

# Harnessing the Power of Virtual Reality

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Advances in physical modeling and computational science will revolutionize the way engineers develop and design new technologies and processes.

Virtual process engineering (VPE) combines computer simulations with real-time, online data to provide engineers with the benefits of so-called virtual reality. Through VPE, engineers will be able to simulate industrial processes with high accuracy and in real time, compare simulation outputs with experimental results online, and visualize relevant results dynamically and in 3D. The realization of VPE will require significant advancements in the accuracy of physical modeling, as well as improvements in the capabilities of computing hardware and software.

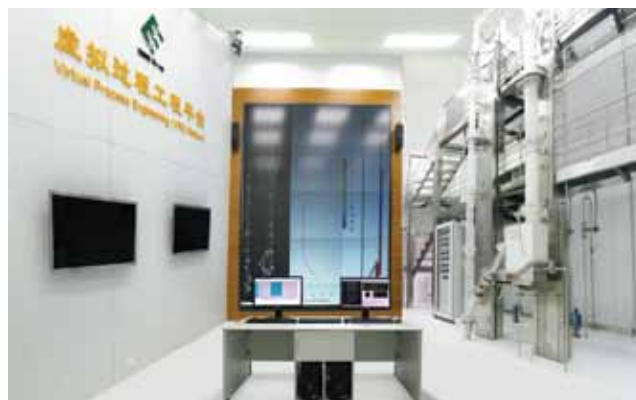
This article builds on a previous *CEP* article (1), which explored the use of advanced computational science in chemical engineering. Despite the progress that has been made in the use of computer modeling — and the realization of virtual process engineering — to accelerate the development of processes and technologies, challenges still exist. These challenges are discussed here along with some of the initial steps being taken to address them.

## Multiple scales

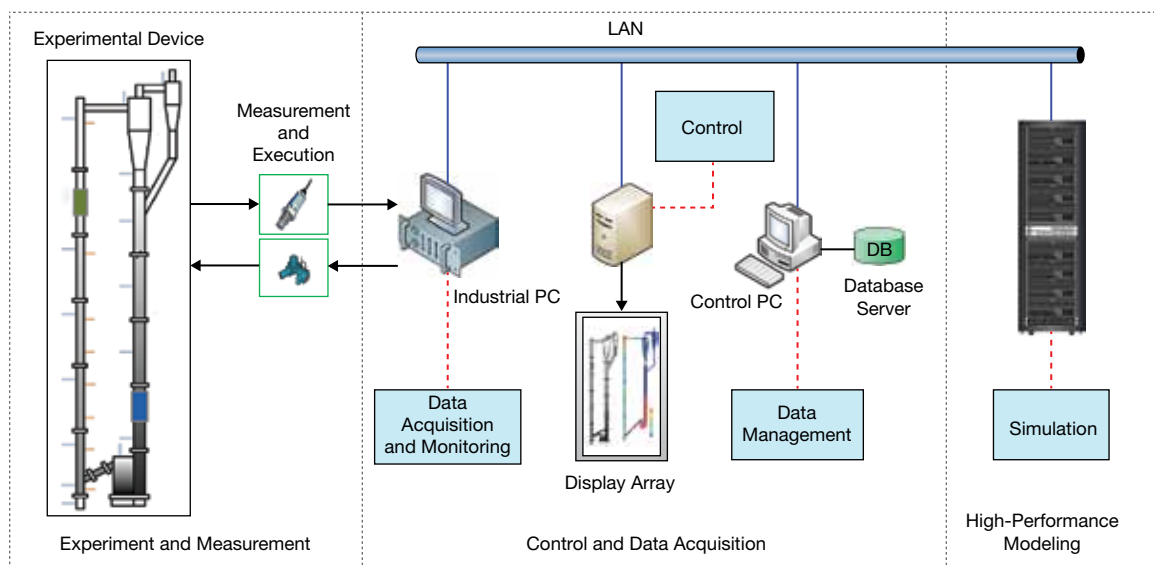
Industrial processes typically consist of a material level, a reactor level, and a system level. Each level, in turn, can be further divided into multiscale structures — intermediate meso-scale structures are bounded by a lower micro scale and an upper macro scale (2). The reactor, which is the main focus of a chemical engineer, involves particles (representing the micro scale), particle clusters (meso scale), and the reactor (macro scale). While the micro scale and macro scale are well understood, the meso scales are

