CONF-9505 28--Summ.

LA-UR-95- 2194

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: **REACTIVE MULTIPHASE FLOW SIMULATION WORKSHOP SUMMARY**

AUTHOR(S): W. Brian VanderHeyden, T-3

SUBMITTED TO: *Distribution to workshop attendees and other interested parties*

DISTRIBUTION OF THIS DOCUMENT IS UNLIMITED

Los Alamos
Los Alamos National Laboratory
Los Alamos, New Mexico 87545

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

DISCLAIMER

Portions of this document may be illegible in electronic image products. Images are produced from the best available original document.

REACTIVE MULTIPHASE FLOW SIMULATION WORKSHOP SUMMARY

A workshop on computer simulation of reactive multiphase flow was held on May 18 and 19, 1995 in the Computational Testbed for Industry at Los Alamos National Laboratory (LANL), Los Alamos New Mexico. Approximately 35 to 40 people attended the workshop. This included 21 participants from 12 companies representing the petroleum, chemical, environmental and consumer products industries, two representatives from the DOE Office of Industrial Technologies and several from Los Alamos. The companies represented at the workshop were:

- Alcoa
- Amoco
- Chevron
- Dow
- Dow Corning
- DuPont
- Exxon
- Molten Metals Technology
- Procter & Gamble
- Shell
- Texaco
- Universal Oil Products

The presentation topics were:

- Introduction - Brian VanderHeyden - LANL
- Introductory Simulation Movies - Bucky Kashiwa - LANL
- Prototype Multiphase Flow Problems - Paul Merz - Chevron Research
- Review of CFDLIB/Current Theory - Bucky Kashiwa - LANL
- Air-Agitated Alumina Crystallizer - Phil Hsieh - Alcoa
- Heat Transfer Mechanisms in Ebullated Bed Reactors - Farshad Bavarian - Texaco
- Review of CFDLIB/Current Theory - Brian VanderHeyden - LANL
- Simulation of Gas Jets in Molten Metal Baths - Jon Wolfe - Molten Metal Technology
- Review of CFDLIB/Current Theory - Nely Padial - LANL
- Multiphase Flow at Procter & Gamble - Joseph Kitching, John McKibben - Procter & Gamble
- Multiphase Flow at Exxon - Bill Heard - Exxon
- KIVA Combustion Simulation - Dan Butler - LANL

- Telluride/Pagosa Codes (Interface Tracking, Object Oriented Programming) - Doug Kothe - LANL
- Review of CFDLIB/Current Theory - Bucky Kashiwa - LANL
- Multiphase Reynolds Stress Transport Modeling - Brian VanderHeyden - LANL
- Spectral Models, Symmetry and Engineering Turbulence Closures - Tim Clark - LANL
- Applications of Group Theory to Turbulence Modeling - Brian Volintine - DOE OIT
- Potential Mechanisms for Collaboration/Oil and Gas Partnership - Bob Hanold - LANL
- Review of 1st Industrial Energy Efficiency Symposium and Expo - Ed Joyce - LANL
- Center for Materials Process Modeling - Richard Lesar - LANL
- A View from Washington - Dan Wiley - DOE OIT
- Tank Flow Simulation - Bert Harvey - Dow Chemical
- Some Thoughts on a Potential CFD Consortium - Tyler Thompson - Dow Chemical
- Brainstorm & Discussion on Consortium or Center of Excellence - Brian VanderHeyden - LANL

The dialog at the meeting suggested that reactive multiphase flow simulation represents an excellent candidate for government/industry/academia collaborative research. A white paper on a potential consortium for reactive multiphase flow with input from workshop participants will be issued separately.

The following is a brief summary of the presentations and discussion at the workshop. The items are summarized in the order of their appearance. The agenda for the workshop is attached as Attachment 1.

Introduction - Brian VanderHeyden, LANL (Attachment 2)

Introductory remarks provided an overview of the Los Alamos National Laboratory Tactical Plan, the Dual-Use concept, the structure of the laboratory, the past and current efforts of the Theoretical Division Fluid Dynamics Group (T-3), current defense related applications of the T-3 CFDLIB multiphase flow simulation flow code library, the workshop purpose and the expected products of the workshop. The purpose of the workshop was to start a dialog between Los Alamos and industry to try to find common needs and complimentary capabilities that could form the basis for the initiation of a coordinated effort on substantially increasing the state-of-the-art of multiphase computational fluid dynamics. Such an effort should benefit both private industry and the US defense complex. If successful, such an effort would involve not only Los Alamos and private industrial partners but also other government laboratories and partners from academia.

Introductory Simulation Movies - Bucky Kashiwa, LANL

Three computer simulation movies were shown to provide a picture of the current capabilities of the CFDLIB codes and the activities of the CFDLIB group.

First, a simulation movie of 3-phase flow and vaporization in an vertical riser was shown. The flow configuration can be seen in Figure 1. Gas and granular solids are introduced in the bottom of the riser. A relatively cool liquid is introduced a few diameters up the riser. As the cool liquid contacts the warmer granular solids the liquid flashes to vapor and propels the mixture up and out the riser. This simulation demonstrates the capability of CFDLIB to handle flows with violent phase change.

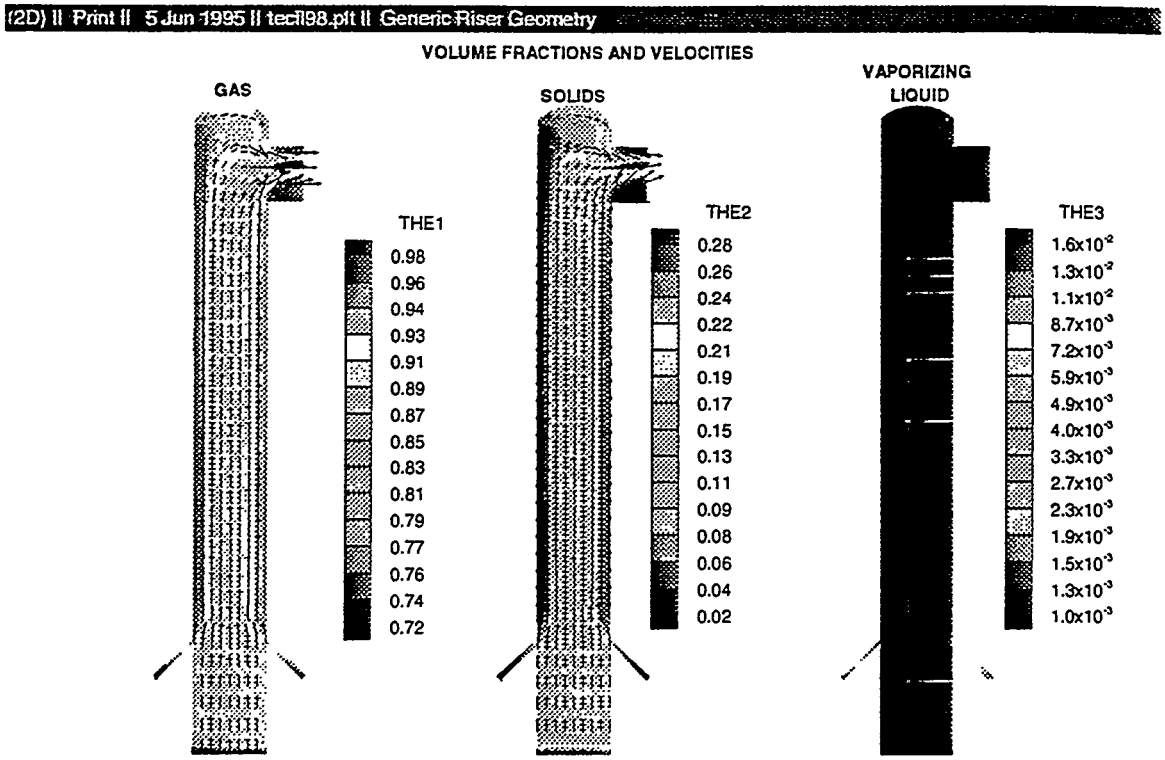


Figure 1 - Velocity vectors and volume fraction fields in a 3-phase riser flow

Second, a movie of a 4-phase simulation of a bath smelter operation. The bath smelter is a proposed alternative to current steel manufacturing methods. The flow configuration is shown in Figure 2.

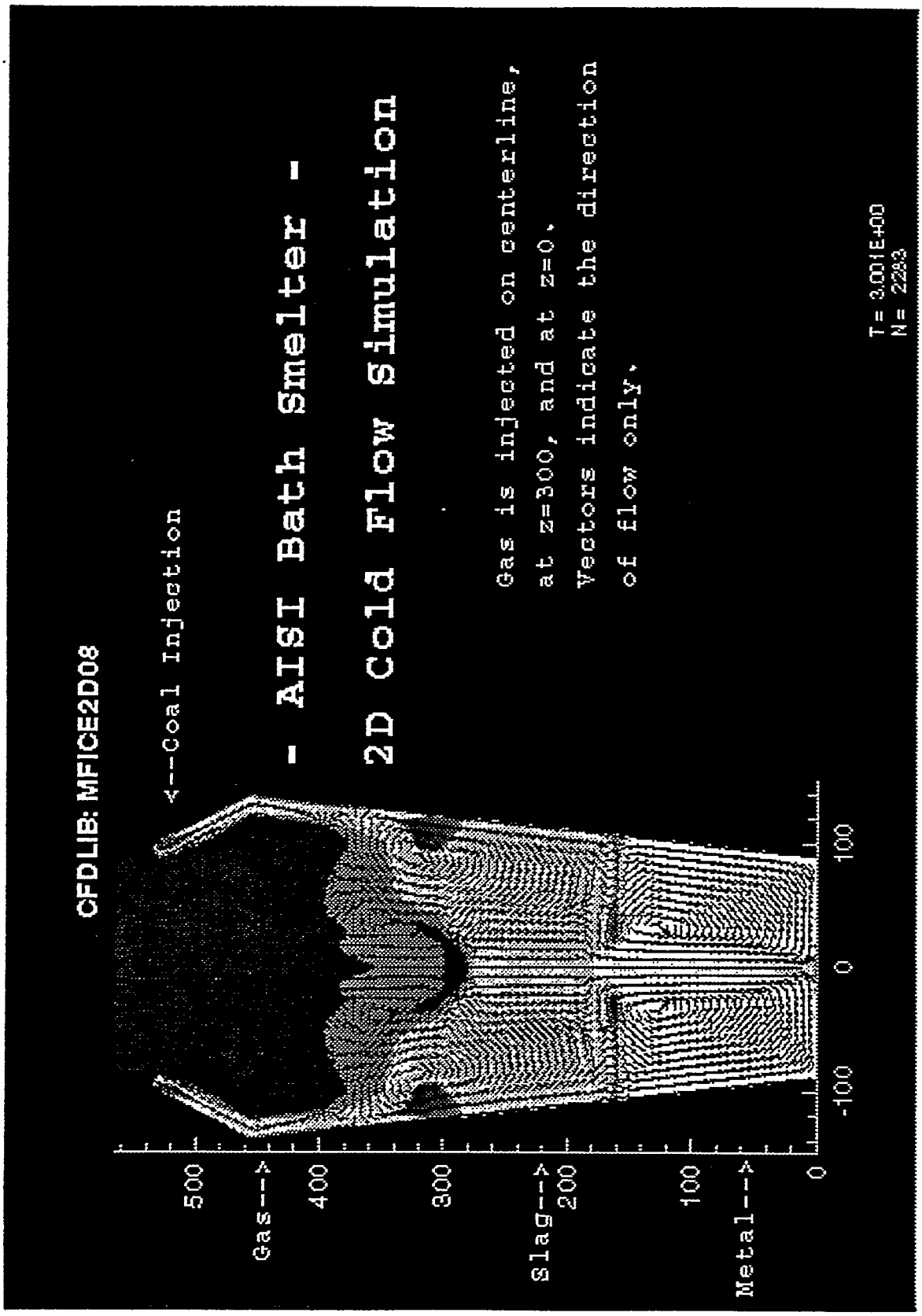


Figure 2 - Bath smelter

The 4 phases in the calculation are molten steel, gas (separate air and nitrogen streams), slag and chunks of coal. The oxygen is injected into the bath smelter at supersonic speeds. The calculation showed the motion and segregation of the separate phases and also tracked the progress of the iron ore reduction. This calculation highlighted several of the capabilities of CFDLIB including simultaneous treatment of 4 phases, compressible flow and finite-rate chemistry.

Third, a movie of the simulation of the oscillatory expansion and contraction of a bubble formed from the gaseous products of an underwater detonation. Figure 3 shows a comparison of the computed and experimentally measured bubble radius as a function of time after the detonation. This calculation highlighted the ability of the code to handle high speed compressible multiphase flows.

