Attachment 8
Spectral Models, Symmetry and Engineering Turbulence Closures
Tim Clark
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TITLE: **SPECTRAL MODELS, SYMMETRY AND ENGINEERING TURBULENCE CLOSURES**

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A8.2

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May 19, 1995

A8.3

Spectral Models

Consider a "Two-Point" Generalization of the Reynolds Stress Tensor (for a Single Fluid)

$$R_{ij}(\mathbf{x}_1, \mathbf{x}_2, t) = \left\langle u_i'(\mathbf{x}_1, t) u_j'(\mathbf{x}_2, t) \right\rangle$$

Derive an exact transport equation via Navier-Stokes, and (1) change coordinates:

$$\mathbf{X} = \frac{1}{2}(\mathbf{x}_1 + \mathbf{x}_2), \quad \mathbf{r} = \mathbf{x}_1 - \mathbf{x}_2$$

(2) Fourier Transform with respect to the relative coordinate, $\mathbf{r}$, and (3) perform angular integrations to reduce the vector-$\mathbf{k}$ space to a scalar k-space;

$$R_{ij}(\mathbf{x}_1, \mathbf{x}_2, t) \xrightarrow{1} R_{ij}(\mathbf{X}, \mathbf{r}, t) \xrightarrow{2} R_{ij}(\mathbf{X}, \mathbf{k}, t) \xrightarrow{3} R_{ij}(\mathbf{X}, k, t)$$

Result: A spectral model of the turbulent Reynolds stress, related to the "single-point" engineering model by integration over wavenumber;

$$R_{ij}(\mathbf{X}, t) = \int_0^\infty R_{ij}(\mathbf{X}, k, t) dk = 2 \int_0^\infty E_{ij}(\mathbf{X}, k, t) dk$$

where the "Energy Spectrum" $E(k,t)$ is $E_{nn}(k,t)$, the turbulent kinetic energy $K(t)$ is

$$K(\mathbf{X}, t) = \int_0^\infty E(\mathbf{X}, k, t) dk$$

Requires no dissipation equation, or length-scale equation.
Permits computation of "non-equilibrium" turbulence.
Cost of direct numerical solution is much more costly than using a spectral model, which is more costly then using an engineering closure.

Turbulence and Symmetry

"A turbulent flow, initialized at t=0 in some arbitrary way, may relax, after some transient period, to a self-similar flow."

The turbulence may satisfy the same symmetries and scalings as the governing equations, i.e., the Navier-Stokes Equations.

Self-Similarity originates in invariance of the turbulence dynamics under a group of transformations, e.g., space-time transformations such as (for isotropic)

$$t' = \rho t, \qquad (time\ \ scaling),$$

$$t' = t + t_0 \qquad (time\ \ translation),$$

$$\ell' = \sigma \ell, \qquad (length\ \ scaling).$$

Consider a scaling subgroup, $\rho^{\gamma} = \sigma$; for which an invariant solution obeys

$$\rho^{3\gamma-2} E(k,t) = E(\rho^{-\gamma} k, -t_0 + \rho(t + t_0)).$$

This can be shown to have a solution of the form (Karman-Howarth)

$$E(k,t) = K(t) L(t) f\big(kL(t)\big),$$

where $f(\xi)$ satisfies an auxiliary equation given by a theory, model, Navier-Stokes etc. Time dependencies are

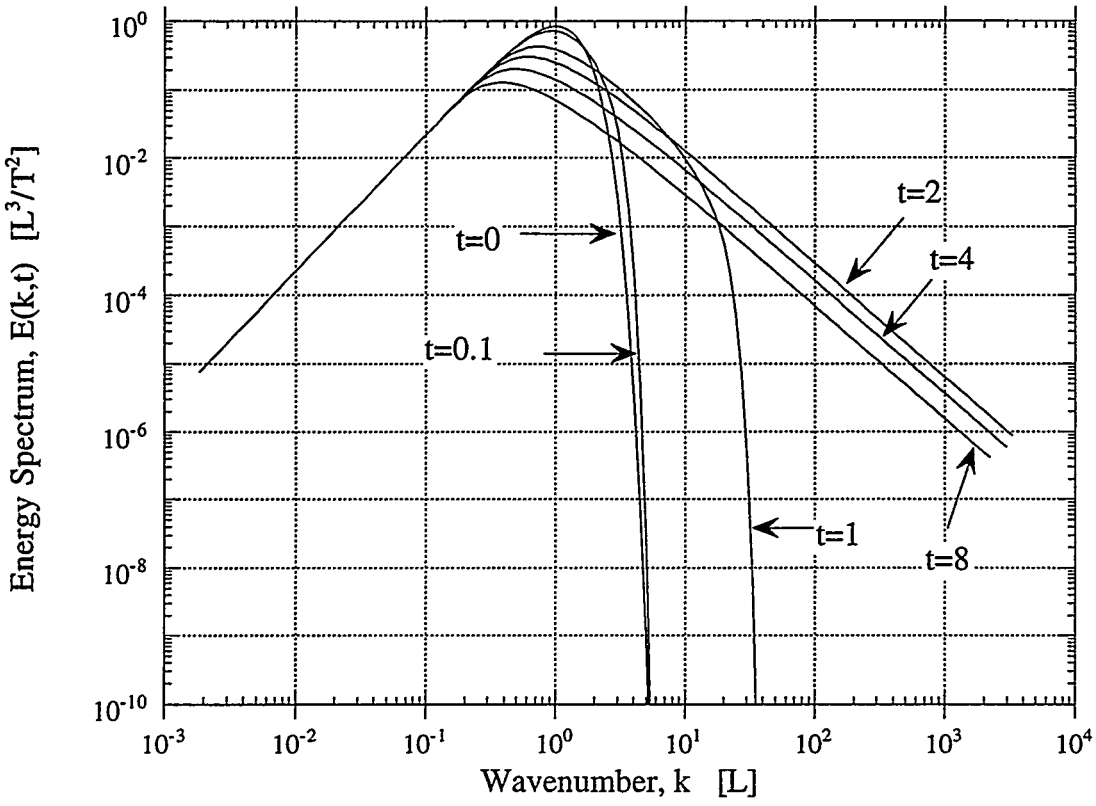
$$K(t) = K_0 \,(1 + t/t_0)^{-\gamma_K}, \;\; L(t) = L_0 (1 + t/t_0)^{\gamma},$$

