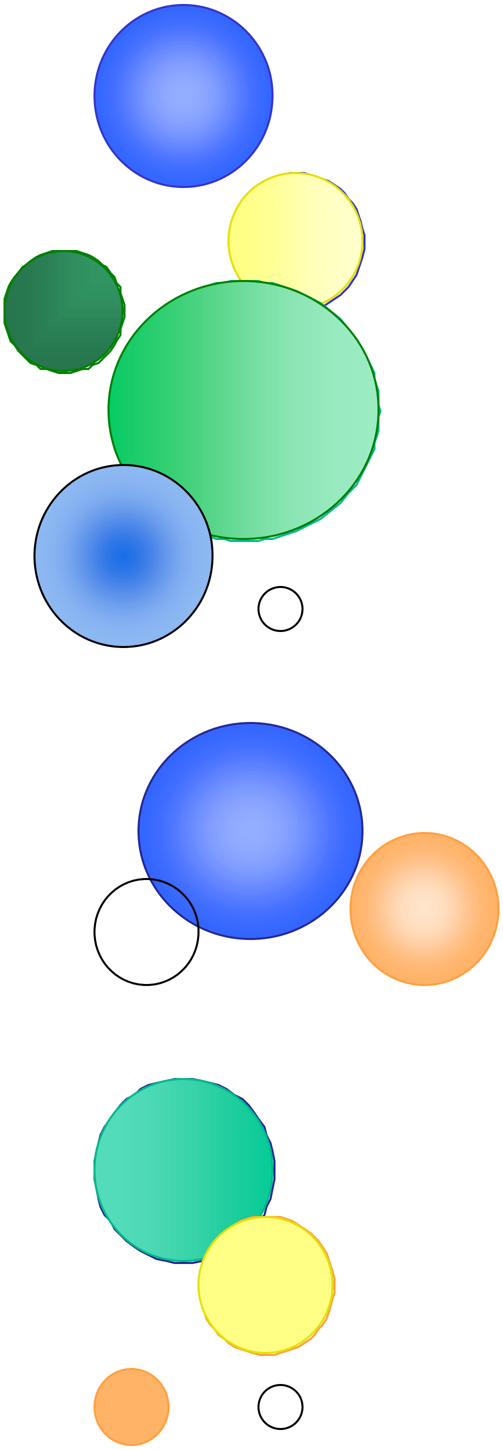

Chemical Industry
of the Future

Technology Roadmap
for
Computational Fluid Dynamics

January 1999

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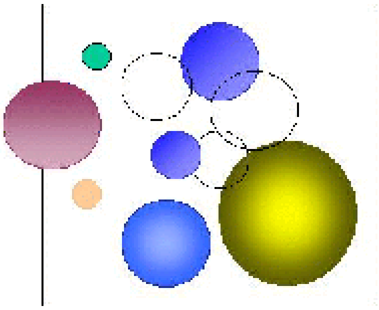


1 Overview

Challenges on the Horizon

As the 21st century approaches, the chemical industry faces considerable economic, environmental and societal challenges [VISION 1996]. Major forces for change include: increased globalization of markets; societal demand for improved environmental performance; the need for increased profitability and capital productivity; higher customer expectations; and changing work force requirements. Technology research, development and deployment will be vital to meeting these challenges and seizing future opportunities for market growth.

Globalization will promote the free movement of people, technology, capital, information and products across international boundaries. While this will create many new market opportunities, it will also require the development of advanced manufacturing technologies that allow the industry to be globally competitive. Improving and sustaining environmental performance will provide opportunities to serve the global population with higher performance and higher quality products. It will also require manufacturing processes that are resource efficient, cost effective, and environmentally sound.

With an ever-increasing emphasis on the creation of products that generate revenues and satisfy stockholder expectations, the industry will need to find ways to increase profitability and capital productivity. Strategically-driven investments in R&D and new technologies can drive the industry towards a higher level of financial performance. An expedient response to customer expectations will be increasingly important in capturing new market opportunities and ensuring financial success for chemical producers as well as customers. To meet this challenge, technology innovation will be needed throughout all phases of R&D, production, and distribution. Finally, to keep pace with rapid technological change and the increased complexity of chemical production technology, a more highly skilled work force will be essential.

Industry's Response

In response to these challenges and to a request from the White House Office of Science and Technology, the chemical industry initiated a study in 1994 to examine the factors affecting the competitiveness of the industry and the R&D essential to meeting their future needs. The results of this study are contained in *Technology Vision 2020*: *The U.S. Chemical Industry*, a collaborative effort representing inputs by more than 200 technical and business leaders from the