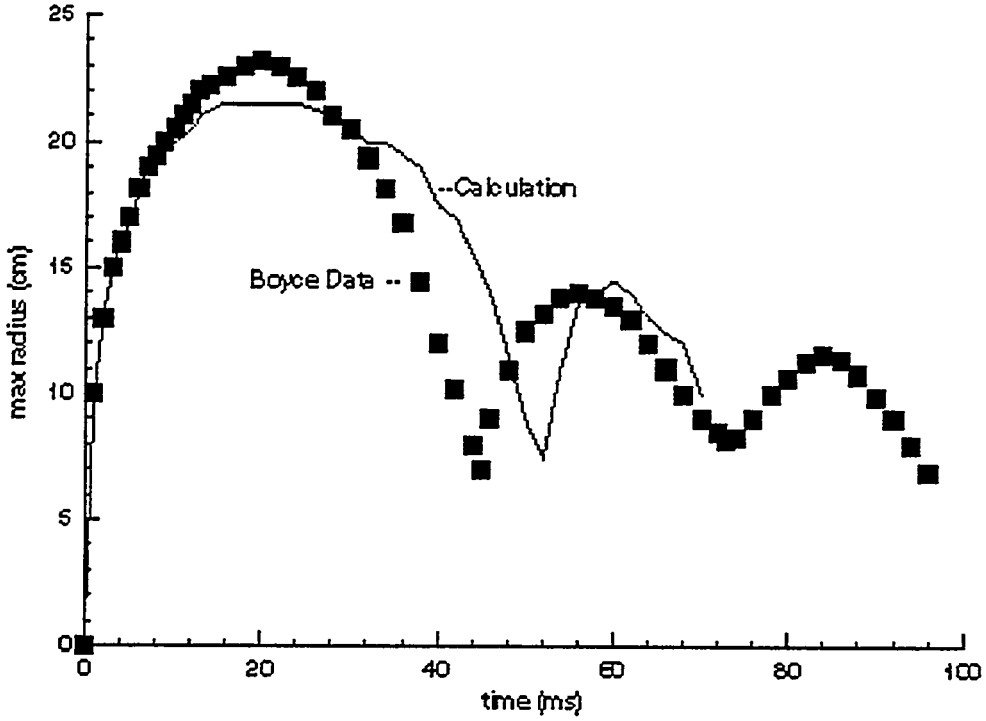


Figure 3 - Bubble Radius vs. Time. Maximum bubble radius vs. time is shown compared to the data of Boyce (1990). The timing and amplitude show very good agreement.

Prototype Multiphase Flow Problems - Paul Merz, Chevron Research and Technology Company

A discussion on single- and multiphase flow computational fluid dynamics experiences at Chevron Research was presented. The central point of the talk was that available commercial software for single phase flow problems is reasonably mature from the

standpoint of the needs of Chevron. On the other hand, a great deal more uncertainty is associated with available multiphase flow codes and therefore more research is needed in this area.

Paul first reported on a successful application of single phase flow (gas) in a packed-bed radial-flow reactor. A commercial computational fluid dynamics package was used to analyze the flow distribution in several commercial reactors. Flow maldistributions, zones of counterflow and regions of high velocity were discovered in the flow simulations. Based on simulation work, modifications were recommended and employed resulting in improved performance of the commercial reactors. Due in part to this success story, Chevron management is becoming more supportive of this sort of work and the technology is being gradually fielded into engineering use.

Paul then discussed a multiphase flow prototype problem that Chevron has used to screen and benchmark commercial software. The prototype problem was similar to a riser separator in a fluid catalytic cracking unit depicted below in Figure 4.

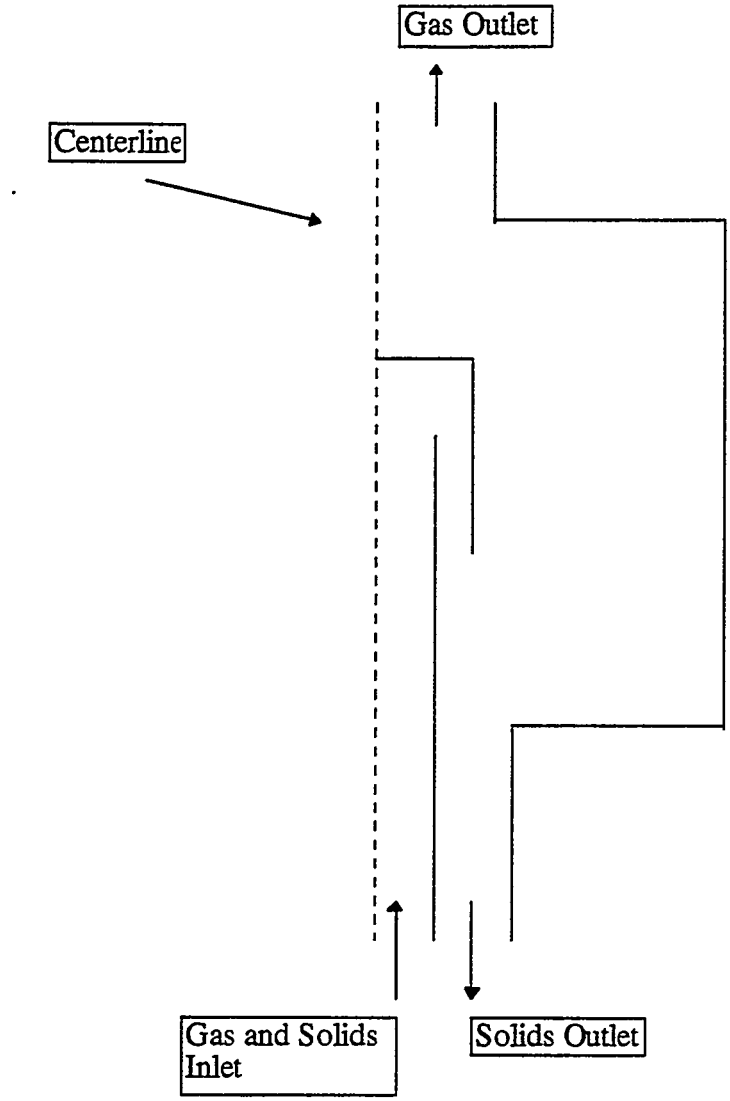


Figure 4 - FCC Riser Separator - Chevron Prototype Multiphase Flow Problem

Chevron Research submitted this problem to a number of commercial vendors. One vendor found a time-varying oscillatory solution while another found a steady solution. It was also found that the pressure boundary condition on the solids outlet had to be lower than what was expected to get outflow. The lesson drawn from this exercise by Chevron was that more research is required for multiphase computational fluid dynamics to bring it to the maturity of the state of the single phase computational fluid dynamics.

A final point was raised on the issue of the speed of available codes. Many available codes, it was felt, were constructed to be "all-purpose,, in order to cut down on maintenance and training costs. At the same time, however, the "all-purpose,, codes tend to carry a great deal of overhead thereby making them slower than a "specialty,, code. A potential solution to this problem might be to construct a code library similar to CFDLIB

which would consist of related but specialized modules. Such a library would enjoy some of the maintenance advantages of an all-purpose code and the speed advantages specialty codes.

Review of CFDLIB/Current Theory - Bucky Kashiwa, LANL (Attachment 3)

The first review session covered the following topics:

- CFDLIB structure
- Multimaterial formalism
- Conservation equations
- Numerical Methods

CFDLIB stands for Computational Fluid Dynamics LIBrary. CFDLIB is a LIBRARY of codes which perform specialized simulation tasks (e.g. single phase compressible flow, multimaterial incompressible flow, etc.) As a result a user can select the library code that best suites his problem. Since many of the codes share common features, data structures, variable names and even subroutines, maintenance of the library and training on different library codes is expeditious.

Then the multimaterial formalism upon which the LANL governing equations for mass, momentum and energy conservation for a multiple, interpenetrating material system are based was discussed. The term multimaterial is used rather than multiphase because multiple material classes can be assigned to a single phase. For example, two classes that might be assigned to a single solid particulate phase such that one class corresponds to particles whose diameter is less than 100 microns with the other class corresponding to particles with diameters greater than 100 microns.

In the multimaterial formalism, mass, momentum and energy conservation equations are derived and solved for each material class. The derivation employs averaging of ensembles of experimental realizations of ordinary points in the flow domain which are surrounded by a pure material. A Boltzmann transport equation for state probability is used to generate transport equations for the expected mass, momentum and energy for each material class. The generated equations are exact but unclosed. The unclosed terms represents phenomena such as multimaterial Reynolds stresses, intermaterial exchange forces and multiphase pressure forces. Models for these terms based either on empirical fits of experimental data or on theoretical microstructure must be introduced to close the equations.

Finally, the numerical methods used in CFDLIB to solve the multimaterial transport equations were outlined. The numerical method is based on the finite-volume approach wherein the discretized equations of motions are obtained by integration around control volumes surrounding the grid points on a given mesh. Unlike the older staggered mesh

schemes in which the scalar data such as pressure and density are stored at cell centers while the velocity components are stored at cell faces, all variables are stored at the cell centers in the CFDLIB numerical scheme. This mode of variable storage necessitates the more complicated averaging operators to achieve conservation than does the staggered mesh approach. On the other hand, the cell centered scheme is much more amenable to non-Cartesian coordinate systems that arise from boundary fitted meshes. Furthermore, the cell centered approach removed some ambiguities that arise from the separate material class trajectories that generally exist in multimaterial systems.

Air-Agitated Alumina Crystallizer - Phil Hsieh, Alcoa

An overview of computational fluid dynamics experiences at Alcoa was given. Alcoa has been a reasonably heavy user of commercial single phase codes. While there are numerous applications in the aluminum and alumina manufacturing processes for multiphase flow analysis, Alcoa is just starting to explore this arena.

The air-agitated alumina crystallizer was given as an example of a multiphase flow problem in aluminum manufacturing to which Alcoa has applied two-phase flow analysis. The air-agitated crystallizer is essentially a tank into which an aqueous caustic slurry of fine alumina is introduced. This is shown schematically in Figure 5.

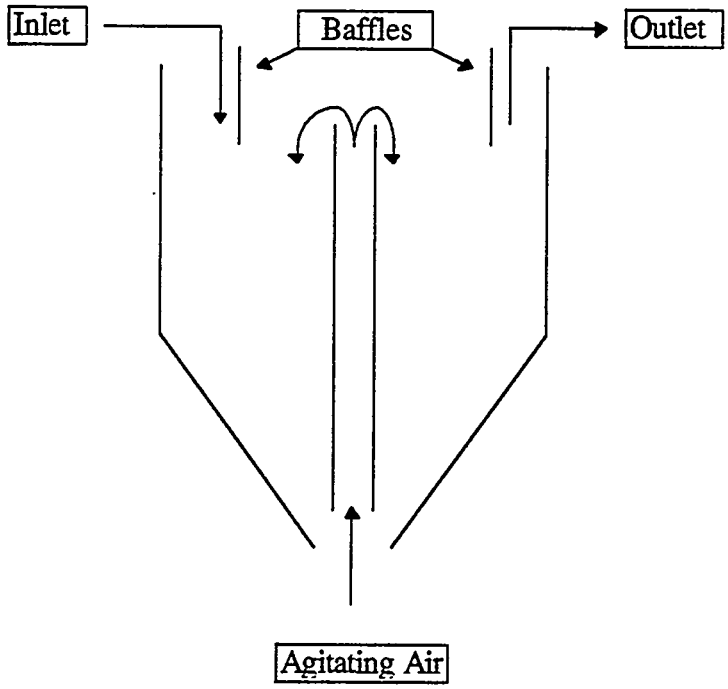


Figure 5 - Schematic Drawing of an Air-Agitated Alumina Crystallizer

Air is also bubbled into the tank to stir the contents. The process objective of the unit is to allow the fine alumina grains to agglomerate into larger particles which are further processed downstream. The extent of the agglomeration and therefore the capacity of a given crystallizer is governed by the concentration of alumina particles and their residence time in the vessel. Increasing either of these increases the capacity and profitability of the crystallizer. Elimination of short circuiting from inlet to outlet and the facilitation of some alumina settling are two keys to achieving these goals.

Alcoa used single-phase computational fluid dynamics to investigate tank baffling strategies for the crystallizers. One proposal involved placing a baffle near the outlet and extending it down into to the crystallizer. The baffle was intended to eliminate short circuiting of uncrystallized alumina across the top of the crystallizer. Analysis using single phase computational fluid dynamics suggested that while the baffle would eliminate short circuiting, the baffle also would decrease average alumina concentration by withdrawing material preferentially from the more concentrated bottom portions of the tank.

To close the talk the following list of "Burning Issues/Needs/Observations,, for multiphase computational fluid dynamics was presented.

- Improved theoretical foundation for the multifluid conservation equations and approach is needed.
- Much improved turbulence models for multiphase flows are needed.
- More efficient solution algorithms are required (the crystallizer problems took 2 weeks to converge on HP and IBM workstations.)
- Multiphase flow problems are abundant.
- There is a need for a coherent voice or set of voices to help sort out the complicated issues of multiphase flow physics and code development and application.

Heat-Transfer Mechanisms in Ebullated Bed Reactors - Farshad Bavarian, Texaco

An overview of Texaco's commercialization efforts and how computational fluid dynamics has been used was given. Computational fluid dynamics was used in the design of a modified gas-liquid separator used in an ebullated bed resid hydrocracker. In addition, computational fluid dynamics has been used to scale-up bubble column reactors directly from the laboratory to commercial scale with a scale-up factor of order 10^5.

