-X Gong of Simprotek Corporation, California will collaborate in this area. Dr Gong and Prof. Mujumdar have published extensive original work in this area.

8. Experimental and Modeling of Thermal Drying Processes

- *Dr ZX Wu and Prof. A S Mujumdar*
- M3TC has expertise in experimental and computational modleing studies of a number of products in diverse type of dryers including microwave, radio frequency, superheated steam, pulse combustion, heat pump assisted dryers etc. We can assist with selection of drying systems, improving energy efficiency, reducing environmental impact and optimization of drying schedules. Companies interetsed in thermal drying of minerals , polymers, coal, biomass, waste sludge etc and a range of diverse materials are invited to contact M3TC through Professor Mujumdar. also visit http://serve.me.nus.edu.sg/arun for resources about drying technology.

9. Modeling of melting, solidification, crystallization processes

- M3TC can call upon necessary expertise through in-house resources and international collaborations to provide consulting services to industry interested in modeling of phase change phenomena as well as crystallization operations which are found in mineral and metal as well as materials process industries.

10. Modeling Thermal Management in Solid Oxide Fuel Cells (SOFC)

- *Dr. A.S. Mujumdar, Dr. H.J. Poh, Dr. ZH Wu*
- Solid oxide fuel cells (SOFC) have attracted much industry attention as promising candidates for future energy conversion systems. They have higher efficiency than the heat engine systems constrained by the Carnot limitation. Internal reforming can occur at the anode this allowing use of natural gas as the fuel. The objective of mathematical modeling SOFC designs is toe predict the concentration of species, temperature distribution, potential distribution and current density for various flow configurations. Nonthermal temperature distribution poses serious problems causing large internal stresses and deformation of cells due to thermal expansion. For cost-effective optimization of the geometric and operating parameters it is essential to have a suitable mathematical model. Ongoing work is concerned with prediction and testing of PEMFC performance utilizing Fluent software with the object of reducing mass transfer resistance and thus enhance fuel cell performance.

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