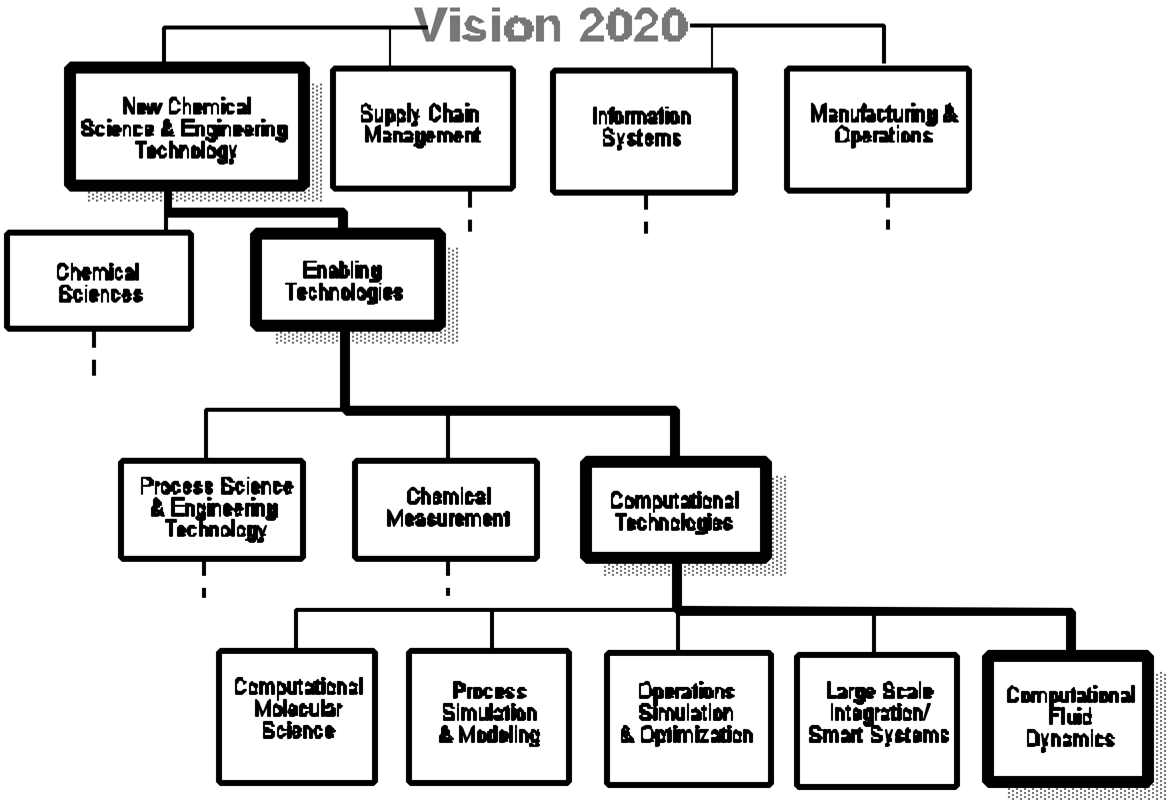


Exhibit 1-1. Selected R&D Areas Identified By *Technology Vision 2020*

chemical community [VISION 1996]. This visionary document identifies major goals for the industry that include, among others, improving operations and the efficient use of resources (e.g., raw materials, energy).

To meet future industry goals, *Technology Vision 2020* advocates the support of R&D in a number of areas, including new chemical science and engineering technologies that will promote more cost-efficient and higher performance products and processes (see Exhibit 1-1). An important component of this R&D is the development of enabling technologies that improve the application of fundamental chemical sciences throughout the industry's process environment.

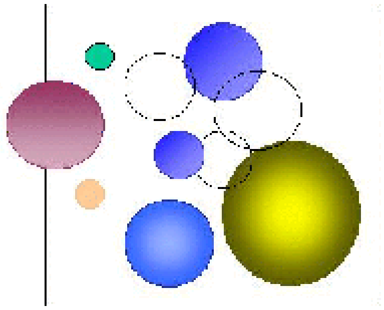
The Role of Computational Fluid Dynamics

Technologies to assist industrial computations may be considered "enabling" in that they are used in nearly every aspect of chemical research, development, design and manufacture. The focus of this report is on **computational fluid dynamics (CFD),** a highly sophisticated integration of applied computer science, physics, chemistry, and engineering science. It is a subset of computational technologies that is critical to meeting the industry's future challenges. A focus on CFD R&D was identified in *Technology Vision 2020* as a high-priority for meeting the industry's future goals.

In 1995, the chemical industry began to define its needs in CFD through a workshop on the computer simulation of reactive multiphase flow [LANL 1995]. Attendees included participants from twelve companies representing the petroleum, chemical, environmental and consumer products industries, along with representatives from the U.S. Department of Energy and Los Alamos National Laboratory. The dialog at this meeting suggested that reactive multiphase flow simulation, a component of CFD, was critical to optimizing a number of chemical processes, and also an excellent candidate for partnership activities involving industry, government, and academia. A white paper was also presented at this workshop to foster discussion on the formation of a consortia to improve the state-of-the-art in computational technologies [DOW 1996]. This white paper outlined the problems with existing computational packages as well as some of the challenges for the chemical process industry in modeling specific chemical systems. The results of this workshop and the white paper later provided input for the discussion of computational technologies in *Technology Vision 2020*.

Following the publication of *Technology Vision 2020* in 1996, another workshop was held to build an industry-wide consensus on the essential research and technology development pathways needed to develop advanced CFD capabilities. The National Workshop on Computational Fluid Dynamics and Multiphase Flow Modeling brought together members of the chemical processing, petroleum refining, aluminum, and computer hardware industries [NATL 1997]. Participants also included representatives from government agencies (U.S. Department of Energy, National Science Foundation), national laboratories, and academia. The first half of the workshop concentrated on the exchange of information between members of the chemical and computer hardware industries regarding needs, future industry direction, and potential developments. The second half included brainstorming sessions to identify specific research needed over the next ten years and to explore the foundation for a cohesive CFD R&D roadmap for the chemical process industries.

A final workshop held in June 1997 completed the roadmap process by further linking technology research needs with practical fluid flow problems, performance targets, and time frames where research could be expected to yield tangible benefits. Together the results of these workshops provide the foundation for this CFD roadmap. It is one of many such efforts to provide a link between the broad-based goals defined in *Technology Vision 2020* and the research portfolio that will be pursued through cooperative R&D partnerships. The research priorities outlined in this roadmap will be used as the basis for making new research investments by government and industry. It is a dynamic document, and will be reevaluated periodically to incorporate new market and technical information and to ensure that the research priorities remain relevant to the needs of both the chemical industry and its customers.



2 What is CFD?

Computational fluid dynamics, or CFD, provides a quantitative description of flowing fluids in relation to the fluid's surroundings. Mathematical equations describe the physical and chemical phenomena that occur as fluids flow. In computational applications the mathematics are translated into computer language so that the thousands of calculations required to describe the fluid flow can be performed.