A discussion was also presented on the heat transfer problems encountered in ebullated bed hydrocracking of non-residual oil material. While metals deposition is a major mechanism of catalyst deactivation in resid hydrocracking, coking of catalyst due to elevated catalyst temperature is the chief deactivation mechanism in petroleum distillate and gas oil hydrocracking. The elevated catalyst temperature is in turn due to the highly exothermic hydrocracking reactions taking place on the surface of the catalyst along with

limited heat transfer rates from the catalyst to the bulk reactor liquid. In order to gain a better understanding of these effects, experiments were performed to measure the heat transfer coefficient in bubble columns under a variety of liquid and gas rates and bubble size regimes. It was found that in large bubble systems such as air-water, the heat transfer coefficient from the liquid to a stationary probe increased with increasing gas rate. This is presumably due to the increased level of agitation which in turn disrupts the insulating boundary layer around the probe. On the other hand, it was also found that in small bubble systems such as those found in a petroleum liquid based bubble column, the heat transfer coefficient decreased with increasing gas rates. This seemingly counter-intuitive result can be understood as follows. In the small bubble system, the boundary layer fluid surrounding the probe is really an effective medium of liquid and bubbles. In the large bubble system, the boundary layer fluid is essentially pure liquid. The heat transfer coefficient is proportional to the boundary-layer fluid thermal conductivity. So the lower heat transfer coefficient of the small bubble system is a reflection of the lower thermal conductivity bubbly mixture versus the pure fluid.

These experimental observations and theoretical explanations are a good example of the sort of efforts that are required to model and close exchange terms that arise in the multi-material conservation equations.

Review of CFDLIB/Current Theory - Brian VanderHeyden, LANL (Attachment 4)

The second review session covered the following topics:

- Species energy conservation equation
- Material Class energy conservation equation
- Pressure force models
- Currently available turbulence models.

A transport equation was derived using the multimaterial formalism for the conservation of the internal energy of species. At this point the notion that a given material class can be composed of multiple chemical species was introduced. The species internal energy transport equation incorporates the effects of compressible work, work due to mass exchange, fluctuational work, exchange of internal energy due to mass exchange, viscous dissipation, conduction and exchange due to conduction. By using the equation for conservation of mass, the thermodynamic expression for material compressibility and the thermodynamic relation between constant pressure and constant volume specific heat, one can manipulate the species internal energy conservation equation into a transport equation for species temperature. The temperature equation is also closely related to a transport equation for species enthalpy. In fact, temperature equation contains a term reflecting the effect of mass exchange that is proportional to enthalpy differences.

To wrap up the discussion of the species energy transport equation, a simple model was presented for the exchange of energy among species due to molecular conduction using the expression for heat transfer coefficient to a sphere.

Species with identical or very nearly identical temperatures and mean velocities can be usefully grouped into classes. By summing the transport equations for all the species in a particular class, the class transport equation is generated. In the case of the temperature equation, the mass exchange term contributes to two effects according to whether the exchange is within or across classes. For species exchanging mass within a class due, for example, to a chemical reaction, the exchange term contributes to a heat of reaction term for the class. For species exchanging mass across classes, the exchange term reflects exchange of energy due to physical processes such as evaporation and condensation.

Models for the expected pressure acceleration for a material class were also reviewed. The expected pressure acceleration at a point can be broken into a mean pressure acceleration, a conservative force and an exchange force. Examples of a conservative force include close packing force that arise when a granular material is compressed beyond maximum packing. Another example is a force that acts on continuous phases whose origin is the Bernoulli pressure departure on the surface of a particulate phase moving relative to the continuous phase.

Examples of exchange forces are drag, added mass and lift arising from unbalanced pressure deviations on, for example, a particle translating or accelerating relative to a continuous fluid. Some models for the drag force on a particle that have been employed in CFDLIB include a model based on the drag experienced by a single sphere in an infinite fluid. This drag law has also been enhanced to include the effects of hindered settling as prescribed by Richardson and Zaki. Another drag model is based on the momentum exchange experienced by clouds of dissimilar particles moving relative to one another due to collisions. Finally another drag law that has been employed in CFDLIB is based on the Ergun formula for pressure drop in packed beds. This model is most appropriately applied to either packed beds or dense fluidized beds.

Finally, the currently available turbulence models were discussed. It is recognized that the multiphase Reynolds stress term in the momentum conservation equation is probably the most complex and least understood term in the governing equations. Dealing with this term can proceed along two lines. The first is to keep the Reynolds stress model as simple as possible and employ the minimum number of parameters. The second line is to try to model the Reynolds stress as rigorously as possible through the use of a Reynolds stress transport equation and theoretical microstructural models. Although we are in the process of following the second approach, we have been using the first approach in our CFDLIB computations to date.

Currently, the Reynolds stress models used in CFDLIB all use the Newtonian Boussinesq closure assumption. The viscosity for each material class in this closure can be taken from one of the following:

- Constant eddy viscosity model. The constant viscosity is specified by the user.
- Prandtl mixing length model. The constant mixing length is specified by the user.
- One-equation turbulent kinetic energy model. A constant mixing length and boundary conditions on turbulent kinetic energy are specified by the user. (This model is still undergoing refinement.)

With the first two choices, the isotropic part of the Reynolds stress is not modeled and is essentially lumped in with the mean pressure. For the case of the one-equation model, the isotropic part of the Reynolds stress is explicitly calculated and used in the material class momentum equation.

An advantage of the one-equation model was demonstrated through a computation of developed flow in a gas-solid riser similar to the situation in the riser of a fluid catalytic cracking unit in a petroleum refinery. By imposing a zero boundary condition on the turbulent kinetic energy at the wall of the riser (energy is dissipated through collisions with the wall) a gradient in the isotropic part of the Reynolds stress is set up which produces a migration of particles toward the walls. As shown in Figure 6, this produces solids holdup profiles similar to what is expected for developed riser flow.

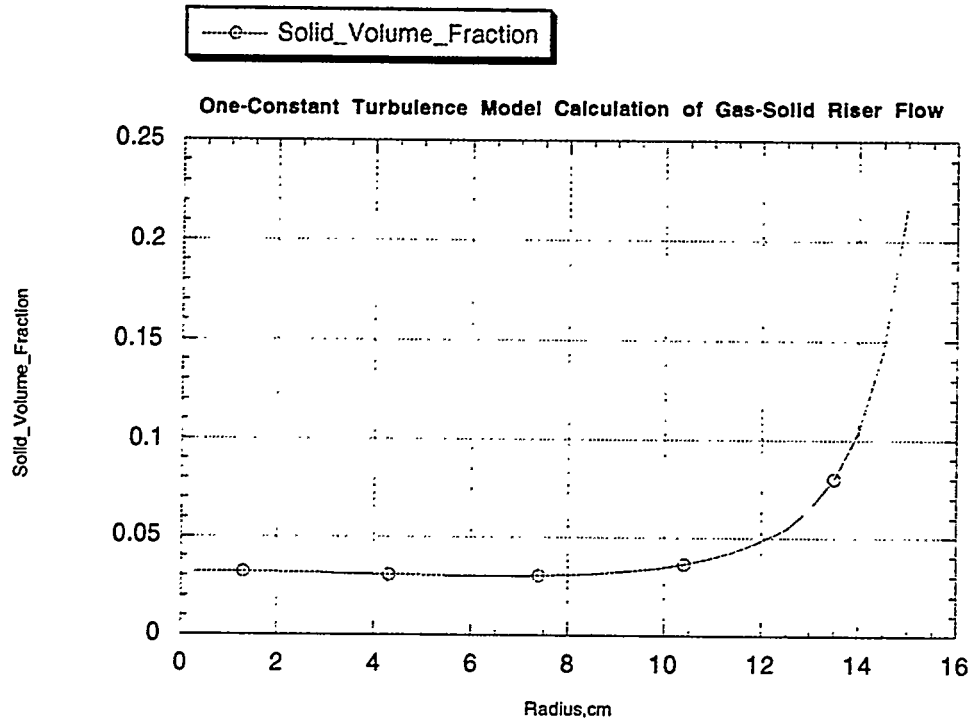


Figure 5 - Radial solids profile from one-equation model simulation of gas-solid riser flow. For comparison, the constant eddy viscosity and constant Prandtl mixing length models cannot produce this solids segregation effect.

It should be mentioned that steady profiles like in Figure 5 were not always obtained. For smaller mixing lengths, the solids tended to slosh back and forth across the radius of the pipe.

A final example calculation was shown in which a 2-dimensional air-water bubble column was simulated to demonstrate the importance of turbulence modeling. The simulations correspond to a set of experiments performed by Chen and others from New Zealand. Chen's bubble column was constructed from two Plexiglas plates positioned in a parallel fashion with a relatively small gap between them. The Plexiglas column was filled with water and air was sparged into the bottom through a simple distributor. Chen observed that the air tended to form a well defined Von Karman-like vortex street in the column.

Computer simulations using CFDLIB and a simple Prandtl mixing length model produced a similar vortex street as shown in Figure 6.

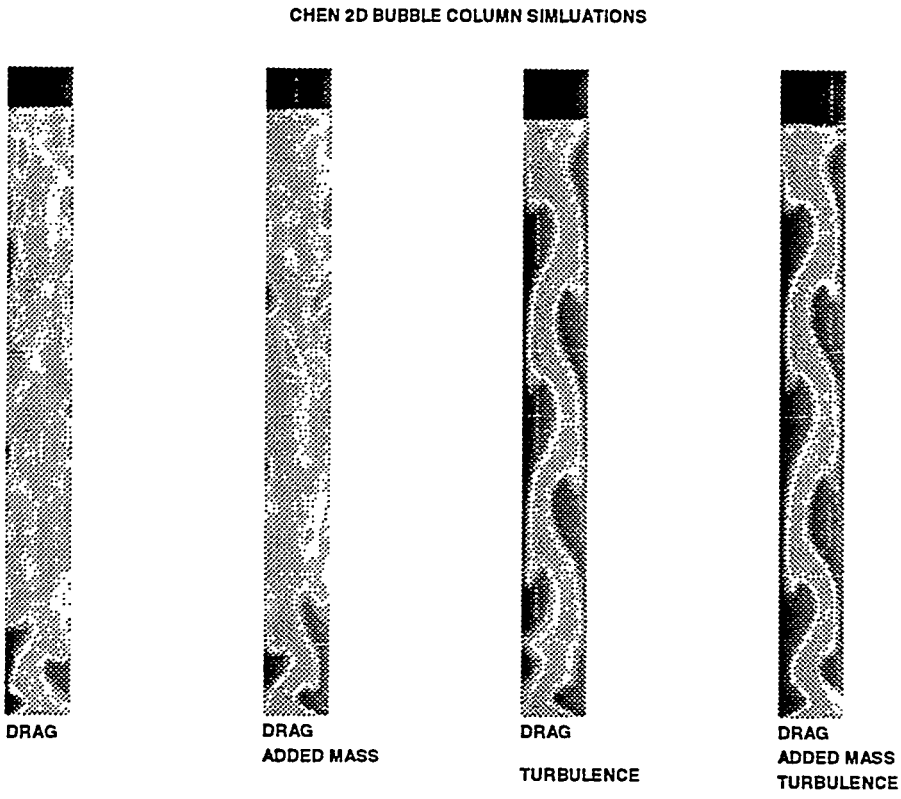


Figure 6 - Gas volume fraction fields from CFDLIB simulation of the 2-dimensional air-water bubble column experiments of Chen et. al. (1989). The lighter areas are relatively gas-rich. Mixing length turbulence is required to obtain experimentally observed Von Karman vortex street. Added Mass affects solutions to a small degree by comparison.

The choice of mixing length was also found to be critical for this problem. Using a too large a mixing length wipes out the vortex street by over-diffusing momentum.

Simulation of Gas Jets in Molten Metal Baths - Jon Wolfe, Molten Metal Technology

Two- and three-dimensional CFDLIB computations of gas jet spreading in a molten metal bath were discussed. Molten Metal Technology, Inc. (MMT) markets a hazardous waste disposal process which involves the jet injection of hazardous materials into a hot molten metal bath. As the hazardous materials contact the hot molten metal, they break down chemically to form a more benign substance. Unit performance is related to mixing and residence time distributions. In order to gain a better understanding of this

phenomena, MMT used CFDLIB to perform 2- and 3- dimensional simulations of gas jet spreading in a liquid pool. The effect of different momentum exchange models and Reynolds stress closures on simulated jet spreading were studied and compared to experimental data. It was found that CFDLIB results accurately match experimental data and other numerical results for jet spread in a liquid bath and that qualitative and some quantitative predictive capabilities are currently possible for MMT applications.

Review of CFDLIB/Current Theory - Nely Padial, LANL (Attachment 5)

Massively parallel supercomputers arrived on the scene several years ago and have the potential of substantially increasing the practical size and speed of large-scale computations. Massively parallel supercomputers work by dividing a given computation into parts and allocating each part to an individual processor. The processors perform the computations on their respective parts simultaneously, or in parallel, to arrive at the solution faster (hopefully) than is possible on a single processor computing the entire problem. Also, massively parallel supercomputers can have much larger memories than a single processor machine so larger problems can be attempted.

One potential bottleneck to speed-up on a parallel computer is communication of data between processors. This is currently a very slow step relative to calculations and data manipulation that take place within a single processor. In fact, it is quite possible to perform a computation that is actually slower on a parallel machine than it is on a comparable single processor because of communication bottlenecks. It is important, therefore that a user configure a parallel computation in such a way to minimize the ratio of inter-processor communication to intra-processor work.