not. For example, consider a multiphase chemical reactor. One can easily describe the hydrodynamics and transport behaviors of a single particle (micro scale), as well as the performance of the reactor as a whole (macro scale), but cannot adequately capture the behavior of gas bubbles or particle clusters (meso scale).

This lack of knowledge of the underlying mechanisms to explain the meso scale has been identified as a bottleneck to scaling up processes efficiently. Thus, laboratory experiments, intermediate tests, and pilot plant and industrial demonstrations are required to develop a new process. Such work is generally empirical or semi-empirical, time-consuming, and costly, and often makes it difficult to obtain optimal design and operational schemes.



▲ Figure 1. Version 1.0 of VPE was developed at the Institute of Process Engineering to demonstrate this type of platform for designing industrial processes.



◀ **Figure 2.** VPE 1.0 contains three subsystems — experiment and measurement, control and data acquisition, and high-performance modeling.

With the rapid development of computational fluid dynamics (CFD) and its ever-increasing application in chemical engineering, computational science is playing an increasingly important role in accelerating technology development (1). However, instead of an accurate prediction of total-system fluid dynamics of industrial processes in real time, existing simulation methods generally provide only a partial description of total-system hydrodynamics of pilot plants, and it takes several weeks or months to obtain such simulation results. Hence, in most cases, computational simulation is an inefficient way to guide process design and scaleup.

The huge gap between the capability of existing computational methods and the capability that will be required for these methods to be useful for engineers can be bridged by performing first global calculations, then regional (meso-scale) modeling, and finally detailed (micro-scale) process evolution (3).

The energy minimization multiscale (EMMS) model for gas-solid fluidization illustrates this approach. The EMMS model represents the gas-solid flow as a particle-rich dense phase and a fluid-rich dilute phase, and describes the system with six hydrodynamic equations and eight structural parameters. The model is closed by a stability condition that is defined by the compromise between the different dominant mechanisms. The dominant mechanisms are the extreme tendencies of individual mechanisms at the macro and micro scales and the compromise between these extremes leads to the dynamic behavior at the meso scale. For example, the compromise between gas behavior and liquid behavior produces bubbles, and the compromise between gas behavior and solid particle behavior brings about particle clustering. The EMMS model theoretically characterizes the meso-scale structures (e.g., particle

clusters in gas-solid two-phase flow) and bridges the gap between micro-scale gas-solid interactions and macro-scale operating parameters (4–6).