Fluid flows found in industrial processes range from simple to highly complex. A simple flow situation is liquid water flowing through a pipe. For this example it is straightforward to predict the properties of the flow (such as the volumetric flow rate) from characteristics of the flow situation (length and material of the pipe, pump pressures, flow temperature). For more complex situations, such as gases, liquids, and solids contacting together in a chemical reactor, it is not possible to determine the properties of the flow (such as concentrations of components, flow rates) by hand calculation. The properties must be calculated from "point to point" in the reactor, meaning that the mathematical relations describing the fluid flow must be solved numerically, with the aid of a computer. The various aspects involved in these calculations are inherent to "CFD."

Characteristics of Fluid Flows

Fluid flow situations comprise liquids, gases, solids or a combination of these phases. Fluid flows can be reactive, turbulent or laminar; steady or unsteady; Newtonian or non-Newtonian.

Reactive Flow - fluid flow where chemical reactions provide important contributions to heat and mass transfer. Combustion situations and many chemical manufacturing processes fall in this category.

Multiphase Flow- fluid flow of more than one phase (e.g. gas-solid, gas-solid-liquid) the properties of which cannot be described by the flow of a single phase alone.

Laminar Flow - flow in smooth, distinct streamlines, such as water flow in a pipe at low flow rates. Steady laminar flow of a single phase is one of the few cases with a relatively straightforward mathematical solution.

Turbulent Flow - Characteristic of higher flow rates (or higher Reynolds numbers) at which, instead of moving in smooth, predictable paths, the fluid motion is chaotic. Turbulent flow is characterized statistically. The time-averaged flow properties can be approximated adequately for some single-phase cases. Expensive experimental methods are currently relied on to analyze and predict turbulent flow, particularly for multiphase flow.

Reynolds Number - a dimensionless number, commonly used in characterizing fluid flow, that is proportional to the inertial force divided by viscous force. Typically it is calculated as (length) x (mass flow rate)/(viscosity). At low Reynolds number the flow is laminar. At sufficiently high Reynolds number it becomes turbulent.

Steady Flow - The spatially averaged properties of which are constant in time.

Newtonian Flow - A flow for which stress is directly proportional to strain rate. Flows of polymer materials (molten plastics, for example) are usually non-Newtonian. In practice non-Newtonian flows require additional energy

More precisely, CFD technical areas include constitutive relations, numerical methods, and experimental validation.

Constitutive relations describe the limitations of the fluids in relation to their surroundings, and the interrelationships of the flow variables. Many constituitive relations are empirical, meaning that they are derived from observations; other constitutive relations are based on theory or fundamental physical principles. It is most common for fluid flow variables (pressure, velocity, temperature) to be related to each other from point to point, infinitesimally close (i.e., in differential form). The corresponding relations are called "differential equations." CFD is applied to find numbers that represent these variables in specified fluid flow situations.

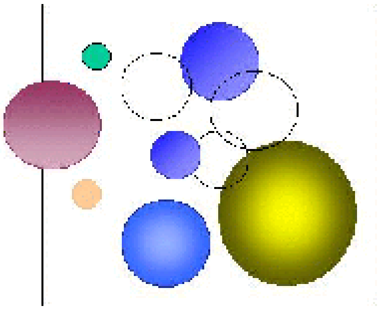
Numerical methods are the tools used to solve the equations described above. The use of numerical methods depends on the particular form of the equations, the desired accuracy of the solution, the type of computer that is used in the calculations, and in many cases, the knowledge and skill of the investigator doing the calculations. Advances in computer technologies are usually accompanied by advances in numerical methods, with the goal of enhanced speed and amount of data that can be processed.

Modeling and simulations mean nothing, of course, independent of the reality they are supposed to represent. The accuracy of the simulation must be checked, or validated, against data obtained from real operating systems. This **experimental validation** is critical to ensuring that the computational tools are meaningful representations of the applications for which they are intended. The role of experiment goes beyond merely confirming the computed results. Experiments must be designed to challenge the model and push it to the limits at which it fails.

By predicting a system's performance in various areas, CFD can potentially be used to improve the efficiency of existing operating systems as well as the design of new systems. It can help to shorten product and process development cycles, optimize processes to improve energy efficiency and environmental performance, and solve problems as they arise in plant operations. There are many potential applications of CFD in chemical processes where predicting the characteristics of fluid flow are important (see inset). CFD has also been applied to determine optimum control strategies, optimize equipment in the automotive and electric power industries, and has been especially successful in the aerospace industry. In some cases, the design to production time for airplanes has been reduced by half or more over the past decade with the development and application of CFD. A concerted effort by industry, in partnership with government and academia is needed to make similar advances in CFD possible for the chemical and other low-temperature process industries.

Applications for Computational Fluid Dynamics in Chemical Processing

- Mixers
- Chemical Reactors
- Packed Beds
- Crystallizing/Dissolving Equipment
- Pneumatic Conveyors & Classifiers
- Flows in Pipes
- Sprays
- Biological Systems



3 Current Situation

Computing Power

Computational tools available today are greatly improved from those developed just a few years ago, and are easier to use. Development of parallel machines and parallel algorithms designed for these machines has allowed the solution of problems that were previously impossible to solve. Advances have also been made that facilitate the handling of the immense amount of data generated by a complex simulation. Distributed and shared-memory computer architectures have both emerged as the way to increase computational power. Visualization of complex three-dimensional flows is now a practical tool for obtaining useful information from simulations.

Computing Hardware

Supercomputer - A system that meets the computer industry's evolving standards at any particular time. A supercomputer must have not only very fast processors but also commensurate memory, internal communications, and data storage technology. For example, in 1998 the U.S. Department of Energy acquired a supercomputer that can perform 3.9 trillion (million million) calculations per second and is equipped with over 2.6 trillion bytes of memory. Such a machine exceeds typical desktop computers by ten thousand fold in both speed and memory.

Parallel Architecture - At least four (and usually more) processors linked together, and controlled by hardware for efficient use of the maximum number of processors at any time. Processors may cooperate or work independently to solve a problem.