Since CFDLIB employed a multiblock structure wherein a given flow domain can be divided into separate, contiguous blocks, it was already in a form that is amenable to parallel computation. To parallelize a CFDLIB computation, different blocks or sets of blocks are allocated to different processors. Interprocessor communication is a natural extension of interblock communication that must occur in any multiblock computation. In order to port CFDLIB from the single processor environment for which it was originally written to a parallel processor environment some code modifications were necessary. Generally, those CFDLIB subroutines that performed calculations within a single block did not require modification. Driver routines that send work to the various blocks or processors had to be modified slightly. Subroutines that handle to interblock communication had to be rewritten completely. Additionally, CFDLIB had to be interfaced with interprocessor communication libraries. Currently, CFDLIB has been interfaced with PVM (Parallel Virtual Machine) a public domain library that can handle many types of architectures including a heterogeneous network of UNIX workstations. CFDLIB has also been interfaced with a specialized proprietary CRAY communication library called F^{--} which has some advanced memory features. This work has been done

and CFDLIB has been run on a CRAY T3D massively parallel supercomputer as well as a networked cluster of IBM RISC 6000 workstations.

The efficiency of the CFDLIB parallel implementation is problem dependent. This was illustrated with two example computations. The first example was a 2-dimensional incompressible 2-fluid simulation of a gas-liquid separator device provided by Amoco. The mesh in this problem was composed of 28 blocks with a variety of sizes and shapes including some high aspect ratio rectangles. The second example was a 2-dimensional compressible single fluid simulation of a Sedov blast wave. The mesh for this problem was composed of 100 identical square blocks. The parallel simulations for both problems were carried out on an CRAY T3D parallel computer using 2, 4, 8 and 16 processors and on an IBM RISC 6000 workstation cluster using 2,4 and 8 processors. Both PVM and F⁻ inter processor communication protocols were used on the CRAY T3D while only PVM was used on the IBM workstation cluster. Computational speed results were presented as the ratio of the parallel machine grind time (real wallclock time per cell per cycle) to the grind time for the same problem on a single vector processor of a CRAY-YMP. Note that the single CRAY-YMP processor is much faster that the IBM processor and the DEC alpha processors used in the CRAY T3D. The scaling was chosen to reflect that practical fact, given the availability of a CRAY-YMP single processor machine, the parallel computer and clusters would have to outperform the YMP to make them an attractive alternative.

Several features emerged from the timing data. First, as expected, the F⁻ protocol computation was generally faster than the PVM protocol on the CRAY T3D. For the 16 processor calculation, the F⁻ calculation was about 1.6 time faster than the PVM. A second observation was that good linear speed up was achieved from the blast wave problem. The grind time for the 16 processor calculation on the CRAY T3D using F⁻ was only 20% of the YMP time. On the other hand, the speed-up for the separator problem was very poor. For 16 processors on the T3D using F⁻, the grind time was 2.5 times that of the YMP. In other words, it was 2.5 time slower. These results are understandable as follows. The blast wave calculation is purely explicit while the incompressible separator problem was implicit requiring a meshwide solution of a Poisson problem for each pressure cycle. The Poisson pressure solution requires a great deal of interprocessor communication. Additionally, the heterogeneity of the mesh blocks and the rectangular shapes produced a couple of inefficiencies. First the processors dedicated to the small blocks were probably idle for a significant amount of time waiting for the large block processors. Also the rectangular blocks produce a less than optimal ratio of communication to intra-block computation.

A final example problem was a 3-dimensional incompressible baffle tank separator problem also contributed by Amoco. For this problem, the grind-time on the CRAY T3D using 64 processor was only 34% of the YMP grind time. The improved results for this problem over the separator problem were attributed to improved meshing and

improvements in the parallel CFDLIB implementation over what was used for the 2-d separator problem.

Multiphase Flow at Procter & Gamble - Joseph Kitching, John McKibben, Procter & Gamble

Application of CFDLIB to a proprietary gas solid flow problem was discussed. The flow domain is depicted schematically in Figure 7.

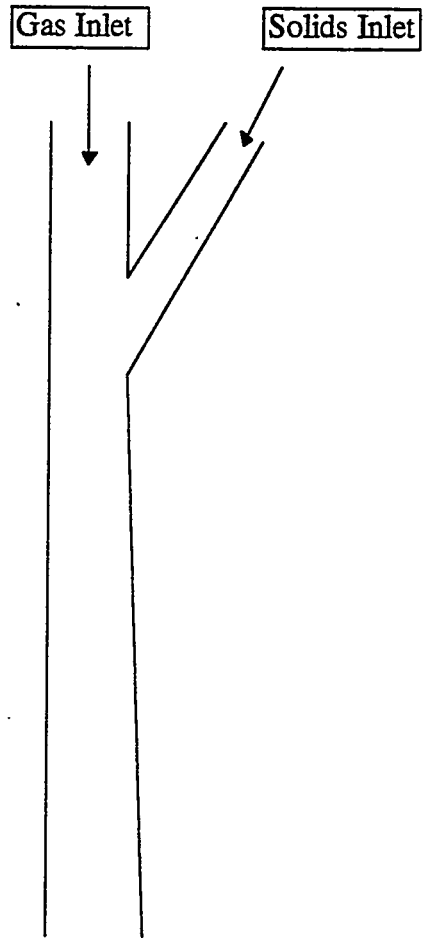


Figure 7 - Procter & Gamble Proprietary Gas Solid Flow Problem

As shown, a primary gas flow enters the device at the top and a solids stream is injected at a given angle from the side. A process objective is to produce a uniform concentration of solids at the outlet. Procter & Gamble will be using CFDLIB to study different strategies to achieve this objective. As a preliminary objective, CFDLIB was used to scope out the effects of a number of process parameters including gas and solids rates,

velocity ratios and solid's injection angles. Both 2 and 3 dimensional calculations were performed. Some of the observations from these runs were:

- Particle size determines if separation occurs between the solids and their delivery streams.
- Injection angle controls the development of a recirculation region downstream of the injection point.
- Gas velocity ratios, particle size and injection angle affect the uniformity of the distribution of the solids.

Procter & Gamble is planning a series of computer runs to increase the current model's complexity and verify its accuracy with physical measurement. The preliminary results indicate that CFDLIB will become an important engineering tool to further optimize its manufacturing process.

Multiphase Flow at Exxon - Bill Heard, Exxon Research & Engineering Company

An overview of multiphase flow simulation research at Exxon Research and Engineering was given. The multiphase flow governing equations used by Exxon are those obtained by Drew of RPI. The method derivation employs a material selector and ensemble averaging quite similar to the multimaterial formalism used by LANL.

Exxon is in the midst of constructing a general boundary-fitted coordinate system multiphase flow simulation code. The code will be used to analyze various problems associated with petroleum refining.

The results of a recent Exxon lagrangian simulation of a hydrofluoric (HF) acid cloud release was shown including the effects of water curtain scrubbing of the cloud. The calculation matched a recent HF release experiment. The simulation reflected the features observed in the experiment generally. It was found that the calculation was sensitive to drop size distribution.

KIVA Combustion Simulation - Dan Butler, LANL

An overview of the LANL T-3 KIVA combustion flow simulation code program was given. The KIVA flow simulation codes are used around the world by auto manufacturers to simulate and study the flow, spray dynamics, turbulence and fuel combustion in internal combustion engine combustion chambers. KIVA flow codes have also been used to simulate water scrubbed convection towers, silicon dioxide condensation in high pressure oxidation chambers, automotive catalytic converters as well a numerous other applications.

The KIVA study of the case of the United Parcel System cavity piston engine was discussed. The engines were built and tested in the late 1970's by UPS as a potentially more fuel efficient engine for their truck fleet. Fleet testing showed that the engines suffered from incomplete combustion. KIVA was used to determine the cause. KIVA simulations clearly showed that the incomplete combustion was the result of fuel being cooled near the walls at the top of the cylinder. This story illustrated how computational fluid dynamics can be used to gain insight into complex situations even though the exact governing equations for the flows are not known. By using reasonable modeling assumptions the KIVA simulations were able to provide information not directly or easily obtainable from experiment. The interaction of experiment and simulation is a paradigm which will exist well into the future.

Even though the KIVA code is relatively mature compared to a full multiphase flow simulation code like CFDLIB, Los Alamos maintains a strong collaborative arrangement with industrial users and other government laboratories. Numerous research topics have yet to be explored. It is hoped that the KIVA experience can serve as a model for a potential reactive multiphase flow consortium or center of excellence.

Telluride/Pagosa, Doug Kothe, LANL (Attachment 6)

The LANL experience with the Pagosa high speed flow simulation code and the newer Telluride free surface flow code was discussed to illustrate Los Alamos capabilities in the area of high speed compressible flows, unstructured grids, parallelization and object-oriented-like programming methods.

Los Alamos has experience with numerous parallel computing environments including the Thinking Machines CM-200 and CM-5, nCUBE2, Cray T3D, Intel Paragon as well as work station clusters. These machines cover the two principle parallel computing strategies, SIMD and MIMD. Pagosa, a high speed multiple material flow simulation code used extensively in weapons research was recently ported to the CM-5 for large-scale computations. As an example, the detailed Pagosa simulation of a missile intercept was shown. In this calculation, detail target and intercept missile components were resolved and all material interfaces were tracked through the collision.

Building on the successes of the Pagosa code, a new state-of-the-art multimaterial interface tracking code called Telluride is under development at Los Alamos. This code employs many advanced features such as unstructured grids, user-friendly graphical interfaces and a highly modular, flexible and portable structure. The code is written in FORTRAN 90 and C++ and takes advantage of the object-oriented-like features of these languages. The code will be able to efficiently handle very intricate mold geometries with fine detail.

Review of CFDLIB/Current Theory - Bucky Kashiwa, LANL (Attachment 3)

The final CFDLIB review session covered the chemical reaction package of CFDLIB and its new immersed boundary/Lagrangian fluid capability. The CFDLIB chemical reaction package is constructed to handle a comprehensive variety of chemical reactions and physical mass exchange processes such as evaporation and condensation. The package uses a fully coupled implicit technique to provide robust integration of the mass and energy equations. This coupled approach avoids time-splitting errors. This implicit treatment allows one to integrate to equilibrium in one time-step if necessary.

The physical-chemical reactions handled by the CFDLIB chemical reaction package are split into three broad classes. These classes are mass action law (Arrhenius gases, burning solids, catalysis), mass-saturation limited (adsorption, desorption, pyrolysis) and mass-thermal-saturation limited (evaporation, condensation). Included in the mass action law class are Langmuir-Hinshelwood kinetics.

A new immersed boundary technique is implemented in CFDLIB which allows a user to input an unresolved moving surface into a given flow. The surface is represented by a collection of lagrangian points which can exchange momentum with the fluids. The particles can be used to simulate an impeller, for example or a stationary distributor plate. The Lagrangian numerical method used to compute the immersed particles has many features in common with the FLIP scheme of Brackbill and Ruppel.

Multiphase Reynolds Stress Transport Modeling - Brian VanderHeyden, LANL (Attachment 7)

Some of the current LANL efforts toward improved closure of the turbulent multiphase Reynolds stress term in the momentum conservation equation were reviewed. The approach is to develop an exact transport equation for the multiphase Reynolds stress using the moment transport equation from our multimaterial formalism. Several of the terms produced by this operation have direct analogs to terms in the single-phase Reynolds stress transport equation such as mean-flow gradient production, diffusion, pressure strain, compressibility production and dissipation. Additional terms appear that have no single-phase analog. These terms represent production due slip between material classes, direct turbulent energy exchange, turbulent energy exchange due to mass exchange and collision effects. The modeling strategy will be to use as much of single-phase theory as possible to model the single-phase-like terms and to focus on the proper handling of the purely multiphase terms. The resulting fully closed Reynolds stress equation will be inverted to find the multiphase analog of the Boussinesq closure.

Spectral Models, Symmetry and Engineering Turbulence Closures - Tim Clark, LANL (Attachment 8)

A brief review of spectral theory, symmetry and engineering closures in turbulence and current LANL research efforts in this area was provided. The starting point for spectral theoretical work is the two-point generalization of the Reynolds stress tensor. The two-point generalization is the ensemble average of the outer product of fluid fluctuating velocities at two distinct points in space. A governing transport equation is derived for the two-point Reynolds stress tensor and is then Fourier transformed with respect to the relative position vector. After integrating the resulting equation over wave-number space, one obtains a spectral model related to the "single-point,, engineering models. Advantages of this equation are that no dissipation or length scale models are needed. Also one-may compute "non-equilibrium,, turbulence with the resulting equation.

Imposition of symmetry and invariance properties of the Navier-Stokes equations produces solutions for the turbulent energy spectrum. These solutions agree with the results from the engineering k-ε turbulence models. The long-time solutions approach a classical spectrum with a peak energy at an intermediate wave number.

Using the spectral theory and equations, it can be shown that single-point engineering closures can be rigorously correct in the limit of spectral self-similarity. It can also be shown using the spectral theory equations and the symmetry and invariance properties of the Navier-Stokes equations that turbulence anisotropy can persist indefinitely in a homogeneous decaying anisotropic turbulence. This is not properly predicted by engineering closures, however, and reminds us not to expect too much from them.

Engineering closures can be constructed from spectral closures by determining the appropriate similarity group for the problem class, determining the self-similar form of the spectra, substituting the self similar spectra into the spectral model equations and taking appropriate k-space moments. As an example, a k-ε deviatoric stress model was derived for homogeneous mean-flow.

Present LANL research on spectral theory is focused on incorporating the effects of swirl. This adds an additional level of complexity to the modeling and direct numerical simulations. Also, multiscale or "reduced spectral,, models are being pursued for use in large computer codes.