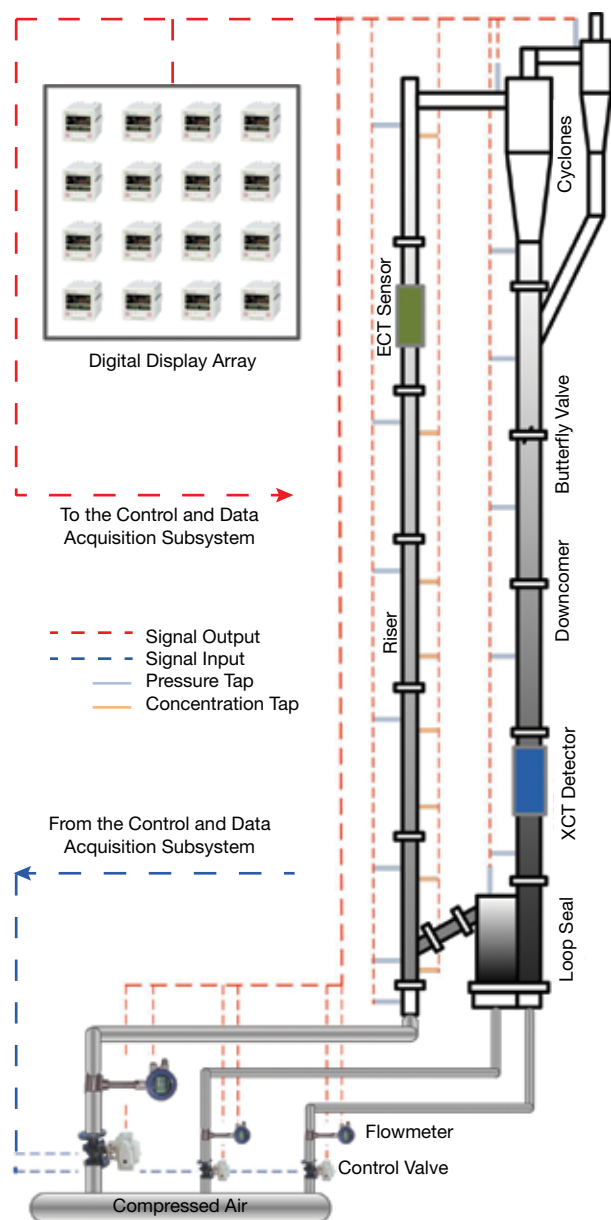
The initial EMMS model applied the so-called three-scale computational method as follows. At the micro scale, particle-fluid interactions were characterized with a common two-phase model — the particle-rich dense phase and the fluid-rich dilute phase are governed by fluid-particle interactions in each phase. At the meso scale, the stability condition was used to model the bulk characteristics of the heterogeneous structure and the interaction between the two phases in a finite element of volume. And, finally, at the macro scale, a global stability condition determined by integrating the meso-scale boundary conditions and the process operating conditions defines the global distribution of flow parameters.

A preliminary version of the VPE platform (based on the EMMS model) — referred to as VPE 1.0 — was developed at the Institute of Process Engineering (IPE), Chinese Academy of Sciences. VPE 1.0 performs a pseudo real-time simulation of the hydrodynamics of an industrial process, which serves as the first step toward using VPE in chemical engineering and industrial chemical process development.

### Under the hood

VPE 1.0 has three main parts: an experiment and measurement subsystem; a control and data acquisition subsystem; and a high-performance modeling subsystem. It also has a large graphical display on which the user can visualize and compare the experimental and simulated results. The actual VPE 1.0 system is shown in Figure 1. Figure 2 illustrates the hardware and software configuration of VPE 1.0 and the integration of the three subsystems.

Article continues on next page



▲ **Figure 3.** The experimental equipment used to demonstrate VPE is a gas-solid circulating fluidized bed reactor equipped with sensors and other monitoring devices that provide hydrodynamic measurements.

The experiment and measurement subsystem is a pilot-scale unit of an actual process equipped with several measurement devices that provide real-time physical property data. The control and data acquisition subsystem consists of three modules:

- *data acquisition module.* This module uses software running on an industrial PC (IPC) to collect data from the process operating in the experiment and measurement subsystem and to control the process.
- *operation control module.* This module, which acts like

a management center of sorts, controls the display of the real-time and offline simulation and experimental data.

- *data management module.* This module, the data center of VPE 1.0, stores all of the data in a customized database, and provides data service for other subsystems over a high-speed network.

Using the operating variables as input parameters, the high-performance modeling subsystem employs the EMMS paradigm for full-loop hydrodynamic simulation of the process on a high-performance computer (HPC) (7).

## Experiment and measurement subsystem

The experiment and measurement subsystem (Figure 3) consists of a multiphase flow reactor, in this case a gas-solid circulating fluidized bed (CFB), that provides real-time hydrodynamic measurements.