Distributed Architecture - A technique to use the capabilities of more than one computer (processors and memory) simultaneously. The technique is usually applied with software controls.

Vector Processing - Calculations are performed in linear, assembly line fashion. Supercomputers based on Vector Architecture include special processor hardware to stage and rapidly execute the repetitive calculations that are typical of matrix arithmetic, as found in most scientific computer programs.

Computational Fluid Dynamics

Considerable effort has gone into the development of single-phase fluid dynamic modeling tools for applications in the aerospace, automotive, and electric power industries. CFD for single-phase non-reactive fluid flows is relatively well-developed, and can be used to model relatively complex flow fields. Reactive single-phase flows can potentially be modeled with existing tools (such as simple combustion systems), provided the computations required are not too large or complex.

Single Phase Numerical Methods

Direct Numerical Simulation (DNS) - provides a numerical solution (description) for all the scales (size) of flow without simplifying or approximating the important physical properties of the flow.

Large Eddy Simulation (LES) - provides a numerical solution for large eddies (whirlpools) in the flow while modeling (simplifying) the effects of very small eddies.

Reynolds Averaged Navier Stokes (RANS) Model -simulates turbulent fluid flow more rapidly than DNS or LES but with limited accuracy.

Currently available numerical methods for single-phase flow include Direct Numerical Simulation (DNS), Large Eddy Simulation (LES), and Reynolds Averaged (RA) models. These models, as well as new approaches coupling full reaction kinetics with turbulence, suggest that modeling turbulent reactive multiphase flows is possible on today's computers. However, development of hardware (parallel architecture), software (advanced numerics for parallel machines, object-oriented modular programming), and theory (submodel development) are required.

Commercial CFD vendors have not given emphasis to problems involving chemical reactions and turbulent reacting flows in particular, primarily because their products have evolved for use in the aerospace, automotive, and power industries. However, a number of existing single-phase CFD packages have been adapted for use in the chemical industry to assist in solving practical problems that arise with chemical processing equipment.

Current Applications of Multi Phase CFD in Chemical Processing

- Gas Scrubbing
- Thermal Oxidation/Waste Treatment
- Packed Bed Reactions
- Crystallization
- Polymer Extrusion
- Mixing and Blending
- Rotary Kiln Incineration
- Drying
- Membrane Separation
- Dust Separation
- Pyrolysis (Cracking)

Limitations of Current CFD Packages
Commercially available CFD tools cannot or do not:

- use available computational horsepower (e.g., parallel computing), as well as they should,
- use leading edge numerical methods (e.g., adaptive gridding, solution-driven grid refinement) or theoretical methods,
- include available submodels of key subprocesses (e.g.,crystal nucleation and growth), or submodels are not coupled properly (i.e., turbulence and chemistry),
- have a common chemical engineering infrastructure to allow linking to programs common in the chemical processing industries (e.g., physical and chemical properties data base).

Chemical Process Design and Operation

The efficient design and operation of multiphase flow systems is currently limited by a number of factors, as shown in Exhibit 3-1. Some of these are due at least in part to the lack of accurate modeling tools for multiphase flow regimes; others result from problems inherent to specific chemical processes.

Exhibit 3-1. Problems Limiting the Efficient Design and Operation of Multiphase Flow Systems

Design	Operation and Control	Process-Related Issues
Current designs are artificially constrained Current designs are based on precedence and empirical methods Data at the macroscopic rather than microscopic level is used in current designs Not all design alternatives are explored—limited possibility thinking is the rule Steady state is often used to explain transient and segregated flows Limited ability to do real reactor design Current design simulations are based on idealized conditions (often quite different from actual) Current codes provide inaccurate predictions when extended to other flow conditions	Lack of means for controlling product attributes Poor utilization of existing process vessels Excessive down-times due to corrosion and erosion Limited ability to optimize existing reactors and separation units, leading to low yields and poor performance High cost of experimenting in full-scale production facilities Poor visualization of process phenomenon	Inefficient pneumatic handling of solids (feeds and products) resulting from poor design and reliability Problems associated with chemical containment and safety General process inefficiencies leading to unnecessary energy consumption, production of waste, and emission of pollutants Limited availability of designs and computational tools that target specific production processes or plants Mass transfer-controlled operations Multiphase flow in channels Viscous and non-Newtonian mass transfer operations Safety pressure relief multiphase discharge designs

Design

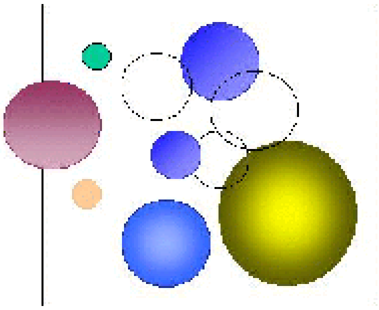
Many current designs are based on precedence and guided by entirely empirical methods (those based on experiment or experience). This is the direct result of the lack of, or inaccuracies associated with, computational methods available for use during the design cycle. Current codes designed for very specific flow conditions often provide inaccurate predictions when applied to other flow conditions. In many cases existing design simulations are based on idealized conditions that are quite different from actual operating conditions. For example, available codes often use steady state simulations (steady over time) to describe flows that are transient (changing with time). In general, the lack of accurate computational packages for multiphase systems results in artificially constrained designs and a limited ability to explore alternative designs.

Operation and Control

While CFD packages for single-phase systems have been used for optimizing operation and control of existing processes in the chemical industry, their use is limited for systems containing reactive and/or multiphase flows. Without the use of simulation tools, the plant engineer’s ability to visualize process phenomena is limited and optimizing operations is made more difficult and time-consuming. Often the only way to identify and solve the problem is to make experimental measurements—a costly proposition in full-scale chemical production. Without an effective way to optimize operations, the result is often poor control of processes and product attributes, poor utilization of equipment, excessive equipment down-time, low yields, and generally low performance.