Applications of Group Theory to Turbulence Modeling - Brian Volintine, DOE Office of Industrial Technologies

Another approach to the turbulence closure problem involves the application of group theory. In many difficult problems in physics, one may obtain approximate solutions by

expanding the solution in terms of an infinite power series in a small physical parameter. Inserting this series into the governing equations generates a hierarchy of simpler problems that can be solved in sequence. The solution to the original problem is then obtained from the series expansion. One usually only computes the first few terms in the series and argues that the remaining terms are negligible. This yields an approximate solution to the original problem.

Something akin to a series solution can be generated for the turbulence closure problem. The Reynolds stress, the product of two fluctuating velocity components first appears in the average momentum conservation equation as an unclosed term. One can in turn generate a conservation equation for the Reynolds stress which will include unclosed terms involving the triple velocity correlations. One can proceed further to a transport equation for the triple correlation which will contain unclosed fourth order correlations. The process can be continued indefinitely. Unlike the power series solution method described above, the higher order correlations do not become negligible compared to their lower order counterparts in this case so one cannot simply neglect these terms to get a valid approximate solution to the problem.

A similar problem was encountered in fundamental particle physics. A solution to this problem was constructed called renormalization group methods. The renormalization group methods have been applied to the turbulence closure problem with some success in single phase flow. Attempts have also been made in the area of turbulent magnetohydrodynamics where, unfortunately, success was not achieved. Nevertheless, the renormalization group method might be successfully applied to the problem of turbulence in multiphase flows to bring new insights into such things as the multiphase analog of the Prandtl mixing length.

Potential Mechanisms for Collaboration/Oil and Gas Partnership - Bob Hanold, LANL

Los Alamos has been involved in a successful lab/industry partnership for research with the oil and gas production industry. This partnership includes the DOE multiprogram national laboratories and many oil and service companies. Some of the research being conducted deals with state-of-the-art processing of seismic data important to oil and gas exploration.

In the Oil and Gas Partnership, projects are proposed by laboratory and industrial partners. The proposals are reviewed and scored by an industry board. The board recommendations are then sent to the DOE which considers this input in their funding decisions. The DOE has consistently followed the recommendations of the industry board.

Funding and project administration can be tailored to the requirements of the industrial partner(s) in each project. Usually cost-sharing from the industrial partners involves some form of in-kind contributions such as the sharing of data, equipment or personnel time. Administrative arrangements can range from informal agreements to formal co-operative research and development agreements wherein many details of the collaboration are spelled out in a legal contract.

Total DOE funding for the Oil and Gas Partnership has grown to over $30 million per year recently. This very successful partnership can serve as a model for a consortium on reactive multiphase flow simulation.

Review of 1st Industrial Energy Efficiency Symposium and Expo - Ed Joyce, LANL (Attachment 9)

The 1st Industrial Energy Efficiency Symposium and Expo held in Washington D.C. on May 1-3, 1995 was reviewed. The meeting was an open symposium involving groups from private industry, federal laboratories and agencies and the academic community. The meeting highlighted the DOE Office of Industrial Technologies "Industries of the Future,, program which covers the chemicals, petroleum refining, forest products, glass, aluminum, metal casting and steel industries.

The proposed structure for future national laboratory/industry collaborations under the "Industries of the Future,, program would involve the formation of "Virtual Laboratories,, and Centers of Excellence. The "Virtual Laboratories,, would be effective laboratories constructed from complimentary groups from the various actual national laboratories. Centers of Excellence could be virtual or real and would incorporate the best talent or laboratory group for a particular research mission. The research would be controlled by a coordinating council with all laboratories represented. Working groups would be established for all stated industry needs would be established and would be governed by laboratory and industry peer review.

Center for Materials Process Modeling - Richard Lesar, LANL

A brief description of the Los Alamos Center for Materials Process Modeling was presented as another example of how collaborative efforts can be structured. The Center's theme has been on tying research on materials process modeling across descriptive length scales from atoms (quantum mechanical and molecular modeling), through unit operations (computational fluid dynamics), process and plant modeling (control and optimization) to large scale enterprise and economic modeling. It is hoped that such a unified approach will bring forth useful synergies. Currently, the focus of the Center has been on the steel industry but the Center is expanding to include the concerns and needs of the chemical industry.

A View from Washington - Dan Wiley, DOE Office of Industrial Technologies (Attachment 10)

The Department of Energy is experiencing a tremendous state of flux currently. Pressures arising from the federal budget deficit and the objectives of the new congress are driving substantial reorganization and re-evaluation of the mission of the DOE. Downsizing of the department is going to occur. Some in congress have even proposed eliminating DOE and moving its core functions to other cabinet agencies.

While these changes are occuring, US industry is also undergoing tremendous change. Increased foreign competition and stockholder pressure to cut costs has prompted many companies to significantly scale back or even eliminate entire segments of their research infrastructure. Many CEO's now look to the federal government to carry on the longer term basic and applied research that the companies can no longer afford due to short-term profit pressures but will need for the technologies of tomorrow (see "A Moment of Truth for America,, in Attachment 10).

While it is difficult to forecast how the DOE will respond to the needs of industry and the budgetary pressures, some new trends are emerging. To avoid the pitfalls associated with "Industrial Policy,, federal research in the future will have to cut across many industry segments such as petrochemical, steel, aluminum, glass, etc. In addition, to avoid the costs associated with unnecessary duplication of effort, federal labs and universities will have to work more cooperatively.

Tank Flow Simulation - Bert Harvey, Dow Chemical Company

A movie made from a 3-dimensional simulation of a stirred tank reactor was shown. The computation of the three-dimensional flow in a baffled tank stirred by a rotating 45 degree pitch-blade impeller was done using a combination of rotating and stationary grid zones. Adjacent grid zone are patched together using an overlapping technique. Grid speed terms are included in the generalized coordinate transformation to account for the motion of the grid.

The simulation was performed using a modified version of the INS3D incompressible Navier-Stokes solver developed at NASA-Ames Research Center by Stuart Rogers. The solver uses the artificial compressibility method of coupling the pressure and velocity fields instead of solving a pressure Poisson equation as done in CFDLIB.

In an incompressible flow, the pressure does not appear explicitly in the continuity equation even though the pressure field has a direct influence on the divergence of the velocity field. The artificial compressibility method involves adding a pseudo-time derivative in pressure to the continuity equation. A pseudocompressibility parameter is then used to adjust the magnitude of pressure disturbances which are made to

propagate at a finite speed throughout the flow field. The solution procedure involves driving the pseudo-time pressure derivative to zero, thus satisfying continuity.

Some thoughts on a potential CFD consortium - Tyler Thompson, Dow Chemical Company (Attachment 11)

Some thoughts on a potential government/industry/academia consortium on computational fluid dynamics research for the Chemical Process Industries (CPI) were presented. The premise of the discussion was that today's tools are inadequate for the needs of the CPI. Needs include vastly improved simulation capabilities in the areas of turbulent reacting flows, multiphase flows and polymer melts and solutions with time dependent 3-dimensional character, free surfaces and non-Newtonian constitutive laws. The inadequacy of today's tools stems from the history of the market, legacy code architectures, slow implementation of advances and the lack of progress in the implementation of the high promises of parallelization.

To address and overcome these problems, a government industry consortium is proposed since no single company or industry group can justify the longer term research to attack this problem. The proposed consortium would be governed tightly by an industry board which would dispense government research money to "subcontractors" according to the perceived needs. The "subcontractors" would include federal laboratories, academic groups and private companies such as commercial software vendors who could ensure the user-friendliness, service and support of the products of the consortium.

Some prior thought would have to be given to the conflicting manner in which industry and government allocates research money. Industry typically allocates solely on the basis of performance and economic need due ultimately to stockholder pressure. Government, on the other hand, often allocates money not only on the basis of performance and economic need but also on the basis of "fairness" which can result in lower efficiency. In order to maximize the return on the research funding, the industry model of allocation should be used.

Brainstorm/Discussion - Consortium/Center of Excellence - Wrap-up - Brian VanderHeyden, LANL (Attachment 12)

To close the workshop, a brainstorming session was held to develop a consensus on the perceived needs that a reactive multiphase flow simulation consortium or center of excellence should address in the areas of theory, experiment, numerical methods and generic simulations. Also consensus on the structure of the potential consortium/center of excellence was sought. In addition, a sample letter of endorsement was distributed to the participants. Using the sample letter as a guide the participants were asked to send LANL a letter stating their support of for the idea of a consortium on reactive multiphase flow simulation. Finally, the participants were given a feedback form.

The following summarizes the needs identified by the industrial participants during the brainstorming session.

On the issue of theoretical needs the effects of turbulent mixing on reaction rates, turbulent grain diffusion, multiphase turbulence, dispersion/coalescence processes, nucleation processes and exchange correlations for packed and fluidized beds were all seen as fruitful areas of research.

On the issue of experimental needs it was agreed that coupling of simulation and experiment is crucial. It was felt that providing experimental data is one potential mode of industrial partner contributions to a consortium. It was also felt that focused non-proprietary fundamental experiments could be designed which would provide information needed to close modeled terms in the governing equations.

On the issue of numerical methods needs it was felt that some current highly specialized academic research could be redirected to help realize the promise of parallelization. It was also pointed out that improved numerical methods such as multigrid techniques rather than parallelization may proved to be a fruitful route to much needed speed-up of multiphase flow simulation codes. State-of-the-art reviews were also offered as a useful product of a consortium.

On the issue of centering a consortium on one or two generic, non-proprietary simulations along the lines of a multiphase flow simulation grand challenge, the group was somewhat split. Some felt the focus should be solely on fluidized gas-solid flows while others felt stirred tanks and packed beds should be the focus. Thermal ethylene cracking units were offered as a widespread and economically very important process in which turbulent mixing and chemical reaction plays an important role. Some felt that the focus of the consortium should be kept quite general.

On the potential structure of a consortium or center of excellence whose mission would be to substantially improve the state-of-the-art, all seemed to agree that it should be comprehensive and include federal labs and agencies, industrial partners, academic researchers and commercial software vendors. It was also felt that "virtual,, centers can be in effective if the governing board or director is not given sufficient power.

At the close of the meeting it was decided that the next step be the issuing of a white paper on the formation of a consortium based on the ideas put forward at the workshop. Several volunteered to help with the white paper. The white paper would be used to explain the mission and structure of a consortium and to lobby the government for funding.

Brian VanderHeyden - June, 1995

Attachment 1
Agenda
Brian VanderHeyden
LANL

WORKSHOP AGENDA - DAY 1, MAY 18, 1995

8:30-9:10	• Greetings/Administrative Items/Schedule • LANL, T-3 Overview • LANL Strategic and Tactical Plan, Dual Use co-operative research • Workshop purpose • Guest introductions	Brian VanderHeyden - LANL
9:10-9:30	Introductory Simulation Movies • Riser flows • 3-phase flows • 3-D bubble columns	Bucky Kashiwa - LANL
9:30-10:00	"Prototype Multiphase Flow Problems"	Paul Merz - Chevron
10:00-10:05	BREAK	all
10:05-11:00	Review of CFDLIB/Current Theory • Multimaterial formalism • Mass and momentum conservation • Numerical methods	Bucky Kashiwa - LANL
11:00-11:30	"Air-Agitated Alumina Crystallizer"	Phil Hsieh - ALCOA
11:30-NOON	"Heat Transfer Mechanism in Ebullated Bed Reactors"	Farshad Bavarian - Texaco
NOON-1:15	Lunch - Otowi Cafeteria	all
1:15-1:45	Review of CFDLIB/Current Theory • Energy conservation • Exchange models • Current turbulence models	Brian VanderHeyden- LANL
1:45-2:15	"Simulation of gas jets in molten metal baths"	Jon Wolfe - Molten Metal Technologies
2:15-2:20	BREAK	

2:20-2:50	Review of CFDLIB/Current Theory • Parallel implementation and results	Nely Padial - LANL
2:50-3:20	"Multiphase Flow at Procter & Gamble"	John McKibben, Joe Kitching- Procter & Gamble
3:20-3:50	"Multiphase Flow at Exxon"	Bill Heard - Exxon
3:50-4:30	"KIVA - Combustion Simulation"	Dan Butler - LANL
4:30	Adjourn	all
6:30-8:30	Dinner at Anthony's on the Delta in Espanola - Party Menu: Chicken Kiev, Prime Rib, Broiled Salmon (also vegetarian with advanced notice), $19.95 per person including salad, dessert and gratuity. Cocktails extra Dinner Speech - "Los Alamos - A Modern Village in an Ancient Setting"	Frank Harlow - LANL

WORKSHOP AGENDA - DAY 2, MAY 19, 1995

8:15-8:30	Plan for the day	Brian VanderHeyden -LANL
8:30-9:00	Telluride/Pagosa • High speed flows • Unstructured grids • Object-oriented programming • Parallelization	Doug Kothe - LANL
9:00-9:30	Review of CFDLIB/Current Theory • Chemical Reaction Package • Immersed Boundaries	Bucky Kashiwa - LANL
9:30-9:45	"Multiphase Reynolds Stress Transport Modeling"	Brian VanderHeyden - LANL
9:45-10:00	"Spectral Models, Symmetry and Engineering Turbulence Closures"	Tim Clark - LANL
10:00-10:05	Break	all
10:05-10:35	"Applications of Group Theory to Turbulence Modeling"	Brian Volintine - DOE Office of Industrial Technologies
10:35-11:00	Potential Mechanisms for Collaborations • User facility agreements • CRADA's • Consortia • Centers of Excellence • Example (Oil & Gas Partnership)	Bob Hanold - LANL
11:00-11:15	Review of 1st Industrial Energy Efficiency Symposium and Expo	Ed Joyce - LANL
11:15-11:30	Center for Materials Process Modeling	Richard Lesar - LANL
11:30-12:45	Lunch - Otowi Cafeteria	all