The CFB, which is constructed primarily of transparent thermoplastic to allow for visibility, consists of a riser, a downcomer, a nonmechanical loop seal, and two cyclones. The CFB is equipped with three control valves with manual and electric integration and three vortex flowmeters, to adjust and measure the fluidization and aeration gases (in this case, compressed air). The equipment can handle fluidized particles with diameters of 50–200  $\mu\text{m}$  at densities of 800–2,500  $\text{kg}/\text{m}^3$ .

An eight-channel optical-fiber concentration analyzer in the CFB measures the instantaneous axial solids-concentration profile in the riser. Electric capacitance tomography (ECT) measures the gas- and solid-fraction distributions within any cross-section of the riser in real time. The solid circulation rate in the CFB (for reference) can be determined manually by using a butterfly valve affixed to the top of the downcomer; in the near future, a dual-plane X-ray computed tomography (XCT) unit will be mounted on the bottom of the downcomer to allow the solids circulation rate to be measured nonintrusively. Sixteen high-accuracy pressure transducers are attached to the CFB to measure pressure throughout the reactor.

The measurements obtained from the ECT and the XCT are processed online by an *in situ* computer and transmitted synchronously to the control and data acquisition subsystem. All standard analog-current signals from other measurement devices are divided into two signals — one is sent to the digital displays for monitoring, and the other is sent to the control and data acquisition subsystem for storage and post-processing. The valves can be automatically adjusted via commands in the graphical user interface (GUI) of VPE 1.0.

## Control and data acquisition subsystem

The control and data acquisition subsystem configures, monitors, and controls all of the VPE components related to data processing, actuator control, and user interaction.

► **Figure 4.** The experiment control window of the graphical user interface shows the real-time local hydrodynamic properties of the CFB and provides a means for changing the operating conditions of the CFB via the graphical “wheels.”

At the front end of this subsystem is the IPC, which is used primarily for data acquisition and process control. Based on real-time measurement signals, users can change operating parameters in real time via the IPC or by issuing commands from the control PC. A timeserver residing in the control PC synchronizes the time among the three subsystems in VPE 1.0 through a local area network (LAN) to achieve a high degree of precision in the experimental and simulation data. A specially designed communication protocol enables all data in VPE 1.0 to be processed and transmitted using a client-server model. The data records can be retrieved and examined on a run-by-run basis, which allows for further data exploration and analysis.

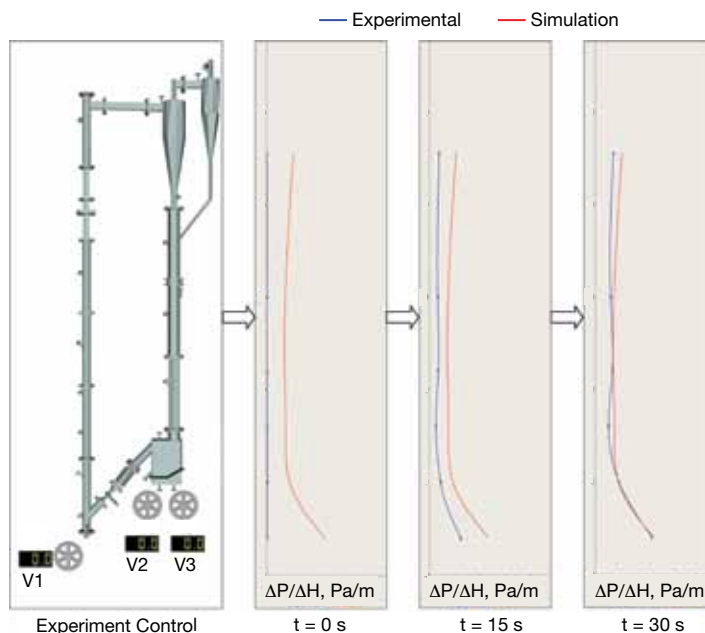
The display array is composed of 15 67-in. screens arranged in a 3-column by 5-row matrix. The height of the display matrix is similar to that of the experimental CFB, so the process characteristics are displayed at near-actual size. The GUI of VPE 1.0 has three types of windows:

- an experiment control and monitoring window, which tracks the operating conditions and exhibits a real-time 2D view of the local hydrodynamics of the process
- a data exploration window, which functions as an interface between the user and the data analysis and results, including statistical charts and plots
- a simulation control and monitoring window, which allows the user to implement the simulation under the given operating conditions, and displays the simulation results in 2D and 3D.