Process-Specific Issues

Several areas of chemical processing are particularly difficult from a design and operational aspect. These include pneumatic handling of solids, chemical containment and safety, and general process inefficiencies. Most of these could be addressed in part by effective CFD packages that model turbulent reacting multiphase flows.



4 Trends and Drivers

Computer Technology

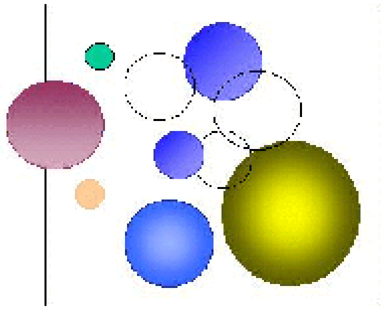
New computing technology is entering the marketplace almost daily. The speed of high performance computing platforms has increased exponentially, and as of 1998 had reached 3.9 TFLOPS in some models. Dramatic advances have been made in highly parallel processing and parallel numerical algorithms and other high performance processors. The rapid advances in computing technology are not expected to slow, and will lend further support to the development and effective use of computational tools like CFD.

Energy Price and Supply

The availability and cost of fossil energy for use as fuel and feedstock is of vital importance to the chemical processing industries. For some products, energy for heat, power, and feedstocks can account for up to 85 percent of total production costs (overall, chemical industry energy costs are about 8 percent of the value of shipments) [DOC 1994, CMA 1996]. Feedstock availability is also a primary concern for many chemical producers—nearly 50 percent of energy consumed is in the form of petroleum-based feedstocks. The industry is highly susceptible to volatility in energy feedstock price and supply, a fact made evident during the oil embargo of 1973. Although energy prices are currently low, history shows they can be subject to rapid change with devastating impacts. Advances in technologies like CFD, which have the potential to improve process energy efficiency, will continue to be of importance to the industry.

Government Regulations and Public Policy

Chemical production, use, storage, transportation, and disposal are heavily regulated by Federal and state laws and regulations. Compliance with these statutes (e.g., Clean Air Act and its Amendments, Toxic Substances Control Act, Resource Conservation and Recovery Act, and others) represent serious challenges to the chemical industry in terms of capital and operating expenses. In 1994 the industry spent about $4.6 billion on pollution abatement and control, nearly double the costs incurred in 1984 [CMA 1996]. New environmental programs are continually being proposed at the Federal, state and other levels of government, and will likely further increase the difficulty and cost of compliance. Consequently, cost-effective technologies that improve the environmental performance of processes will be increasingly important.



5 Performance Targets

Improvements in computational fluid dynamics can contribute directly to the goals stated in the chemical industry vision. Specifically, the application of computational technologies could promote:

- Shortened product-process development cycles;
- Optimization and control of existing processes to improve yield and energy efficiency;
- Efficient design of new products and processes; and
- Improvements in health, safety, and environment.

With these broad goals as a base, specific performance targets (both quantitative and qualitative) have been identified for CFD, as shown in Exhibit 5-1. These targets illustrate how improvements in computational fluid dynamics can have a wide-reaching impact throughout the entire chemical industry. The basic tools of numerical modeling and simulation of fluid flows are broadly applicable and can lead to improvements in nearly all unit operations and processes.

Exhibit 5-1. Performance Targets for Computational Fluid Dynamics

Quantitative Targets

- Shorten lead times (from research to final plant design) to 3-5 years.
- Reduce plant down times to 1%.
- Reduce separation energy and improve separation efficiency by 20%.

Qualitative Targets

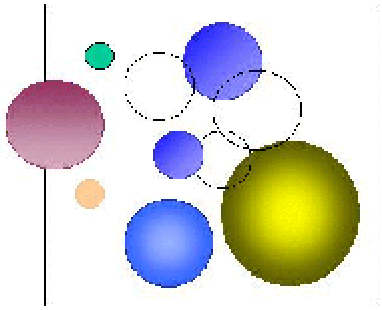
- Increase reliability of design (reduce risk).
- Reduce/eliminate design errors.
- Promote innovation.
- Reduce fuel consumption per unit of product.
- Improve heat transfer (waste-heat recovery).
- Optimize processes to increase yield and aid incremental expansion.
- Create a library of computational tools with both single-phase and multiphase flow capability.

The primary advantage of CFD is the potential to shorten lead times for process development (and plant designs) as well as new product development. Using conventional development methods without CFD, lead times can be as long as 7 to 10 years. The impact of CFD on the process and product development cycle is greatest in the earliest phases (i.e., experimental optimization and scale-up). CFD facilitates the design process by increasing the reliability of the design, reducing or eliminating design errors, and allowing developers to visualize the results of a process design or innovation. It promotes innovation by making the design process shorter, less risky, and easier to accomplish.

Using CFD to resolve problems with existing processes can reduce equipment failures and minimize poor operational performance, decreasing process shut-down time. When used to optimize plant and equipment operation, CFD can increase yields, providing a mechanism for incremental expansion.

Applying CFD to the optimization of energy-intensive processes (e.g., separations) can improve separation efficiency, reduce energy requirements, and improve environmental performance. CFD can also provide a way to improve heat transfer (e.g., recovery of waste heat) and better integrate heat transfer needs within the chemical plant.

The creation of a library of computational tools that are relatively easy for a non-specialist research plant engineer to use is a key target. Such a library would greatly promote the use of CFD tools in the chemical plant to solve real problems and optimize process and product designs. These tools would be designed with a “plug-and-play” code to allow easy insertion of new submodels and new solution algorithms on various computing platforms, including high performance desktop workstations; large, fast vector-processor machines; and highly parallel processors. Proposed codes would be built independently of current computer architecture, since architecture will change and code must change along with it to retain usability. A CFD library with the above features will be more widely acceptable and usable throughout the chemical community, and will help to promote environmentally safe, efficient chemical production processes.