and

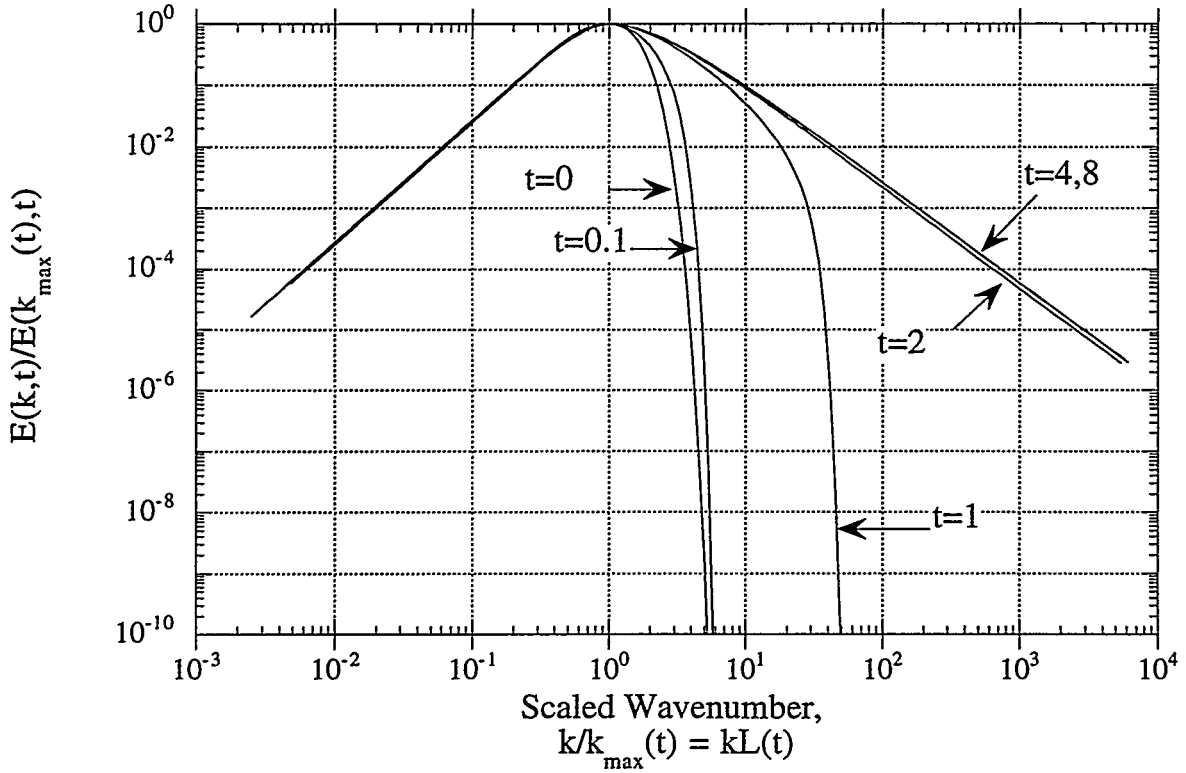
$$\gamma_K = 2 - 2\gamma.$$

This agrees precisely with K-ε closures and with results from (all?) spectral models for isotropic turbulence.

A8,5



Energy Spectrum



Energy Spectral Shapes

A8.6

Self-Similarity and Engineering Closures

Assertion: Single-Point (Engineering) closures can be rigorously correct in the limit of spectral self-similarity.

Consider the self-similar form for turbulence at high Reynolds number subjected to a homogeneous mean flow velocity gradient;

$$E_{ij}(k,t) = K(t)L(t)f_{ij}\big(kL(t)\big).$$

In general, each f_{ij} is different. During free decay, (upon releasing the mean flow strain or shear) the spectrum tends asymptotically towards the form

$$E(k,t) = K(t)L(t)f\big(kL(t)\big).$$

and

$$\tilde{E}_{ij}(k,t) = E_{ij}(k,t) - \frac{1}{3}\delta_{ij}E(k,t) = \tilde{K}_{ij}(t)L(t)\tilde{f}\big(kL(t)\big)$$

where

$$\tilde{K}_{ij}(t) = \frac{1}{2}\tilde{R}_{ij}(k,t) = \frac{1}{2}\left(R_{ij}(k,t) - \frac{1}{3}\delta_{ij}R_{nn}(k,t)\right)$$

Simple Group analysis (and the spectral model) predicts the same time dependencies of $\tilde{K}_{ij}(t)$ and $K(t)$. Hence the anisotropy, given by

$$b_{ij}(t) = \frac{\tilde{K}_{ij}(t)}{K(t)},$$

asymptotes to a constant--No Long-Term Return to Isotropy!

Conclusion: The detailed process of "Return Toward Isotropy" is a non-equilibrium process, not accurately depicted by engineering closures.

Example: Experiment of Uberoi & Wallis (J. Fluid Mech. **24**, 1979).

Lesson: One should not ask "too much" of an engineering closure.

Construction of Engineering Closures From Spectral Closures

(1) Determine the appropriate similarity group for the problem class.
- -Might be an approximation.
- -In conjunction with direct computation of the spectral model, and direct numerical simulation.

(2)Determine the self-similar form of the spectra.

(3) Substitute the self-similar expression into the spectral model equations, and take "appropriate" k-space moments.

> "Appropriate" moments may be a product of the tastes of the researcher. E.G., does one want a dissipation rate equation or a length scale equation?

(4) Model coefficients will depend on spectral moments and are determined by the details of the self-similar forms produced by the spectral model.

Example: K-ε -b_{ij} models constructed from self-similar form for homogeneous mean-flow form.

K-Equation

$$\frac{\partial K(t)}{\partial t} = -2\frac{\partial U_n}{\partial x_m} b_{nm} - \varepsilon$$

where

$$b_{ij} = \int_0^\infty \tilde{f}_{ij}(\xi) d\xi .$$

ε-Equation

$$\frac{\partial \varepsilon}{\partial t} = -\left\{ g_{\varepsilon 0} b_{nm} + g_{\varepsilon 1} \phi_{nm} \right\} \frac{\partial U_m}{\partial X_n} \varepsilon - g_{\varepsilon 2} \frac{\varepsilon^2}{K}$$

where

$$g_{\varepsilon 0} = \frac{3m-2}{m},$$

$$g_{\varepsilon 1} = \left(\frac{3c_{F2}m+2}{m} \right),$$

$$g_{\varepsilon 2} = \frac{1}{m} \left(\frac{3m-2}{2} + \frac{1}{\alpha} \frac{J(m)}{I_{nn}(m)} \right),$$

$$\phi_{ij} = \frac{\tilde{I}_{ij}(m)}{I_{nn}(m)},$$

$$I_{ij}(m) = \int_0^\infty \xi^m f_{ij}(\xi) d\xi,$$

and

$$J(m) = \int_0^\infty \xi^m \frac{d}{d\xi} F_f(\xi) d\xi.$$

b_{ij}-*Equation* (Algebraic)

$$(c_B - 1)\left\{\frac{\partial U_i}{\partial x_n} b_{nj} + \frac{\partial U_j}{\partial x_n} b_{ni} - \frac{2}{3}\delta_{ij}\frac{\partial U_m}{\partial x_n} b_{nm}\right\}$$

$$+c_{B1}\left\{\frac{\partial U_n}{\partial x_i} b_{nj} + \frac{\partial U_n}{\partial x_j} b_{ni} - \frac{2}{3}\delta_{ij}\frac{\partial U_m}{\partial x_n} b_{nm}\right\}$$

$$+c_{B0}\left\{\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i}\right\} + 2\frac{\partial U_n}{\partial x_m} b_{nm} b_{ij}$$

$$= \frac{\varepsilon}{K}\left\{\frac{c_M}{\alpha}\beta_{ij} - b_{ij}\right\},$$

where

$$\beta_{ij} = \int_0^\infty \xi^{3/2} f_{nn}^{1/2}(\xi)\tilde{f}_{ij}(\xi) d\xi .$$

Conclusion

Symmetry considerations and transformation groups provide a frame work to view the behavior of turbulence and closures without resort to ad-hoc modeling hypothesis.