12:45-2:00	Brainstorm/Discussion - Consortium/Center of Excellence	all

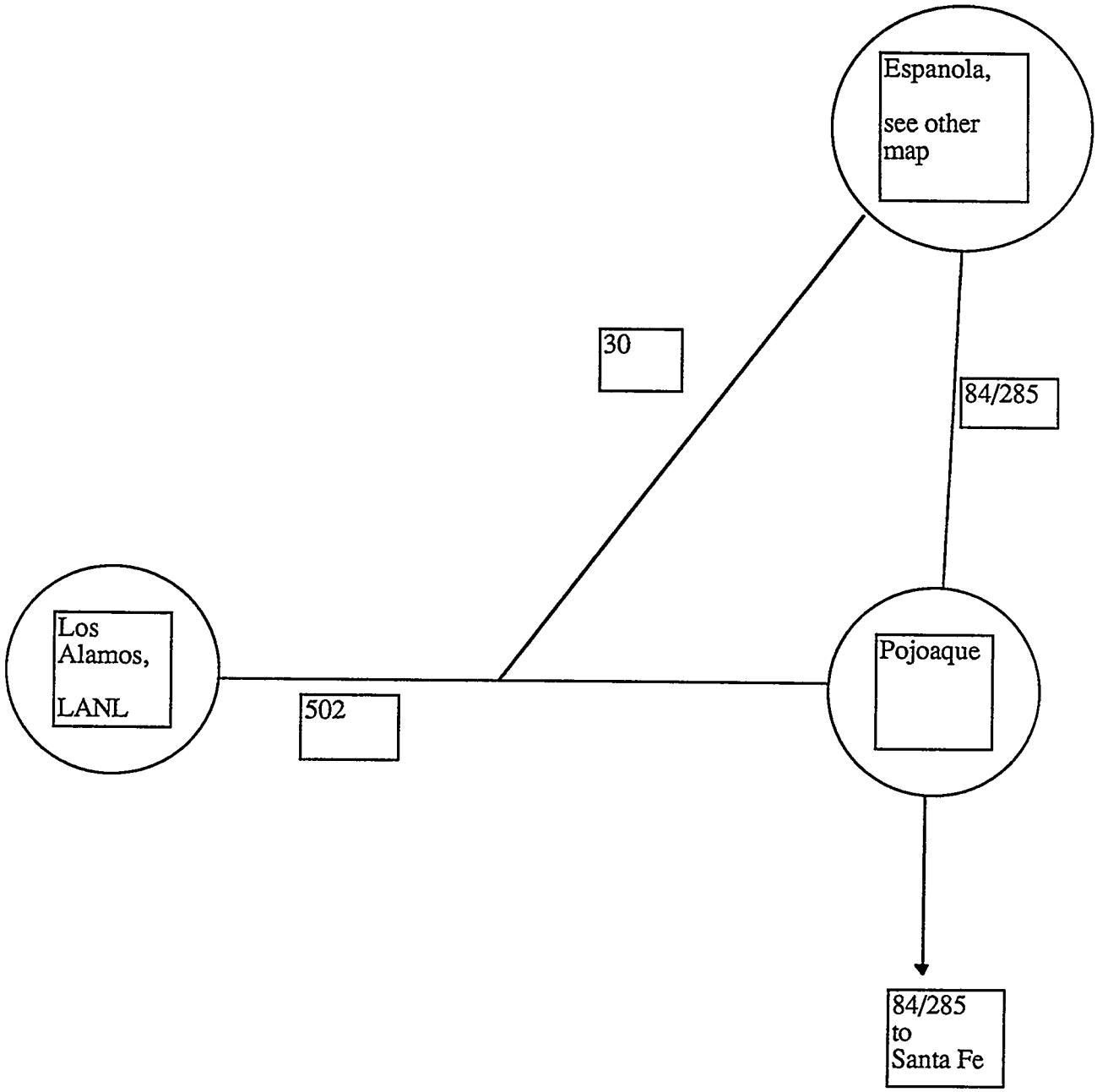
- Needs
  - Theory
  - Experiment
  - Numerical methods
  - Generic simulations
- Potential Consortium/Center of Excellence
  - Vision/Mission
  - Structure

2:00-2:10	BREAK	all
2:10-2:30	Wrap-up	all

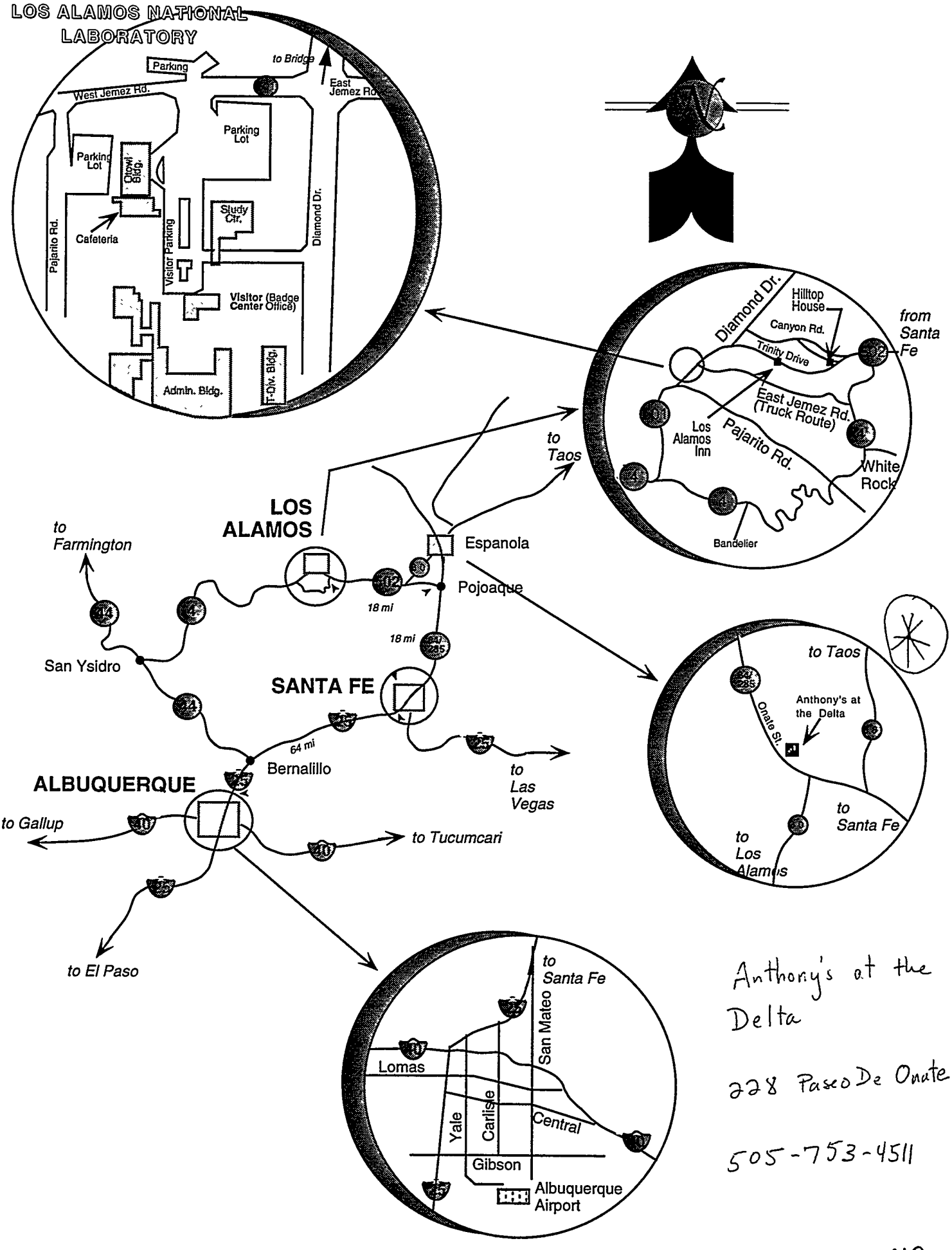
- Meeting documentation
- Feedback (another, expanded workshop?)
- Protocol

2:30-2:45	Tour of Computational Testbed for Industry	all
2:45-3:15	Tour of Advanced Computing Laboratory	all
3:15	Adjourn	

Anthony's at the Delta
228 Paseo De Onate
Espanola, NM
505-753-4511



A1.6



Anthony's at the Delta

228 Paseo De Onate

505-753-4511

A1.7

Attachment 2
Workshop Introduction
Brian VanderHeyden
LANL

LA-UR-95-1724

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: **REACTIVE MULTIPHASE FLOW SIMULATION WORKSHOP**

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*

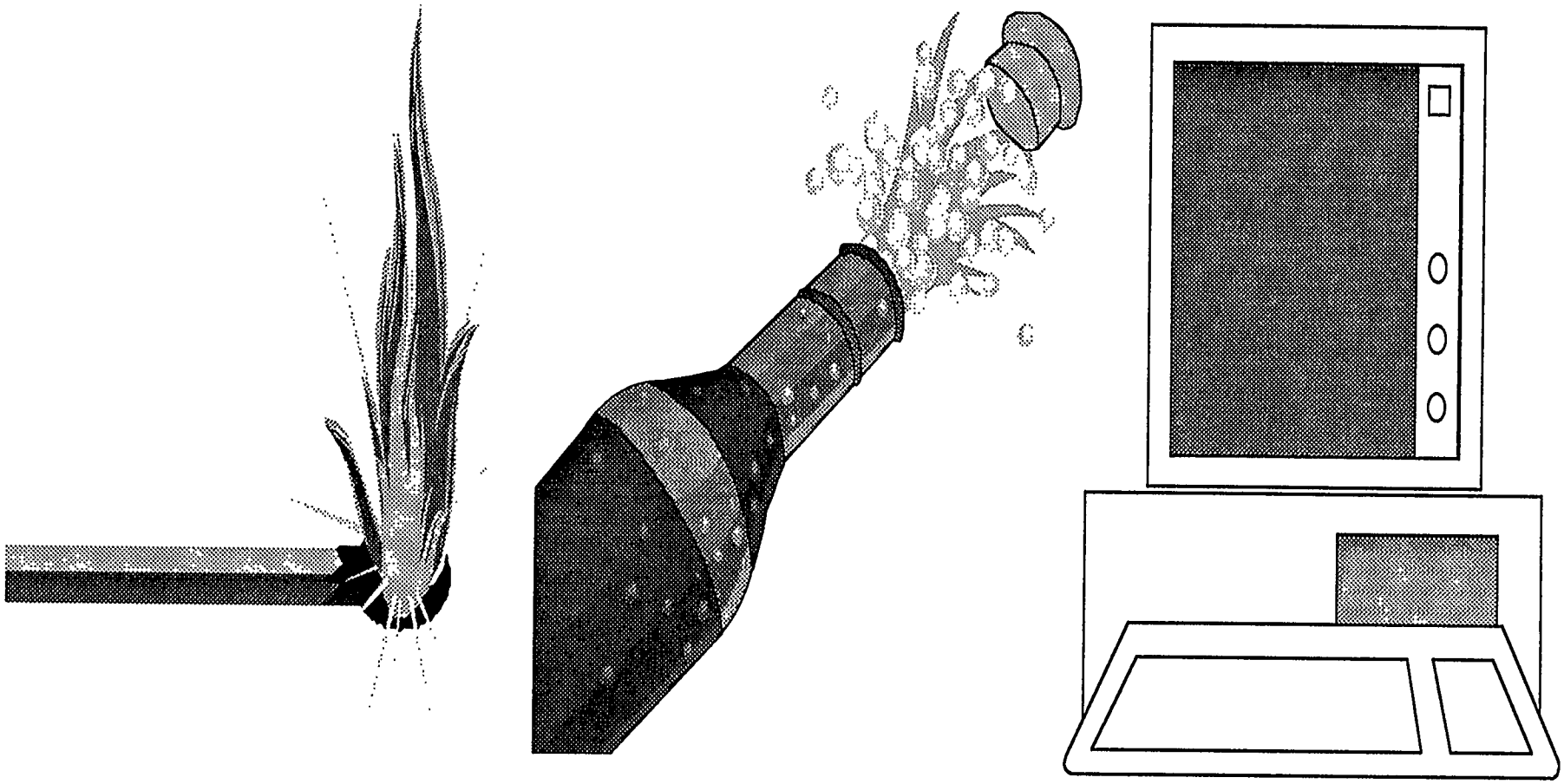
Los Alamos

Los Alamos National Laboratory
Los Alamos, New Mexico 87545

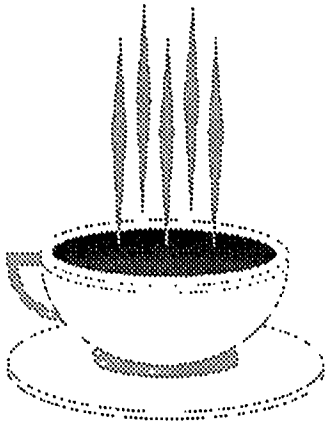
FORM NO. 836 R4
ST. NO. 2629 5/81

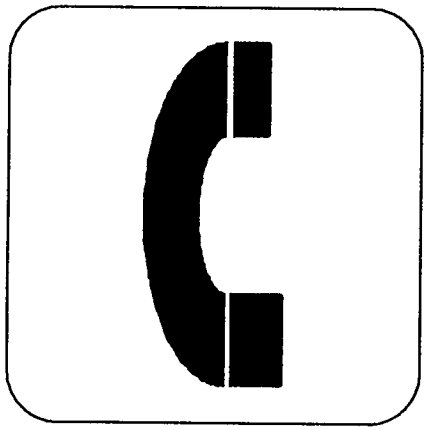
A2.2

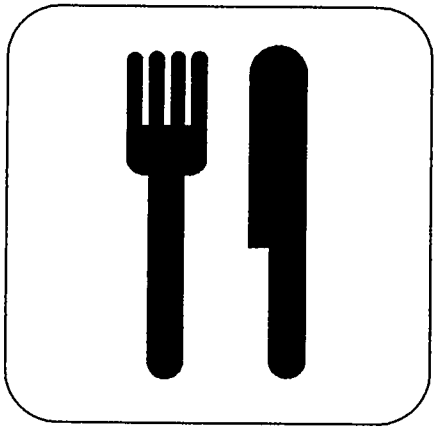
Reactive Multiphase Flow Simulation Workshop