6 Technology Barriers

There are a number of barriers that inhibit the development and use of CFD. These are shown in Exhibit 6-1, organized by topic.

Practical Usability

The practical use of current CFD packages by engineers in chemical plants is limited primarily by the excessive time currently required for the engineer to set up the calculation. Furthermore, current CFD tools do not always provide results that are easily used or interpreted by the plant engineer. In many cases the plant engineer initially wants to use CFD to solve a problem arising with existing equipment or processes. He/she then finds that the solutions provided by CFD are not conveniently accessible. Another limit is the lack of CFD tools that can model simple versus complex situations. For example, some problems or design issues could be resolved by easily accessible submodels of a larger CFD package rather than setting up an entire simulation. These types of modular packages are currently not available. In general, many personnel involved in plant operations have a poor perception of modeling tools as a means of solving practical problems, primarily because of a lack of good information dissemination concerning these tools, their usability, and the validity of results.

Data/Basic Sciences

Inadequate understanding of the basic chemistry and physics related to fluid flows is a limiting factor to the advancement of CFD, particularly for reactive and/or turbulent multiphase flows. Lack of knowledge of residence times, interfacial phenomenon, distribution of materials in the flow, interphase coupling, turbulence, and general flow characteristics inhibits the development of relations needed to model fluid flows in more complex situations. Experimental data and physical properties data that could provide empirical relations for multiphase flows are also lacking.

Computational Limits

While computing power has increased dramatically, many computational tools have not been upgraded to take advantage of new capabilities. Current computational methods place limits on the size of the problem that can be simulated—limiting the development of CFD for many important problems (e.g., coupling of turbulence and interfacial chemistry, modeling complex polymer rheology). A more generic limitation applicable to many higher level simulations is the inability to integrate multi-disciplinary problems in a single computational tool. For multiphase flow simulations, the lack of general relations for the coupling of turbulence, chemistry, phase

Exhibit 6-1. Technology Barriers to the Development and Use of Computational Fluid Dynamics

Practical Usability	Data/Basic Sciences	Computational Limits	Commercial Software Development	Computer Hardware/ Architecture
Excessive time required for engineer to set up the simulation Inadequate usability of computational tools/results by plant support engineers Solutions are not conveniently accessible Lack of different levels of modeling and simulation (simple vs. complex) Poor transfer of information about computational tools and their usefulness Poor perception and acceptance of modeling tools and results by plant personnel Lack of support to link current CFD tools to chemical engineering infrastructure	Lack of data/knowledge of residence times, interfacial area, distribution of materials, scaling Insufficient knowledge of fluid flow characteristics Lack of appropriate coupling of chemistry to multi-phase physics Poor understanding of underlying physics of multi-phase conditions (e.g., turbulence, interfacial phenomenon) Lack of experimental data for multi-phase flows Lack of physical properties data for multi-phase flows	Limits on the size of the problem that can currently be simulated, such as - turbulence - interfacial chemistry - segregation - complex polymer rheology - complex processes - time dependence Inability to integrate multi-disciplinary problems in a single computational tool Lack of closures for turbulence, chemistry, phase interfaces, and boundary conditions Inadequate mathematical methods Fine-scale physical features of multi-phase flow are not captured in any canonical set of equations	Chemical manufacturers lack the resources to effectively commercialize software Chemical manufacturers lack the resources to support software documentation, help files, on-line help, and training In-house codes developed by industry are typically usable only by specialists, not general Few chemical companies are motivated to refine models for general use Developing commercial software for small markets is cost-prohibitive for a single vendor	Inadequate speed of computation Lack of solution-dependent grid refinement (relates to computing efficiency) Inadequate data management devices for the enormous data sets generated

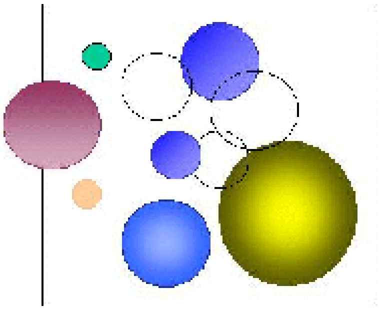
interfaces and boundary conditions is a limiting factor in CFD development. In general, mathematical methods are still inadequate for complex CFD.

Commercial Software Development

The manufacturing industries, particularly the chemical industry, are avid users of sophisticated scientific and engineering software, but seldom develop it for commercial use. Manufacturing companies do not have the resources needed to commercialize software, which includes support for auxiliary functions (e.g., documentation, help files, on-line help support, training, debugging, and upgrading) to meet customer needs. Commercial software companies find it difficult and expensive to develop, support, and sell specialized programs for relatively small markets. While the market for CFD in the chemical processing industries is potentially very large, current CFD packages are not “usable” enough to capture that market. A number of manufacturers have developed CFD codes for in-house use, but many are only usable by the researchers who developed them (specialists), rather than by the broader chemical engineering community (generalists). These in-house codes often become orphans and fall into disuse because they are not updated to keep up with newer science, better concepts in software architecture, or improved paradigms for user interfaces.

Computer Hardware/Architecture

In spite of the many advances in computer hardware and architecture, computer hardware still places limits on highly complex computational tools like CFD. Current computer systems are still not quite fast enough to effectively perform the many thousands of calculations required for a multiphase flow simulation. The promise of parallel computing has been limited in general by software development and code portability issues related to the lack of a parallel computer architecture standard. Computing efficiency is also currently limited by the lack of solution-dependent grid refinement in commercial CFD programs. In addition, while new storage mechanisms are emerging continually, none are entirely adequate for managing the enormous sets of data generated by reactive, multiphase CFD solutions.