Spectral models provide a much richer picture of the dynamics of turbulence and mix than do engineering closures, but at a greater computational cost.

In the limit of self-similarity (where a group transformation applies) engineering closures can be derived rigorously from spectral closures.

Likewise, the absence of any such self-similarity might indicate that the engineering closure is, at best, approximate.

Future

Presently incorporating effects of helicity ("swirl") which adds an additional level of complexity to the modeling and direct numerical simulations.

Additional self-similarities ?

Derivation of multi-scale models or "reduced spectral" models for use in large computer codes;

Applicable to non-self-similar turbulence.

More tractable than full spectral closure.

Attachment 9
Review of 1st Industrial Energy Efficiency Symposium and Expo
Ed Joyce
LANL

Bryan just a "Draft" for Tomorrow.

Review of the 1st Industrial Energy Efficiency Symposium and Expo

- **Industry/Federal/ University Symposium, Highlighting the DOE-OIT "Industries of the Future" Program, which includes:**
  - **Chemicals**
  - **Petroleum Refining**
  - **Forest Products**
  - **Glass**
  - **Aluminum**
  - **Metal Casting**
  - **Steel**

A9.2

Industry/National Laboratory Collaborations for the "Industries of the Future"

- "Virtual Laboratories"- Centers of Excellence
  - Coordinating Council with All Laboratories Represented
  - Working Groups for All Stated Industry Needs with Laboratory Peer Review
  - One Stop Shopping

Attachment 10
A View from Washington
Dan Wiley
DOE Office of Industrial Technologies

A MOMENT OF TRUTH FOR AMERICA.

Imagine life without polio vaccines and heart pacemakers. Or digital computers. Or municipal water purification systems. Or space-based weather forecasting. Or advanced cancer therapies. Or jet airliners. Or disease-resistant grains and vegetables. Or cardiopulmonary resuscitation (CPR).

We take for granted these and thousands of other technological breakthroughs that have made American society the most advanced in history. They have made our economy more competitive, created millions of jobs, and underpinned our entire standard of living. They have vastly improved our health and extended our life span. In a very real sense, they epitomize the American Dream.

But these breakthroughs didn't just happen. They are the products of a long-standing partnership that has, as a matter of national policy, fostered the discovery and development of new technologies. For many years, Administrations of both parties, working with Congress, have consistently supported university research programs as a vital investment in our country's future. Industry has played an equally critical role, carefully shepherding these new technologies into the marketplace.

This partnership — the research and educational assets of American universities, the financial support of the federal government and the real-world product development of industry — has been a critical factor in maintaining the nation's technological leadership through much of the 20th century.

Just as important, university research has also helped prepare and train the engineers, scientists and technicians in industry whose discipline and skill have made technological breakthroughs possible. It has sparked innovation and prudent risk-taking. And as a result of the opportunity afforded such skilled workers in our technologically advanced economy, many disadvantaged young people have used high-tech jobs as a "stepping stone" to more productive and satisfying lives.

Unfortunately, today America's technological prowess is severely threatened. As the federal government undergoes downsizing, there is pressure for critical university research to be slashed.

University research makes a tempting target because many people aren't aware of the critical role it plays. It can take years of intense research before technologies emerge that can "make it" in the marketplace. History has shown that it is federally sponsored research that provides the truly "patient" capital needed to carry out basic research and create an environment for the inspired risk-taking that is essential to technological discovery. Often these advances have no immediate practical usability but open "technology windows" that can be pursued until viable applications emerge. Such was the case with pioneering university research done on earthquakes in the 1920s, which led over time to the modern science of seismology and the design of structures that better withstand earthquake forces.

Today, we, the undersigned — executives of some of America's leading technology companies — believe that our country's future economic and social well-being stands astride a similarly ominous "fault line." We can personally attest that large and small companies in America, established and entrepreneurial, all depend on two products of our research universities: new technologies and well educated scientists and engineers.

Technological leadership, by its very nature, is ephemeral. At one point in their histories, all the great civilizations — Egypt, China, Greece, Rome — held the temporal "state of the art" in their hands. Each allowed their advantage to wither away, and as the civilization slipped from technological leadership, it also surrendered international political leadership.

For all these reasons, it is essential that the federal government continue its traditional role as funder of both basic and applied research in the university environment. If we want to keep the American Dream intact, we need to preserve the partnership that has long sustained it. As we reach the final years of the century, we must acknowledge that we face a moment of truth:

Will we nurture that very special innovative environment that has made this "the American century"? Or will we follow the other great civilizations and yield our leadership to bolder, more confident nations? As the Congress makes its decisions on university research, let there be no mistake: We are determining the 21st century *today*.

W. Wayne Allen
Chairman & CEO
Phillips Petroleum Company

Norman R. Augustine
President
Lockheed Martin Corporation

John L. Clendenin
Chairman & CEO
BellSouth Corporation

Robert J. Eaton
Chairman & CEO
Chrysler Corporation

George M. C. Fisher
Chairman, President & CEO
Eastman Kodak Company

Robert W. Galvin
Chairman, Executive Committee
Motorola, Incorporated

Louis V. Gerstner, Jr.
Chairman & CEO
IBM Corporation

Joseph T. Gorman
Chairman & CEO
TRW, Incorporated

Gerald Greenwald
Chairman & CEO
United Airlines

George H. Heilmeier
President & CEO
Bellcore

Jerry R. Junkins
Chairman, President & CEO
Texas Instruments, Incorporated

John McDonnell
Chairman
McDonnell Douglas Corporation

Randall L. Tobias
Chairman & CEO
Eli Lilly and Company

P. Roy Vagelos, M.D.
Former Chairman & CEO
Merck & Company, Incorporated

John F. Welch
Chairman & CEO
General Electric Company

Edgar S. Woolard, Jr.
Chairman & CEO
E.I. DuPont DeNemours and Company

From WSJ

A10.2

Attachment 11
Some thoughts on a potential CFD consortium
Tyler Thompson
Dow

"In those days there was
no king in Israel;
every man did that which was
right in his own eyes."