Administrative Items

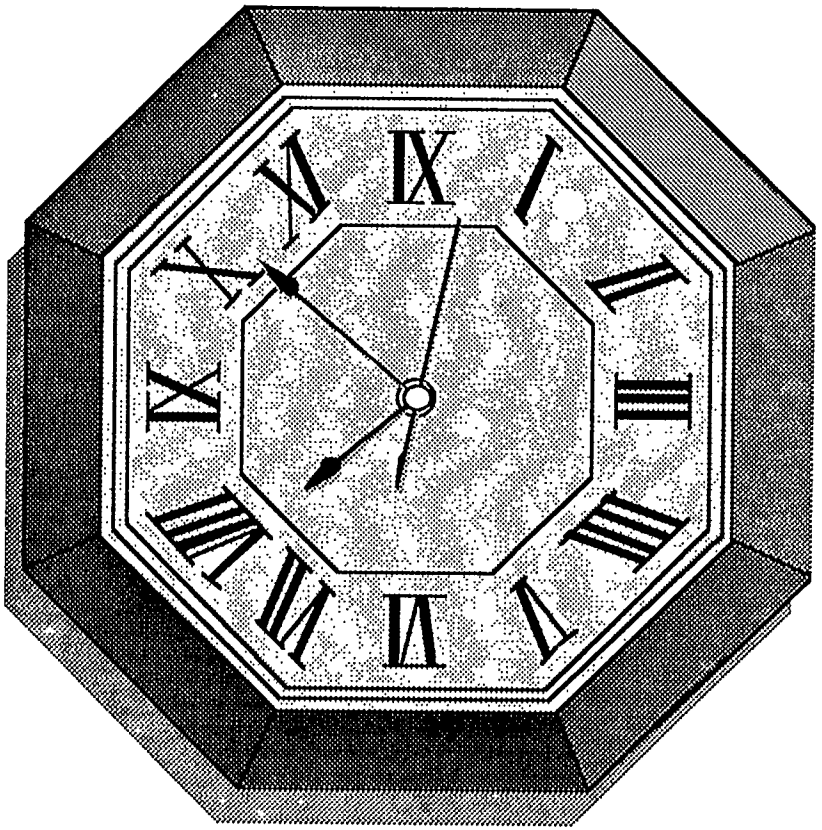






Schedule

- Today
  - » Orientation
  - » Technical Presentations
  - » Dinner
- Tomorrow
  - » Technical Presentations
  - » Organizational Information
  - » Brainstorming
  - » Tours



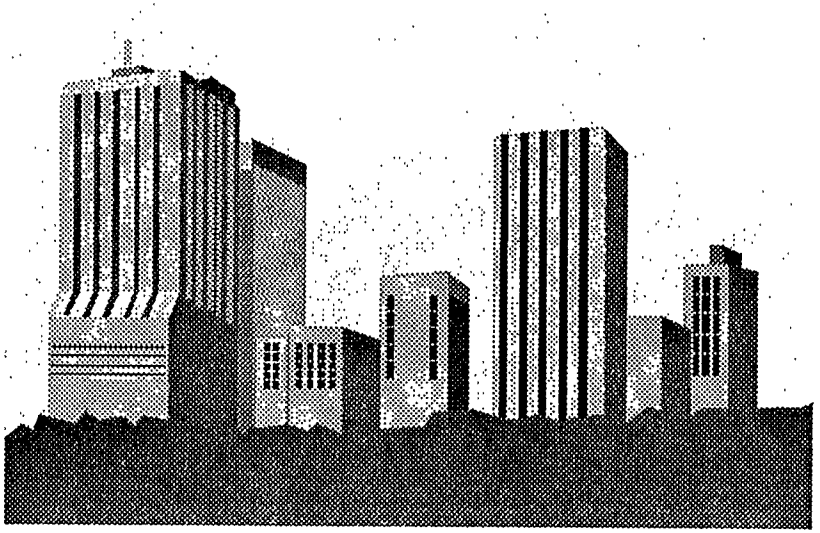
LANL Technical Goals

- Science-Based Stockpile Stewardship
- Neutron Laboratory
- Plutonium Legacy
- Great Science
- Modeling, Simulation and High-Performance Computing
- Industry

A2.6

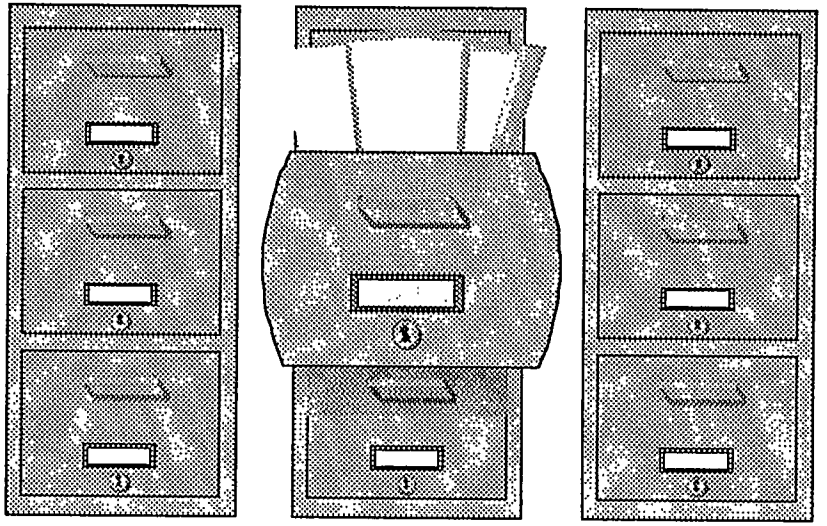
LANL STRUCTURE

- Administrative/ Business
- Technical



Administrative / Business

- Divisions
  - » Business Operations Division
  - » Environmental, Safety & Health
  - » Facilities, Security & Safeguards
  - » Human Resources
  - » Non-proliferation & International Security
- Programs
  - » Industrial Partnership
  - » Quality & Planning
- Offices
  - » Audits & Assessments
  - » Government Relations
  - » Public Affairs
  - » Laboratory Council



Technical Divisions

- Accelerator Operations & Technology
- Applied Theoretical Physics
- Chemical Science & Technology
- Computing, Information & Communications
- Dynamic Experimentation
- Earth & Environmental Sciences
- Engineering Sciences & Applications
- Life Sciences
- Materials Science & Technology
- Nuclear Materials Technology
- Physics
- Technology & Safety Assessment
- **Theoretical**

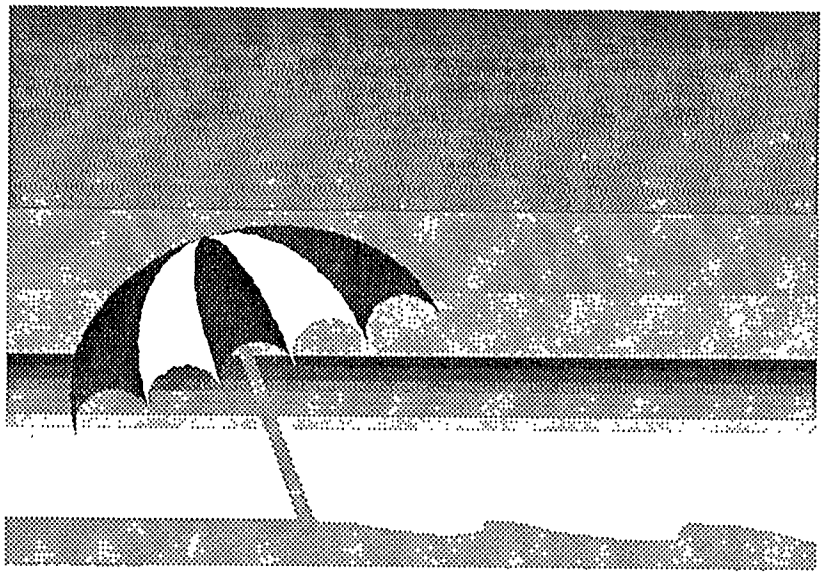
Technical Programs

- Department of Defense
- Energy Technology
- Environmental Management
- LANSCE/Energy Research
- Nuclear Materials & Reconfiguration Technology
- Nuclear Weapons Technology
- Science & Technology Base

A2.10

T-3

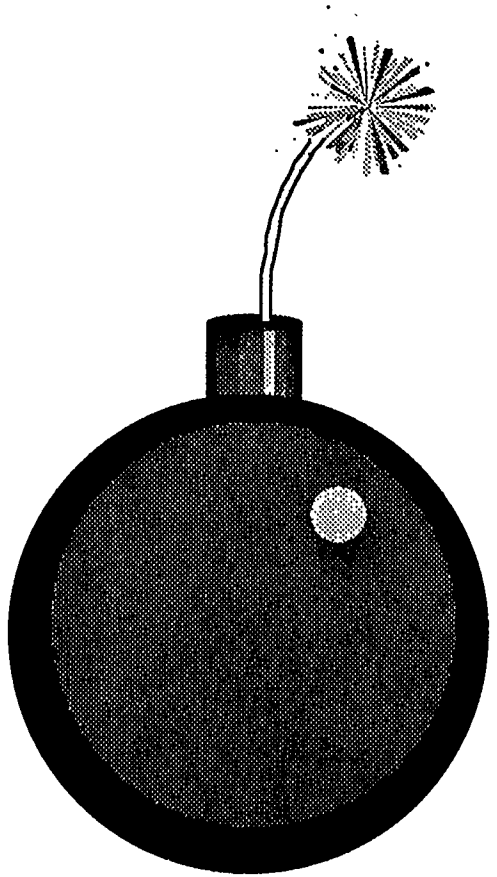
- Theoretical Division Fluid Dynamics Group
  - » Weapons
  - » Materials
  - » Single and Multiphase Turbulence theory
  - » Geophysical Flows
  - » Combustion flows (KIVA)
  - » Multiphase flows (CFDLIB)



A2.11

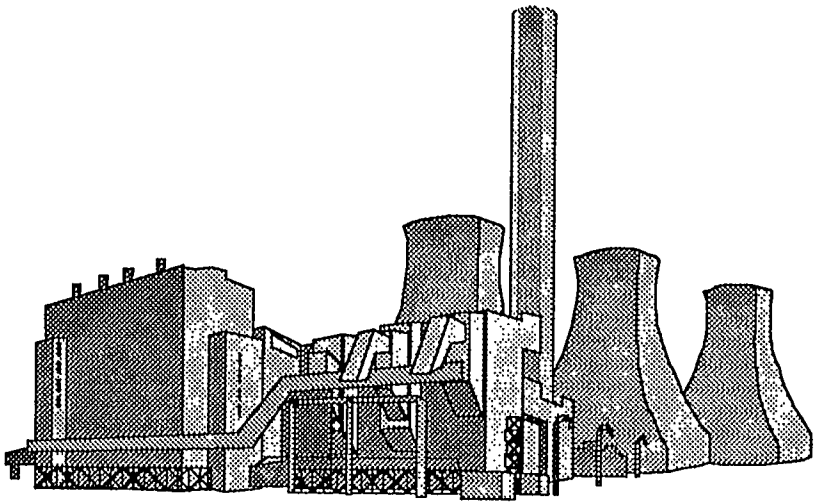
Defense Applications

- DARHT
- Near-miss missile intercept
- Jumbino



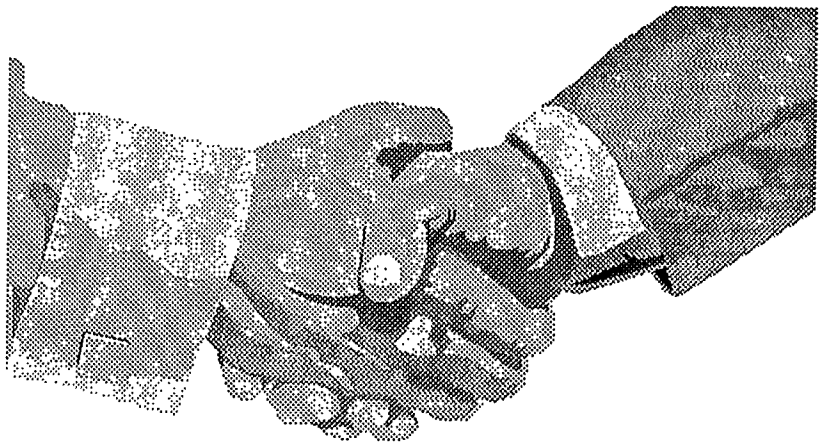
Industrial Applications

- Circulating Fluidized Beds
- Bubble Columns
- Gas-Liquid-Solid
- etc, etc.