7 Research Needs

The primary goal of research in CFD is to extend current CFD capabilities to accurately model multiphase flows, including reactive and/or turbulent flows. Some of the physical models and advanced numerics needed to address these flows exist, but commercial CFD vendors have been slow to incorporate them into readily available and fully supported CFD tools that are compatible with the needs of the chemical industry. The following areas are of particular importance to chemical processing:

- **Turbulent/Reacting Flow** - simulation of turbulent flows with chemical reactions, including gas phase, liquid phase, and multiphase reacting flows. For example, prediction of turbulence and its effect on fast reactions in a liquid phase stirred tank reactor remains an unsolved problem. Applications include turbulent combustion, chemical reactors with mixing, gasification of solids, and hydrocarbon production.

- **Multiphase Flow** - simulation of flows containing solids in gas, solids in liquid, gas bubbles in liquid, liquid emulsions, and liquid sprays in gas. Applications include design of safety relief devices for reactors and tanks, optimizing burners and waste incinerators, eliminating wear failure in pneumatic conveyors, controlling crystallization of fine chemicals, and improving reactor performance.

- **Viscoelastic Polymer Flow** - simulating flow of polymers with non-Newtonian rheology into a mold, through a die, extruder barrel, or gear pump. Applications include coating and fiber spinning.

Three-Phase Flow Problems

- Mixing
- Packed Beds
- Crystallizing/Dissolving
- Sprays
- Three-phase Flows in Pipes
- Biological Systems
- Bubble Column Catalytic Reactors

Two-Phase Flow Problems

- Riser Reactors
- Fluidized Beds
- Spray Dryers
- Pneumatic Conveyors/Classifiers
- Gas-Solid Jets

Research needed to overcome barriers to the development of CFD tools that can be effectively applied to the simulation of chemical processes is shown in Exhibit 7-1, with different priority levels identified. Exhibit 7-2 illustrates the time frame (near, mid, and long term) in which various R&D activities are expected to be accomplished.

Exhibit 7-1. Research Needs for Computational Fluid Dynamics

Numerical Methods	Phenomenology and Constitutive Relations	Experimental Validation
Characterize/model dilute to dense phases ✪ Develop relevant data sets for code verification and scaling ✪ Incorporate complex geometry ● Develop adaptive computational grids ● Design modules to customize complexity for different user needs ● Improve parallelization techniques ● Develop more efficient, accurate algorithms and solvers ● Characterize/model chemistry and chemical coupling phenomenon for multi-phases ❍ Develop algorithms to treat the changing position of a free surface (e.g., molten polymers) ❍ Develop wrap-around optimization using large-scale CFD simulation and small parameter models ❍	Characterize/model dilute to dense regimes (e.g., laminar/turbulent flows) ✪ Characterize/model interactions between phases ✪ Develop reliable turbulence closures for multi-phase flows ✪ Characterize boundary conditions and interactions (e.g., inlets and wall and interior surface interactions) ✪ Develop chemistry models for volume and surface phenomenon ● Characterize/model polydisperse systems ❍ Incorporate population balance ❍ Characterize/model multiphase heat transfer ❍	Design/develop multiphase flow test beds ✪ Perform experimental validation at small scale ✪ Conduct small and large scale separate effects tests ✪ Develop new diagnostics and sensors for experimental measurement of multi-phase flows ✪ - Non-invasive - Full-field, rather than local or averaged - Increase spatial and temporal resolution Enhance capability for analysis of results ● Develop new experimental methods applicable to large scale flows ●

Key: ✪ = Top Priority ● = High Priority ❍ = Medium Priority

Numerical simulation capabilities for multiphase CFD should be developed at three levels which parallel those used in single phase CFD. These include direct numerical simulation (DNS), large eddy simulations (LES), and Reynolds Averaged (RA) simulations (see Section 3 - Current Situation). Extension of these single phase methods to multiphase systems will require an integrated effort that involves development of numerical methods, constitutive theory and concurrent experimental validation.

Numerical Methods

Ultimately, the goal is to develop numerical capabilities that are efficient, accurate and allow simulation of the complicated patterns involved in chemical processes (e.g., mixing), with the ability to model conditions as they change over time. Research needs in numerical methods will help to overcome some of the more critical barriers associated with current computational limits and advanced computer architectures. For example, the development of adaptive computational grids and improved parallelization techniques will enable better integration of CFD with high performance computing platforms. The development of more efficient, accurate algorithms and

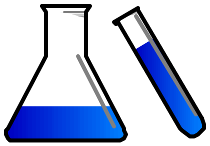
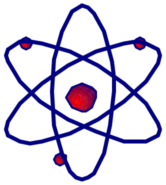
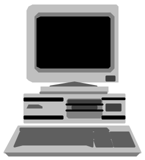
	Near Term (0-3 years)	Mid Term (3-5 years)	Long Term (5-10 years)	All Time Frames
Experimental Validation 	Develop multiphase flow test beds		Develop new experimental methods applicable to large scale flows 💣 Enhance capability for analysis of results 💣	Perform experimental validation at small scale ✪ Conduct small and large scale separate effects tests ✪ Develop new diagnostics and sensors for experimental measurement of multi-phase flows ✪
Phenomenology and Constitutive Relations 		Characterize/ model dense phases (e.g., laminar / turbulent flows ✪ Characterize/ model interactions between phases ✪ Develop reliable turbulence closures for multi-phase flows ✪ Characterize boundary conditions and interactions (e.g. inlets and wall and interior surface interactions) ✪	Incorporate population balance ☞	Develop chemistry models for volume and surface phenomenon 💣
Numerical Methods 		Characterize/ model dense phase ✪ Develop more efficient, accurate algorithms and solvers 💣	Incorporate complex geometry 💣 Develop adaptive computational grids 💣 Improve parallelization techniques 💣 Model changing positions of a free surface ☞ Develop wrap-around optimization using large-scale CFD simulation and small parameter models ☞	Develop models to customize complexity for user needs Develop relevant data sets for code verification and scaling ✪ Characterize/ model chemistry and chemical coupling phenomenon for multi phase ☞

Exhibit 7-2. Research Needs Time Frame

mathematical solvers will enhance computational efficiency and speed. Research will also strive to overcome barriers created by the lack of understanding of basic chemistry and physics of multiphase flows (e.g., characterization of chemistry and chemical coupling phenomenon).