Figure 4 provides more details about the GUI.

### High-performance modeling subsystem

The EMMS model could not be implemented with any existing commercial hardware until IPE proposed the development of the powerful three-level hybrid CPU and GPU computing system on which VPE 1.0 is based (2). This computing system, named Mole-8.5, reaches a peak performance of 1 double-precision petaflop. Its three-level design reflects the structure of the physical model and the numerical algorithm. At the top level, a few servers with only high-speed CPUs are equipped to conduct complicated operations and branchings to search for the global stability conditions through optimization. At the middle level, more servers with a balanced configuration of CPUs and GPUs are introduced to carry out simple and massive mathematical operations to compute the meso-scale



continuum. At the bottom level, a majority of the servers, which consist of multiple GPUs but only a few CPUs, are assigned to implement a large number of primitive and intensive computations for micro-scale discrete simulation.

Using this computing system, the global stable distribution of complex fluidization systems can be calculated in real time (8). However, general parallel-discrete simulation software needs to be developed further before the three-scale computing method of the EMMS paradigm can be fully implemented for real-time detailed hydrodynamic evolution.

One way to implement the EMMS approach (at least partially) on EMMS-based CFD software running on a CPU cluster is to partition the calculations. First, the software calculates the macro-scale steady-state hydrodynamics, and these results serve as the initial conditions for calculating the micro-scale hydrodynamics. This strategy significantly reduces computational cost and increases simulation accuracy compared with the traditional two-fluid model (TFM) simulations (9). VPE 1.0 is based on this strategy.

### VPE 1.0 test drive

We used VPE 1.0 and FLUENT 6.3 software, with the gas-solid drag coefficient calculated from the EMMS model, to simulate the full-loop hydrodynamics of the CFB, and compared those results with the *in situ* CFB experiments. In the simulation, the EMMS-based drag coefficient, which replaces the traditional drag coefficients based on the assumption of homogeneity, was used to close the Eulerian multiphase model. By considering the heterogeneity in the finite element of volume, this simulation scheme enables the calculation of the meso-scale