Judges 21: 25 (KJV)

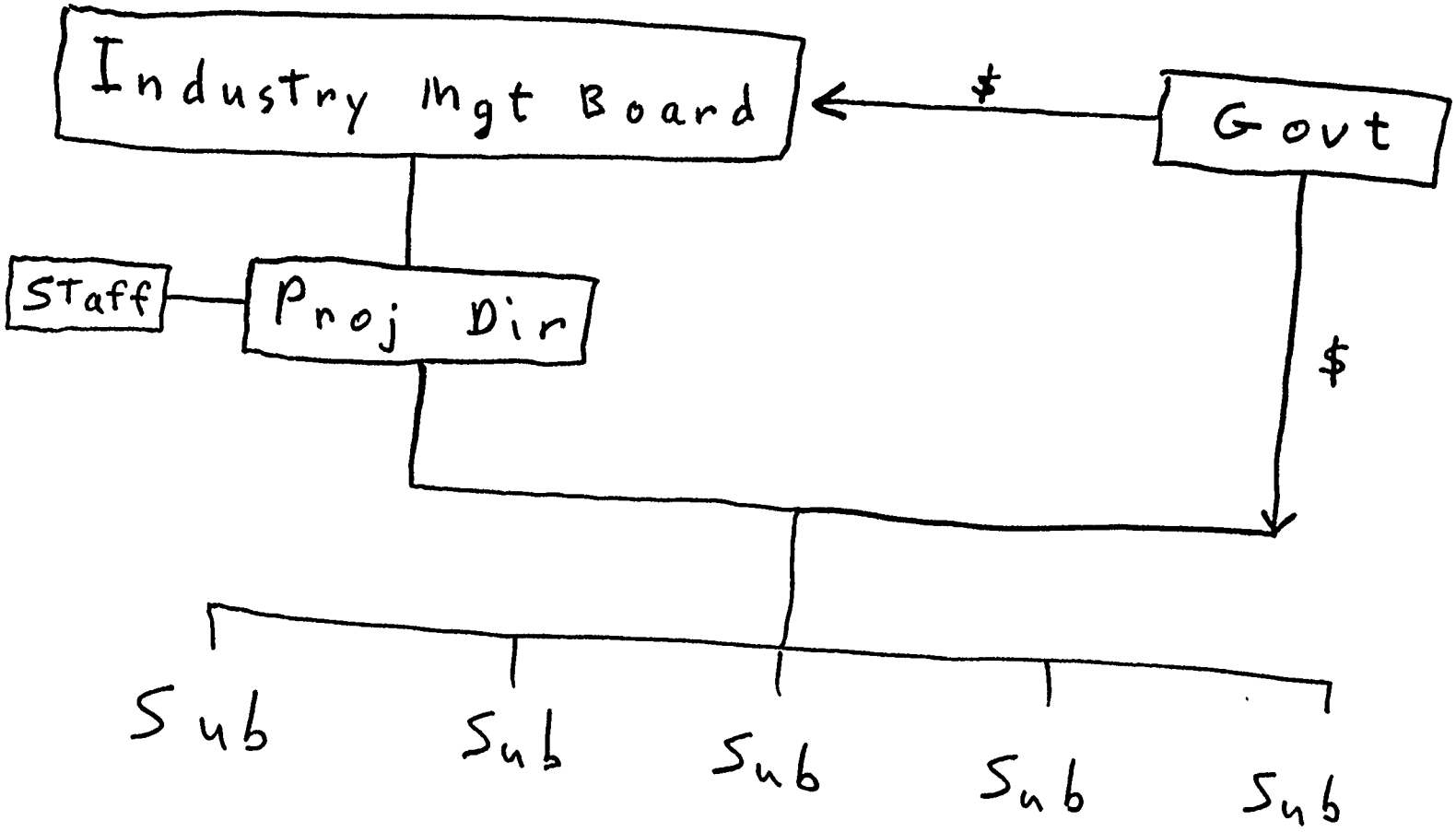
Premise

- Existing tools inadequate
  - Turbulent Reacting Flow
  - Multiphase Flow
  - Polymer melts & solutions
    - 3 D
    - Time-dependent
    - Non-Newtonian rheology
    - Free surface

Why inadequate?

- Historical market
- Legacy architecture
- Slow to implement advances
- Promise of Parallel

Model



A11.5

Essentials

Govt. support

Industry direction

effectiveness vs fairness

Commercial vendors

Deliverables

National best

Who's Heard?

Univ. Utah - Phil Smith

REI - Mike Heap

PNL - Jim Fort
Don Trent
Nick Lombardo
Marv Clement
Steve Weiner

LANL - Jeff Salzman
Dan Butler
Dick Siemon

LLNL - John Bell

Univ. CA Berkeley - Phil Colella

DOE - Dale Schaeffer

Al McLauchlin

Du PonT - Hank Morneau

HoechsT - Celanese

From
Tyler B Ronson, Dow Chemical

May 1995

Computational Fluid Dynamics (CFD)

Situation A wide variety of CFD tools developed for other industries (aerospace, automotive, and power) are currently being used to solve problems in the chemical process industry (CPI). Although CFD is having an impact, the available tools clearly have limitations for many applications unique to the CPI. This is especially true for applications that require coupling of chemical reactions with fluid mechanics. Examples of CPI specific problems that are not satisfactorily addressed include:

- fully turbulent reacting flow
- multiphase flows (reacting or not)
- viscoelastic laminar flows with free surfaces (polymer melt into a die)

Many of the physical models and advanced numerics needed to address these problems exist, however they are slow to be incorporated into readily available and fully supported CFD tools. Another general limitation of available CFD tools is the lack of a common chemical engineering infrastructure to allow linking with CPI programs for physical and chemical property databases.

Vision In the CPI of the future, CFD will be used along with other modeling tools for optimization of existing product lines and for reduced time to market for new products/processes. In this role, CFD will be specifically used to help guide and shorten the cycle for experimental optimization and scaleup.

Challenges The principal challenge is to produce a CFD tool that is tailored to the needs of the CPI. This will require effective collaboration between those with technology (CPI and federal labs), those with need (CPI), those with resources (industry and federal government), and those that can provide support (commercial software vendors). Success will also require progress in the areas of software and computing. Common to applications of CFD in other industries, progress is paced by growth in computational power and its effective use. The promise of parallel computing has been limited by software development and code portability issues that are caused mainly by the lack of a parallel computer architecture standard.

Critical Success Factors We will know we are successful when we can use CFD to model a significantly wider range of CPI-specific problems, with turnaround times that facilitate its use in the design process. Examples of CPI-specific problems that CFD should solve include:

- Combustion and related high temperature gas-phase systems (e. g., incineration, thermally activated reactions, gasification, light hydrocarbon production)
- Multiphase mixing in a tank with baffles and an impeller (e. g., polymer

production)
- Polymer processing with non-Newtonian rheology in extruders and dies (e. g., plastic film production)
- Dense multiphase turbulent flows (e. g., solids conveying)
- Dense multiphase turbulent reacting flows (e. g., ceramics production)
- Crystallization with particle nucleation and growth (e. g., caustic production)

Second, we will know we are successful when this software tool is in the form of a single commercial quality CFD platform that is not only usable by dedicated specialists, but by knowledgeable generalists, as well. Finally, we will know we are successful when this software platform allows rapid incorporation of new developments as CPI needs evolve and as simulation technology matures (software, hardware, numerics, models).

Strategy and Recommendations The initial task is to prioritize CPI simulation needs. This would be followed by a general state-of-the-art assessment of available codes and of current knowledge, theory, and methods relative to these needs. In parallel, flexible software paradigms would be explored for a new base code. Based on the results of these tasks, a clearly defined development path could be defined for the new CFD tool.