In terms of time frames for R&D (see Exhibit 7-2), early progress in the development of dense phase models will be essential to the overall research program in numerical methods. Development of relevant data sets for validation and scaling is needed throughout the program. The same is true for chemistry and chemical coupling models—development should begin with less-detailed models that are continually improved in terms of model complexity and flow coupling. Parallelization is an important part of the research plan, but is not the primary focus of early work. In the area of optimization, both direct optimization using large-scale CFD simulations and "small parameter" models that can be run separately from the simulation will be explored. Modeling the changing position of a free surface (for polymer flows), developing adaptive computational grids and the ability to model flows around complex geometries will be a long-term effort.

Phenomenology and Constitutive Relations

Constitutive relations are needed to accurately describe the chemical and physical phenomenon occurring in specific fluid flows. The development of accurate constitutive relations is a continuing process of interactions between derivations based on theory, simulations, and experiments. The accuracy of constitutive relations must be demonstrated through a verification process in which simulation results are carefully compared with detailed experimental data. Verification requires simplified, idealized experiments which allow one feature of the process to be isolated and examined. In general, the desire is to obtain constitutive relations that are accurate, verified, simple, consistent, hierarchical, general, and theoretically based.

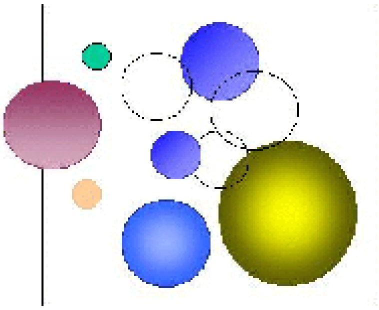
Ideally research in this area will progress along with an increased understanding of the chemistry and physics of multiphase flows (e.g., modeling of dense phases, characterization of boundary conditions, development of chemistry models). The development of reliable turbulence closures for multiphase flows and the incorporation of population balance will enhance computational efficiency and improve the accuracy and reliability of results.

Early progress in dense phase models, along with development of reliable turbulence closures, characterization of boundary conditions (inlets and wall and exterior surface interactions), and modeling of interactions between phases will be essential to this research activity. Chemistry models will be important throughout this research, including development of models of increasing complexity from reduced models to full chemistry with surface chemical effects.

Experimental Validation

A well-planned experimental program will provide validation of model results for complex multiphase flows and increase the usefulness of results to plant engineers, enhancing overall CFD usability. Experimental validation goes hand in hand with research in numerical methods and constitutive relations. Experimental tests at a small scale are needed for model development as well as closures for turbulence, chemistry, phase interfaces, and boundary conditions. Large scale experimental measurements will be equally important for validating model performance. A strong experimental program is essential to the overall research plan, as the experimental measurements of multiphase flows are extremely difficult to obtain and require careful analysis when comparing with model results.

The optimal multiphase flow diagnostic for validation of multiphase flow models provides non-invasive, full-field, spatially (in space) and temporally (over time) resolved measurements of velocity, pressure, temperature, material phase, and chemical composition. A portion of the research program is designed to overcome the lack of diagnostics currently available for providing information at this level. A wide variety of physical techniques (e.g., acoustic, electrical, optical, radiation) should be examined as possible diagnostic tools. Development of advanced multiphase-flow test beds will be essential for evaluating a wide range and scale of flows (e.g., size, velocity) and controlling flow regimes. They will serve as platforms for evaluating diagnostics as well as acquiring data for model development and validation.



8 Summary

CFD Goals

CFD can assist the design and optimization of new and existing processes and products. CFD can also be used for reducing energy costs, improving environmental performance, and increasing productivity and profit margins. Although single-phase CFD has been applied to great advantage in the aerospace, automotive, and power industries, the current packages available are limited for use in the chemical industry, particularly for reacting and/or turbulent multiphase flows. The chemical industry needs advanced CFD software that can be used by a broad segment of the chemical community to solve more complex flow problems. CFD tools for the chemical industry need to be:

- Versatile — portable to various machines, usable by generalists rather than just specialists, scalable, reliable, and compatible with current chemical industry data bases.
- Fundamentally Based — containing more and better physics coupled with chemical reactions, rather than non-mechanistic correlations that are not scalable.
- Experimentally Verified — simulations validated with experimental results.
- Computationally Efficient — adaptable to multiprocessor work stations and clusters of processors, able to expediently provide useful results.
- User Friendly — accompanied by professional technical support that is appropriate for industrial engineers as well as researchers.
- Information Transfer — include mechanisms for information dissemination and educational support.

The Road to Follow

Workshop results have demonstrated that precompetitive research and development is needed to advance the state of the art and to build capabilities for computing multiphase flows. Research should include activities in numerical methods and constitutive theory to advance computational capability for reactive and turbulent multiphase flows. The research agenda should include a well-integrated experimental program that will allow validation of models developed for practical chemical processes.

For effective resource leveraging, risk minimization, and providing a stable baseline for funding, precompetitive research should be cooperatively supported through the chemical industry, commercial software vendors, and the Federal government (Department of Energy and Department of Defense).

For maximum use by industry, the development process will be directed by the technology users - the U.S. petrochemical industry.

Industry has identified the Federal R&D Laboratory system as a candidate for leading CFD technology development. As such, Federal support of R&D laboratories for CFD development, on behalf of industry, could maximize the returns on the R&D investment. Project selection, control, and evaluation should be carried out by a broad cross-section of potential industrial users. Federal laboratories can partner with individual industries for technology development, and universities can address fundamental issues in the development of this technology.

The technology cannot be widely applied without the customer service and support base of the software business, and these businesses must be brought into the technology program as soon as possible.

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