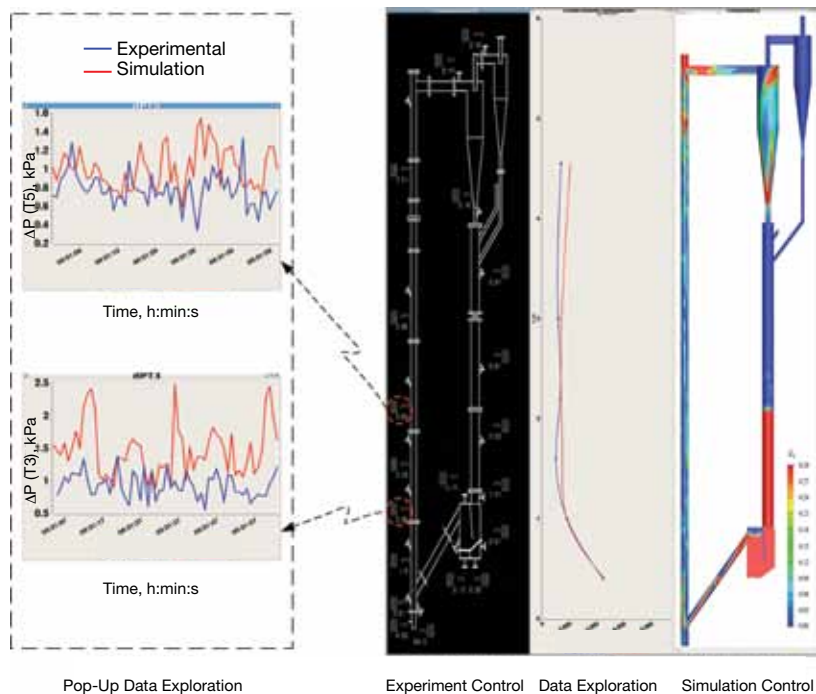
## On the Horizon

structures (*e.g.*, particle clusters) and their influence on CFB hydrodynamics (7). The EMMS-predicted global distribution of particles improved the calculation efficiency and also decreased the appearance of gas channeling in the total-system simulation, because the optimized initial field is much closer to the so-called pseudo steady state than either the common homogeneous distribution or close packing used in traditional continuum simulation.

### Moving forward with VPE

While VPE 1.0 — its simulation scheme and hardware architecture — only partially implements the EMMS paradigm, it does reveal the benefits associated with such a platform for fast, high-accuracy, total-system simulation of industrial chemical processes. VPE 1.0 not only functions as a comprehensive platform to provide basic data and design guidelines for the development of industrial processes, but it could be an effective tool for training new operating staff at much lower cost.

The existing VPE 1.0 system takes about one week to simulate a one-minute physical process; in the future, the computation time will likely be reduced to about one day or even one hour for the same process. With further development and maturity of the general parallel-discrete simulation software and the multiscale computing hardware platform defined by the EMMS paradigm, a total-system, real-time simulation of complex chemical systems can be expected.



▲ **Figure 5.** The data exploration window of the graphical user interface lets the user view data, including statistical charts and plots, in real time.

In the long term, virtual process engineering will be able to deal with the flexibility of different processes. At that time, the design, scaleup, and optimization of chemical processes could be completed in several days via a computer, thus bringing about a revolution in the development of chemical processes and realizing so-called virtual reality for process engineering.

IPE is conducting further work to improve the computational speed and functionality of VPE 1.0.

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### LITERATURE CITED

1. Syamlal, M., *et al.*, "Computational Science: Enabling Technology Development," *Chem. Eng. Progress*, **107** (1), pp. 23–29 (Jan. 2011).
2. Li, J., *et al.*, "Meso-Scale Phenomena from Compromise — A Common Challenge, Not Only for Chemical Engineering," ARXIV, 0912.5407v3, <http://arxiv.org/abs/0912.5407v3> (Dec. 2009).
3. Ge, W., *et al.*, "Meso-Scale Oriented Simulation Towards Virtual Process Engineering (VPE) — The EMMS Paradigm," *Chem. Eng. Science*, **66** (19), pp. 4426–4458 (Oct. 2011).
4. Li, J., "Multi-Scale Modeling and Method of Energy Minimization for Particle-Fluid Two-Phase Flow," PhD Thesis, Institute of Chemical Metallurgy, Chinese Academy of Sciences, Beijing, China (1987).
5. Li, J., *et al.*, "Multi-Scale Modeling and Method of Energy Minimization in Particle-Fluid Two-Phase Flow," Proceedings of the Second International Conference on Circulating Fluidized Beds, Compiègne, France, pp. 89–103 (Mar. 1988).
6. Li, J., and M., Kwauk, "Particle-Fluid Two-Phase Flow: The Energy-Minimization Multi-Scale Method," Metallurgical Industry Press, Beijing, China (1994).
7. Lu, B., *et al.*, "Multi-Scale CFD Simulation of Gas-Solid Flow in MIP Reactors with a Structure-Dependent Drag Model," *Chem. Eng. Science*, **62** (18–20), pp. 5487–5494 (Sept.–Oct. 2007).
8. Liu, X., *et al.*, "A Method to Fast Predict Macro Hydrodynamics of Complex Fluidization Systems," Chinese Patent, No. 201110122298.X (2011).
9. Liu, Y., *et al.*, "Acceleration of CFD Simulation of Gas-Solid Flow by Coupling Macro-/Meso-Scale EMMS Model," *Powder Technology*, **212** (1), pp. 289–295 (Sept. 2011).

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