Ref. March 2, 1995 letter from Tyler Thompson (Dow Chemical) to Dale Schaefer (DOE) and attachment: Computational Fluid Dynamics for the Chemical Processing Industry

Computational Fluid Dynamics for the Chemical Processing Industry

Introduction

Significant efforts have been made to develop CFD packages that are applicable to the aerospace, the automotive, and the electric power industries. These packages have been used to solve problems in the Chemical Process Industry (CPI). However, like other industries, the CPI has special types of problems not addressed by current packages. Recent work at Dow sought to define projects of interest to the CPI, and to identify limiting shortcomings in commercial CFD software. This work has demonstrated the value of CFD to the CPI, and has identified three broad areas of application in which the available computational tools are not adequate for our needs. (1) Simulation of fully turbulent reacting flow systems. Since efficient chemical production is based upon transport processes of reacting systems, this ability is critical to applications in the CPI. (2) The simulation of several types of multi-phase flows (reacting or not). (3) Time-dependent, three-dimensional viscoelastic laminar flow with a free surface, such as flow of a polymer melt into a die. Collaborative efforts between the CPI, several federal research laboratories, and established hardware and software vendors could help facilitate development and implementation of new CFD packages focused on problems specific to the CPI.

Dow, Battelle Pacific Northwest Lab, and other parties are trying to assess the CPI's interest in organizing a research team and funding to address the development and implementation of the next generation of CFD, focused on reacting flow systems, multiphase systems, and polymer systems. Information presented here details issues important to the CPI related to this proposal. Results from an informal survey of Dow CFD users and their counterparts from other chemical companies are also presented.

Issues of Developing CFD for the CPI

A critical issue of this effort is identifying the technical objectives and approach. Questions such as: "why a new CFD package for the CPI?", "what's wrong with existing commercial programs?", and "what are the great 'challenges' the CPI must solve to be competitive in the next century?" must be considered.

Why a new CFD package for the CPI?

Developing a new code is driven by the need to solve "hard" problems important to the CPI. A "Hard" problem might include: (1) a complex 3-D geometry with sharp gradients (e.g., shock waves, highly exothermic reactions, or low-concentration non-accumulating reactive intermediates that are both produced and consumed at high rates); (2) non-trivial reaction kinetics confounded with turbulence; and (3) non-steady-state multiphase reacting flow with radiative heat transfer. Implementing one commercial-quality CFD computer program throughout a company, with provision for future support and further development is also central to this project.

Why not existing commercial packages?

A difficulty with current CFD codes is the time required to bring new technology to market. Generally, work at research laboratories is not incorporated into commercial codes for many years. This is due, in part, to the current architecture of CFD codes — implementation means a "new rewrite"! Generally, current CFD packages:

* do not fully utilize available computational horsepower (e.g., parallel computing);
* do not include available submodels of key subprocesses (e.g., crystal nucleation and growth), or the submodels aren't coupled properly (i.e., turbulence and chemistry);
* do not fully utilize leading edge numerical methods (e.g., adaptive gridding) or theoretical methods (e.g., advanced pdf-based turbulence models);
* do not have a common chemical engineering infrastructure to allow linking to common CPI programs (e.g., physical & chemical properties databases).

What are the "Grand Challenges" for the CPI?

Some of the "hard" problems that CFD should solve include:

* Combustion and related high-temperature gas-phase systems (e.g., incineration, thermally activated reactions, gasification, light hydrocarbon production).
* Multi-phase mixing in a tank with baffles and an impeller (e.g., polymer production).
* Polymer processing with non-Newtonian rheology in extruders and dies (e.g., plastic film production)
* Dense multiphase turbulent flows (e.g., solids conveying)
* Dense multiphase turbulent reacting flows (e.g., ceramics production)
* Crystallization with particle nucleation and growth (e.g., caustic production)

CFD Today and Tomorrow

Current work at Dow shows that CFD is used to solve real problems today! Typical applications included: rotary kiln incinerators, gas scrubbing, drying ovens, thermal oxidation, packed bed reactors, storage bin ventilation, crystallization, polymer extrusion, general mixing vessels, dust separation, impeller design, caustic evaporators, ceramic production, retention basin flow, membrane flow, liquid flow in polymer beds, degassing, and atomization nozzle design. In many of these projects, a key limitation has been coupling reactions with the fluid mechanics.

Recent development of new approaches to modeling turbulent mixing (e.g., pdf methods, linear eddy methods, large eddy simulations) and to coupling full reaction kinetics with turbulence (e.g., dynamic mechanism reduction) suggests that modeling turbulent reacting flows on today's computers is possible. However, given the rapid rate of development for hardware (parallel architecture), software (advanced numerics for parallel machines), and technology (submodel development), together with recent advances in object oriented programming it would be wise to develop a "new" base code on which to build.

It is desirable to design a "plug-and-play" code to allow easy insertion of new submodels and new solution algorithms on various hardware platforms. This is done using an object-oriented structure so a user selects sub-models and applicable solvers for the available hardware platform when developing a specific model for a problem. The new "plug-and-

play" approach would reduce effort needed to move new technology from the laboratory to industrial application. Presently, incorporation of new technology can take years — the suggested approach reduces this greatly.

However, development of a new CFD paradigm means starting over — no more band-aid approaches. This would require several partners from the CPI, the research community, the software vendors, and computer hardware vendors. Another critical ingredient is government support. The cost of long-range tool development is difficult to justify and sustain in an industry whose purpose is producing chemicals and materials. The increasing level of international competition and decreasing operating margins make it even harder.

Results of Initial CPI Survey

Results of an informal survey of both Dow and other CPI users are listed with follow-up comments.

Comments from Dow CFD Users

Initial responses from Dow's CFD user community are listed below:

* *The project scale seems ambitious; is too much promised?* The proposed project is based on current work at several U. S. research institutions.
* *Will this project be directed by members of the chemical industry to help focus the work on problems relevant to industry?* A close working relationship between industrial and research laboratories is critical to successful completion of this goal — a steering team is a reasonable approach.
* *Will this be a totally new code, not based on an existing code?* Given the proposed code structure, it would be impossible to modify an existing code. Of course, experience will form a basis for future efforts to reduce development time.
* *If the resulting code is totally "new", who will support it after the development phase?* This will be decided by the partners — but it most likely will be an existing software vendor with their support staff and facilities.
* *Given our limited understanding of turbulence, and its effect on reactions, can we hope to accomplish this project?* We are solving real problems with turbulent reacting flow today — we do our best with the tools we have. A platform that allows rapid implementation of new understanding is a critical concept of this project.
* *How will partners be identified, specifically software and hardware vendors?* The idea is to solicit proposals from each vendor and allow the CPI partners to select those that bring the most to the project.

Comments from CFD Users from Other Chemical Companies

The following comments were gathered at a recent meeting of representatives from several chemical companies.

* *The project goals reflect current CPI wants.* Not surprising, since the main goal of the project is aimed at the CPI.
* *There are no parallel architecture standards upon which enduring codes can be built.* The proposed code must be built independent of current computer architecture since architecture will continue to change and the code must change along with it to be usable.

* *Why not just hire a code developer to implement selected enhancements for the CPI into existing codes?* The band-aid approach is costly and does not allow timely utilization of new understanding and technology.

* *Would additional site presentations to member companies be possible to facilitate further discussion?* Both possible and desirable since the member companies are critical to the success of this project. This is not just a research project; it represents development of a critical technology for the CPI.

* *A technical assessment of current capabilities of existing CFD codes, both commercial and from the federal laboratories, should be performed.* A general state-of-the-art assessment of available codes and of current knowledge, theory, and methods should be the initial task. Even to get started, though, will require funding for up to a year for a highly expert and experienced core staff of perhaps two or three scientists.

* *Government support is essential if this project is going to happen!* Industry is not able to support this level of non-proprietary research project individually or collectively. Government support would provide an effective mechanism and encouragement for collaboration.

Conclusions

In conclusion, CFD is being used to solve "real" problems today at Dow and in the CPI. However, given the focus on chemical production, a special class of problems represents a "Grand Challenge" to the chemical industry. It appears that there is a need for a new CFD package specifically designed to address these problems for the CPI. To successfully develop this tool in a timely fashion will require several key ingredients including: government support, close collaboration between industrial and research laboratories, participation by both software and hardware vendors, and a basic paradigm shift in CFD code structure. A new "plug-and-play" tool that will allow the rapid implementation of new technology for industrial application is proposed. This new tool could help address key issues needed to support environmentally safe chemical production in efficient, profitable processes.

Additional Discussion

The following material provides some additional discussion of the importance and application of computational fluid dynamics in the chemical industry. It also addresses in more detail the need for government funding.

Computational fluid dynamics critical needs

Flow of matter and heat, with or without chemical reaction, is modeled and simulated in many areas of process research and development, and as part of environmental stewardship. The following three topics have been identified by research engineers in one chemical company as key needed capabilities that are lacking or inadequate in commercial software packages.

1. Turbulent reacting flow

Although CFD shows great promise for improving the productivity and reducing the environmental impact of chemical processes, the needs of the chemical industry have not been adequately served by the existing commercial CFD vendors. Because their products have evolved mainly from the aerospace, automotive, and power industries, they have given short shrift to problems involving complex chemical reactions, and turbulent reacting flows in particular. There is much active research in universities and federal labs on adaptive and moving grid methods, on modeling turbulence and multiphase flows, and on improved algorithms for new high-performance computers. The commercial vendors have been slow to implement these advances in their products. Chemical companies might ally with partners in the petrochemical industry, with aid from government, to develop a new CFD code or improve an existing one to meet our needs.

2. Multiphase flow

This includes solids in gas, solids in liquid, gas bubbles in liquid, liquid emulsions & latexes, liquid sprays in gas. Multiphase flows are ubiquitous in the chemical processing industry. Our ability to analyze and simulate these flows is important for:

a. designing safety relief devices for reactors and tanks

b. optimizing burners and waste incinerators to minimize hazardous emissions

c. eliminating wear failures in pneumatic conveyors

d. controlling crystallization of fine chemicals

e. improving performance of liquid-phase hydrogenation, oxidation, or chlorination reactors

3. Time-dependent modeling of viscoelastic polymer flows with free surface

Flow of molten polymer into a mold or through a die is a typical application. The calculation is particularly challenging when it must:

a. treat all three geometrical dimensions

b. simulate the flow varying with time rather than at steady state

c. handle non-Newtonian (viscoelastic) rheology

d. treat the changing position of a free surface

Development & support of sophisticated technical software with a limited market

The manufacturing industries in general, and the chemical process industry in particular, are increasingly avid users of advanced, specialized scientific and engineering software. We are reluctant occasional developers of it. We value the quality of commercial application software, with its refined user interfaces, user support, documentation, and sustained development. Nevertheless, many companies have developed their own in-house codes because it was essential to their business and unavailable commercially. The Dow Chemical Company has made some efforts to commercialize two such computer programs, but we wish it hadn't been necessary. Seldom does a single manufacturing company have either the incentive or the resources to do a good job at it. There has been much duplicated effort in many companies developing specialized software that is inferior compared to commercial standards. Such codes often become orphans and fall into disuse because they do not keep up with newer science, better concepts in software architecture, or improved paradigms for user interfaces. And yet, further development of such codes to implement the latest scientific advances and raise them to the quality of fully commercial software could have a major impact on the competitiveness of American manufacturers. Besides the cost savings from avoiding redundant efforts, major gains are available from wider use of fully supported, continuously improved, well documented, user-friendly software. Typical in-house codes may only be used by specialists, and sometimes only by the small group of scientists who developed the code. The best commercial software is usable by generalists: scientists and engineers who have a problem to solve or a project to finish, and don't want to make a career out of technical computing.

1. Cost

Manufacturing companies derive value from the application of technical software, not from the exclusive ownership and sale of it. Commercial software companies, on the other hand, find it difficult and expensive to develop, support, and sell specialized programs for such small markets. Because of this gap between the needs of the manufacturing industry in general and the economic priorities of individual companies, financial aid from government would have the potential for major impact. Aid might include CRADA funding for federal laboratories in consortium with several chemical companies to aid them in developing pre-commercial versions of scientific and engineering software. Such an effort would include partnership with scientific software companies who would subsequently commercialize the products. It may involve further development of existing federal lab codes, or it might fund creation of a new code to meet an unmet need in a segment of the industry. Some of the work could be subcontracted to commercial software developers and universities, but direction of projects should be under the control of the manufacturing companies. After a certain period of technical development, the commercial version of such software would be offered for sale

openly. By underwriting part of the development cost, the government would enable the sale of the software to a much wider market and promote use by other manufacturers. The benefit to the U. S. economy would come from productive application of the software.

2. Documentation, training, other support

The chemical industry has neither the resources nor the focus to support the high-quality documentation, help files, training, and help-line telephone support that are necessary to extend the use of technical computing beyond the dedicated specialists.

3. Upgrades, debugging

Few chemical companies have the incentive to refine their codes to the desired high level of quality necessary for use by the generalist. Continued development, responsive to active, demanding customers, is necessary and very beneficial. It is thus that new methods, new features, and new science are added to established packages and come to be applied routinely by the general users.

4. Practical access by knowledgeable generalists vs. state-of-the-art capabilities for the dedicated specialists

This issue is addressed explicitly above, and is the key to profitable use by the widest segment of industry. It is the defining difference that elevates a computational approach to the level where it can affect the productivity of the whole industry. Research engineers of The Dow Chemical Company particularly recognize need and opportunity in computational fluid dynamics (CFD) with chemical reactions, aimed at better meeting the needs of the chemical process industry.

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Envisioned scope of program:

5 yrs, $2 million /yr govt. funding, 10 FTEs program developers

5-10 chemical co. partners, each contributes:

$50,000 - $100,000 /yr cash

0.5 - 1.0 FTE (Full Time Equivalent) in-house in-kind

for industrial steering board

provide sample problems

"friendly early users" for code

Sub contract awards to Natl. Labs, universities, small companies

Commercial CFD software vendors role to be defined. All.17

Attachment 12
Brainstorm/Discussion on Consortium/Center of Excellence /Wrap-up
Brian VanderHeyden
LANL

LA-UR-95-1722

Los Alamos National Laboratory is operated by the University of California for the United States Department of Energy under contract W-7405-ENG-36

TITLE: **BRAINSTORM/DISCUSSION ON CONSORTIUM/CENTER OF EXCELLENCE**

AUTHOR(S): William Brian VanderHeyden , T-3

SUBMITTED TO: *Viewgraphs for Reactive Multiphase Flow Simulation Workshop, Los Alamos National Laboratory, Los Alamos, New Mexico, May 18–19, 1995*

Los Alamos

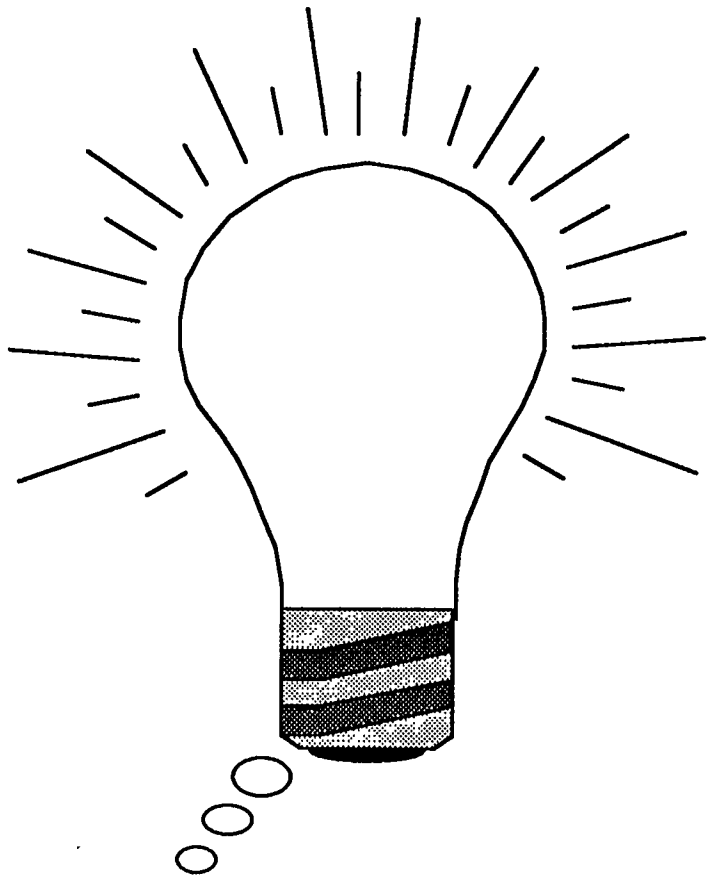
Los Alamos National Laboratory
Los Alamos, New Mexico 87545

FORM NO. 836 R4
ST. NO. 2629 5/81

A12.2

Brainstorm / Discussion on Consortium / Center of Excellence

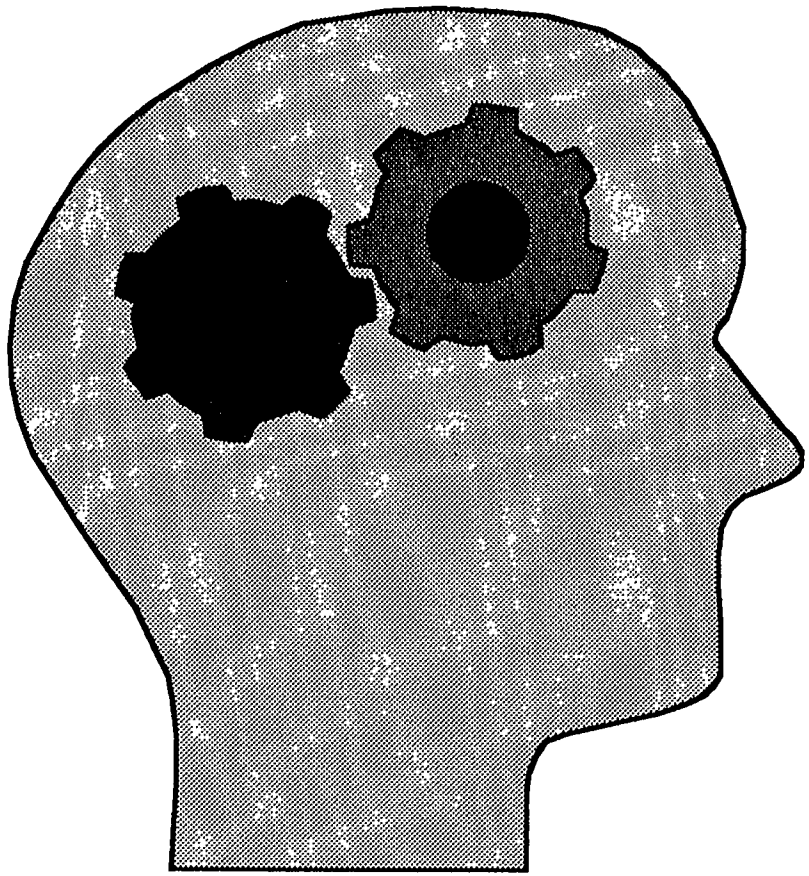
- Needs
- Potential Consortium/Center of Excellence



A12.3

Needs - Theory

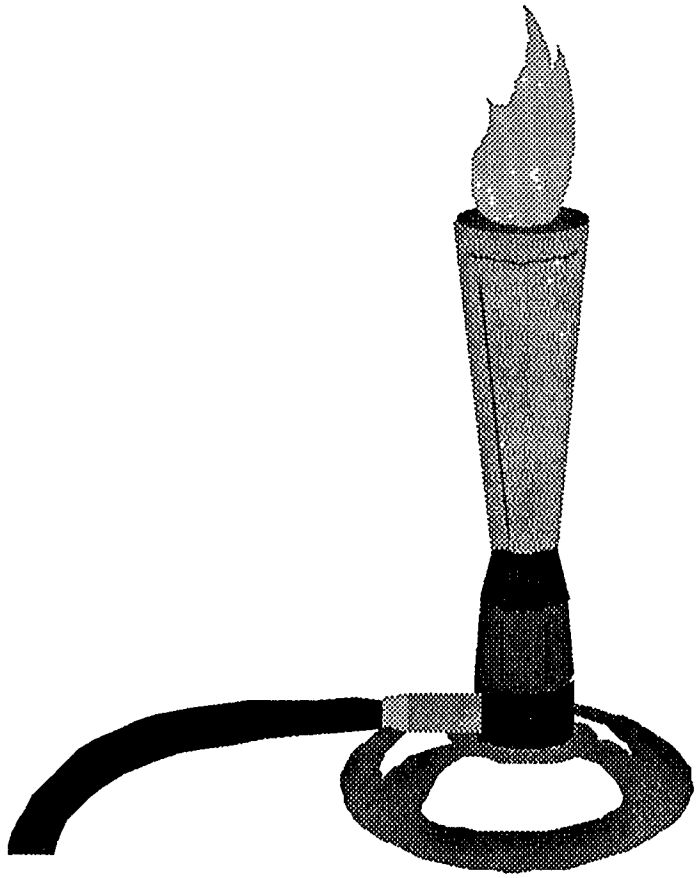
- Multiphase Turbulence
- Exchange
- Granular stresses
- Electromagnetic fields
- Radiation Transport



A12.4

Needs-Experiment

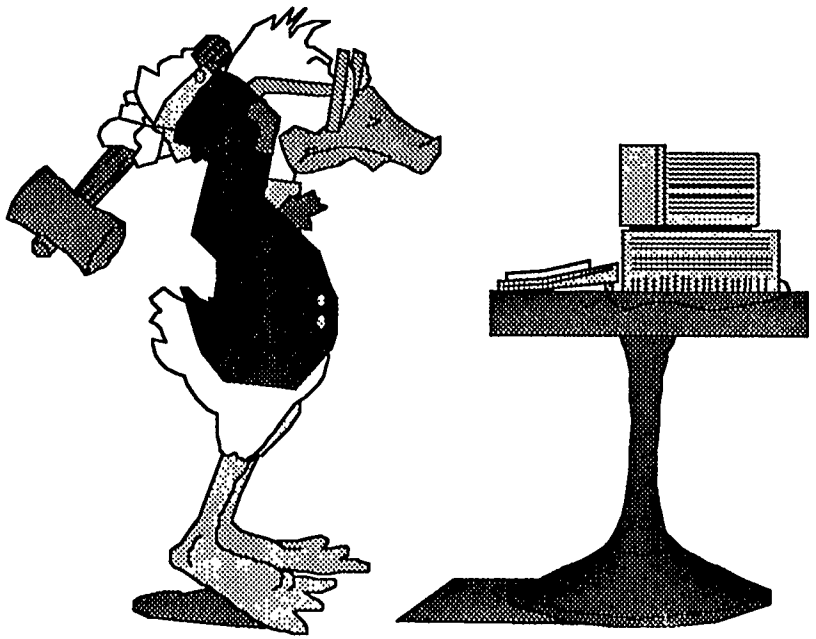
- Tomography
- Probes
- Turbulence
- Multifluid exchange



A12.5

Needs-Numerical Methods

- Parallel methods
- Immersed boundaries
- Implicit transport
- Lagrangian fields
- Unstructured Grids
- Special boundaries
- Higher level languages



A12.6

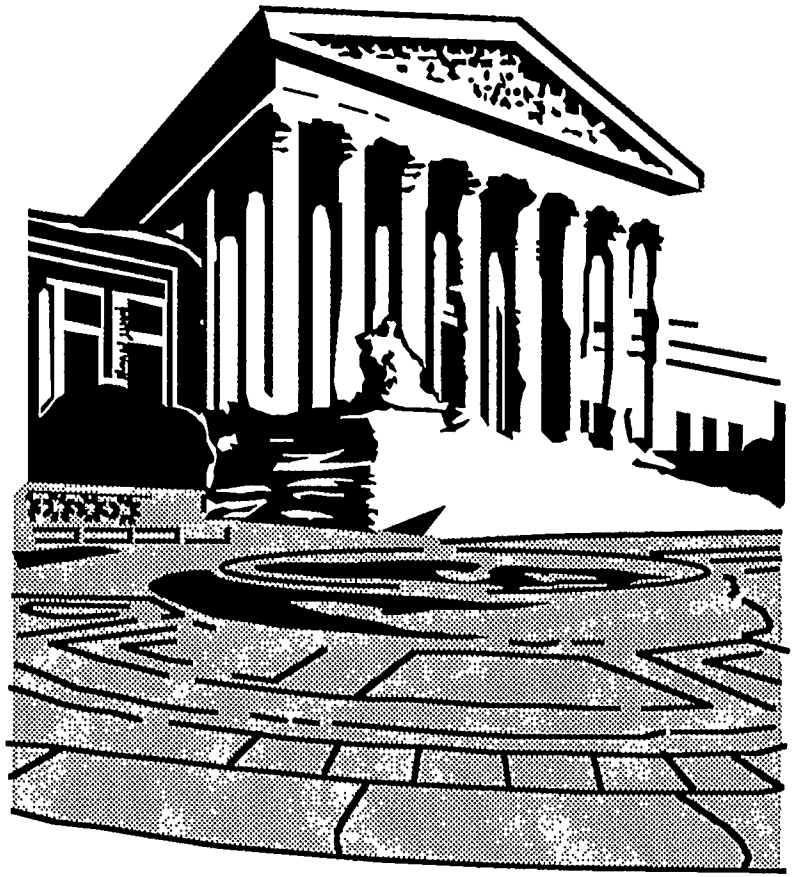
Needs-Generic Simulations

- Bubble Columns
- Stirred Tanks
- Risers
- Immiscible liquids
- Packed Beds
- Fluid beds
- Fractionation equipment

A12.7

Potential Consortium / Center of Excellence

- Vision/Mission?
  - » advance state-of-the-art
  - » target computation/grand challenge?
- Structure
  - » physical center?
  - » virtual center?
- Leadership/direction
  - » board?
  - » top dog?
- Membership
  - » industry
  - » academia
  - » sister labs



Wrap-up

- Meeting documentation
- Protocol/Letter of support
  - » Company letterhead
  - » Value of workshop
  - » Interest in an expanded workshop with academia/ sister labs
  - » Interest in further collaboration
  - » Interest in consortium or center of excellence

A129

XYZ COMPANY
LETTERHEAD

May 22, 1995

W. Brian VanderHeyden
Theoretical Division Fluid Dynamics Group
Los Alamos National Laboratory
Los Alamos, New Mexico 87545

Re: Protocol Letter on Reactive Multiphase Flow Simulation Workshop & Consortium

Dear Mr. VanderHeyden:

As you know, I attended the Workshop on Reactive Multiphase Flow Simulation held at Los Alamos National Laboratory on May 18 & 19, 1995. I found the workshop very interesting and informative. Without obligating myself or my company in anyway I would like to stipulate that I see potential value in collaborative research between industry and Los Alamos on reactive multiphase flow simulation where dual-use benefits exist. I further support the idea of a more structured formal arrangement such as a consortium between Los Alamos, industry, academia and other government laboratories whose mission would be to substantially advance the state-of-the-art in reactive multiphase flow simulation. The product of such an endeavor would certainly yield significant benefits to both industry and the government.

Please keep me informed of further developments along these lines.

Sincerely,

Dilbert Q. Engineer
XYZ Company

A12.10

Reactive Multiphase Flow Simulation Workshop Feedback Form

The part of the workshop I liked best was:

The part of the workshop I liked least was:

This workshop could have been improved by:

An industry/government consortium on reactive multiphase flow simulation should:

FAX (505-665-5926), e-mail (wbv@lanl.gov), or mail to Brian VanderHeyden, Mail Stop B216, Theoretical Division Fluid Dynamics Group, Los Alamos National Laboratory, Los Alamos, NM 87545

A12.11