Workshop Purpose

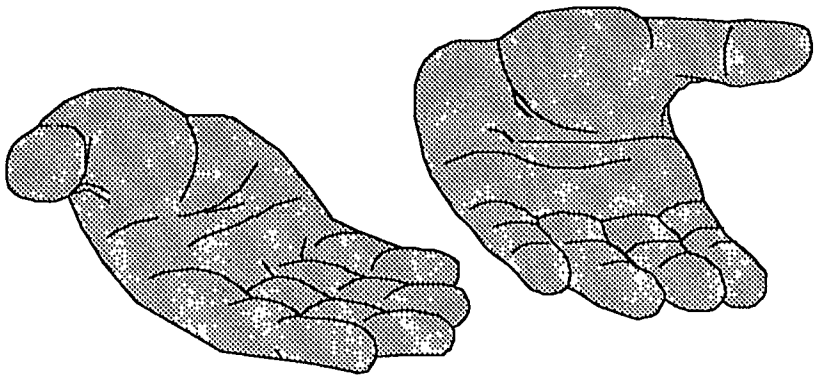
- Needs and capabilities
  - » Industry
  - » LANL
- Future collaboration possibilities



A2.14

Workshop Products

- Workshop Document
  - » Summary
  - » Guest Feedback
- Springboard



Attachment 3
Review of CFDLIB/Current Theory
Bucky Kashiwa
LANL

Multimaterial Formalism
Mass and Momentum Conservation
Numerical Methods

LA-UR-95-1745

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: **MISCELLANEOUS NOTES ON MULTIPHASE FLOW THEORY**

AUTHOR(S): Bryan Kashiwa, 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

A3.2

Miscellaneous Notes on Multiphase Flow Theory

Bryan (Bucky) Kashiwa
Los Alamos National Laboratory
Theoretical Division, Group T–3
(505) 667–8812, bak@lanl.gov

Presented at the LANL Workshop
on
Supercomputer Simulation
of
Industrial Reactive Multiphase Flows
18–19 May 1995
Los Alamos, NM

A3.3

Very Broad–Brush Overview

- A Multimaterial Formalism.
- Mean–Flow Conservation Equations.
- Frames of Reference.
- Numerical Solutions.
- Physical–Chemical Kinetics.
- The "Immersed Boundary" Method.

What we mean by A Multimaterial Formalism.

- A general method for developing averaged conservation equations for multiple materials, any *one* of which may be at a point, at a given instant.

- Definition of a "material" is up to the analyst.

- Requires knowledge of a continuum law for the dynamics at any point. This means that one has already averaged over individual molecules, at an "ordinary" point.

- This is a procedure by which the most likely state at a point, as well as which material is most likely to be found at a point, are determined simultaneously.

- Closure modeling is still up to the analyst; the exact equations, like laboratory experiments, help guide the modeling process.

How it works for a single material.

- Define the probability distribution function:

$$f(t, \mathbf{x}, \rho_0, \mathbf{u}_0, e_0) \cdot d\rho_0 d\mathbf{u}_0 de_0 = f d\Gamma_0$$

- Write down its total change:

$$\frac{\partial f}{\partial t} + \mathbf{u}_0 \cdot \boldsymbol{\nabla} f + \dot{\Gamma}_0 \cdot \frac{\partial f}{\partial \Gamma_0} = \frac{Df}{Dt}$$

- Define the general moment:

$$\langle Q_0 \rangle = \int Q_0(\Gamma_0) f d\Gamma_0$$

- This yields a moment generating equation:

$$\frac{\partial \langle Q_0 \rangle}{\partial t} + \boldsymbol{\nabla} \cdot \langle Q_0 \mathbf{u}_0 \rangle = \left\langle \dot{Q}_0 + Q_0 \boldsymbol{\nabla} \cdot \mathbf{u}_0 \right\rangle + \int Q_0 \frac{Df}{Dt} d\Gamma_0$$

- Define moments of interest:

$$\rho = \langle \rho_0 \rangle\,, \quad \rho \mathbf{u} = \langle \rho_0 \mathbf{u}_0 \rangle\,, \quad \text{and} \quad \rho e = \langle \rho_0 e_0 \rangle$$

- Use the continuum law for pure material:

$$\dot{\rho}_0 = -\rho_0 \nabla \cdot \mathbf{u}_0$$

$$\rho_0 \dot{\mathbf{u}}_0 = -\nabla p_0$$

$$\rho_0 \dot{e}_0 = -p_0 \nabla \cdot \mathbf{u}_0$$

- Turn the crank:

$$\frac{\partial}{\partial t} \begin{bmatrix} \rho \\ \rho \mathbf{u} \\ \rho e \end{bmatrix} + \nabla \begin{bmatrix} \rho \mathbf{u} \\ \rho \mathbf{u}\mathbf{u} + \langle \rho_0 \mathbf{u}_0' \mathbf{u}_0' \rangle \\ \rho e \mathbf{u} + \langle \rho_0 e_0 \mathbf{u}_0' \rangle \end{bmatrix}$$

$$= \begin{bmatrix} 0 \\ -\nabla p \\ -p \nabla \cdot \mathbf{u} - \langle p_0 \nabla \cdot \mathbf{u}_0' \rangle \end{bmatrix}$$

Extension to multiple materials.

- Extend the phase space of f:

$$f(t, \mathbf{x}, \rho_0, \mathbf{u}_0, e_0, \alpha_1, \alpha_2, \ldots, \alpha_N) \cdot$$
$$d\rho_0 d\mathbf{u}_0 de_0 d\alpha_1 d\alpha_2 \ldots d\alpha_N$$

- Define moments of interest:

$$\rho = \langle \alpha_k \rho_0 \rangle, \quad \rho \mathbf{u} = \langle \alpha_k \rho_0 \mathbf{u}_0 \rangle, \quad \text{and} \quad \rho e = \langle \alpha_k \rho_0 e_0 \rangle$$

- Turn the crank:

$$\frac{\partial}{\partial t} \begin{bmatrix} \rho_k \\ \rho_k \mathbf{u}_k \\ \rho_k e_k \end{bmatrix} + \boldsymbol{\nabla} \cdot \begin{bmatrix} \rho_k \mathbf{u}_k \\ \rho_k \mathbf{u}_k \mathbf{u}_k + \langle \alpha_k \rho_0 \mathbf{u}_k' \mathbf{u}_k' \rangle \\ \rho_k e_k \mathbf{u}_k + \langle \alpha_k \rho_0 e_0 \mathbf{u}_k' \rangle \end{bmatrix}$$
$$= \begin{bmatrix} \langle \rho_0 \dot{\alpha}_k \rangle \\ \langle \alpha_k \rho_0 \dot{\mathbf{u}}_0 \rangle + \langle \rho_0 \mathbf{u}_0 \dot{\alpha}_k \rangle \\ \langle \alpha_k \rho_0 \dot{e}_0 \rangle + \langle \rho_0 e_0 \dot{\alpha}_k \rangle \end{bmatrix},$$

- Use the continuum law for pure material:

$$\rho_0 \dot{\mathbf{u}}_0 = -\nabla p_0 + \nabla \cdot \boldsymbol{\tau}_0 + \rho_0 \mathbf{g}$$

$$\rho_0 \dot{e}_0 = -p_0 \nabla \cdot \mathbf{u}_0 + (\boldsymbol{\tau}_0 : \boldsymbol{\varepsilon}_0)/2 - \nabla \cdot \mathbf{q}_0$$

- Consider the pressure acceleration term:

$$\begin{aligned}\langle \alpha_k \rho_0 \dot{\mathbf{u}}_0 \rangle &= -\langle \alpha_k \nabla p_0 \rangle \\ &= -\langle \alpha_k \rangle \nabla p - \langle \alpha_k \nabla p_0' \rangle \\ &= -\theta_k \nabla p - \langle \nabla \alpha_k p_0' \rangle + \langle p_0' \nabla \alpha_k \rangle\end{aligned}$$

- In which the equilibration pressure satisfies:

$$1 - \textstyle\sum_k \rho_k v_k(p, T_k) = 0$$

and we identify

$$\theta_k = \rho_k v_k$$

as the volume fraction, in the equlibrium case.

Summary of Exact, Averaged, Equations.

$$\frac{\partial \rho_k}{\partial t} + \nabla \cdot \rho_k \mathbf{u}_k \quad k \text{ mass accumulation}$$

$$= \langle \rho_0 \dot{\alpha}_k \rangle \quad k \text{ mass conversion}$$

$$\frac{\partial}{\partial t} \rho_k \mathbf{u}_k + \nabla \cdot \rho_k \mathbf{u}_k \mathbf{u}_k \quad k \text{ momentum accumulation}$$

$$= \langle \rho_0 \mathbf{u}_0 \dot{\alpha}_k \rangle \quad k \text{ momentum conversion}$$

$$-\nabla \cdot \langle \alpha_k \rho_0 \mathbf{u}'_k \mathbf{u}'_k \rangle \quad \text{Reynolds stress}$$

$$-\theta_k \nabla p \quad \text{equilibration pressure}$$

$$+\rho_k \mathbf{g} \quad \text{body force}$$

$$-\nabla \theta_k (p_k^0 - p) \quad \text{nonequilibrium pressure}$$

$$+\nabla \cdot \langle \alpha_k \boldsymbol{\tau}_0 \rangle \quad \text{average stress}$$

$$+ \langle [p'_0 \mathbf{I} - \boldsymbol{\tau}_0] \cdot \nabla \alpha_k \rangle \quad \text{momentum exchange}$$

$\frac{\partial}{\partial t}\rho_k e_k + \nabla \cdot \rho_k e_k \mathbf{u}_k$	k energy accumulation
$= \langle \rho_0 e_0 \dot{\alpha}_k \rangle$	k energy conversion
$-\nabla \cdot \langle \alpha_k \rho_0 e_0 \mathbf{u}'_k \rangle$	fluctuational transport
$- \langle \alpha_k p_0 \nabla \cdot \mathbf{u}_0 \rangle$	multiphase work
$+ \langle \alpha_k \boldsymbol{\tau}_0 : \boldsymbol{\varepsilon}_0 \rangle / 2$	average dissipation
$-\nabla \cdot \langle \alpha_k \mathbf{q}_0 \rangle$	average conduction
$+ \langle \mathbf{q}_0 \cdot \nabla \alpha_k \rangle$	energy exchange

Frames of Reference.

- Consider Leibnitz' Rule relative to material k:

$$\int_V \frac{\partial q_k}{\partial t} dV + \int_S \hat{\mathbf{n}} \cdot q_k \mathbf{u}_k dS = \frac{d}{dt} \int_V q_k dV$$

- And again relative to the mesh:

$$\int_V \frac{\partial q_k}{\partial t} dV + \int_S \hat{\mathbf{n}} \cdot q_k \mathbf{u}_m dS = \frac{d_m}{dt} \int_V q_k dV$$

- Now subtract:

$$\frac{d_m}{dt} q_k V + V \boldsymbol{\nabla} \cdot q_k (\mathbf{u}_k - \mathbf{u}_m) = \frac{\Delta(q_k V)}{\Delta t}$$

- A "Lagrangian" scheme comes from letting

$$\mathbf{u}_m = \mathbf{u}_k$$

and using the kinematic rule

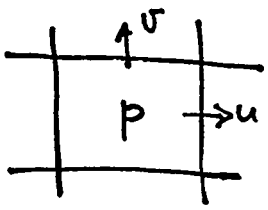
$$\dot{\mathbf{x}}_k = \mathbf{u}_k$$

to establish the location of material k.

Highlights of the CFDLIB method.

- Finite–Volume scheme.
- State vector cell–centered.
- Coupling accomplished with space–centered, time–advanced fluxes of volume and momentum.
- Implicit in pressure acceleration, like the ICE method; extension is to cell–centered variables.
- Implicit in exchange terms.

- Consider Classical MAC, with $\rho = const.$:



$$\widetilde{\mathbf{u}} = \mathbf{u}^n - \Delta t \nabla_f \cdot \mathbf{u}^n \mathbf{u}^n$$

$$\mathbf{u}^{n+1} = \widetilde{\mathbf{u}} - \Delta t \nabla_f p$$

$$\nabla_c \cdot \mathbf{u}^{n+1} = 0$$

- Restate by eliminating $\mathbf{u}^{n+1}$:

$$\nabla_c \cdot (\widetilde{\mathbf{u}} - \Delta t \nabla_f p) = 0$$

- Solve for p:

$$p = \frac{1}{\Delta t} (\nabla_c \cdot \nabla_f)^{-1} \nabla_c \cdot \widetilde{\mathbf{u}}$$

- Backsubstitute for $\mathbf{u}^{n+1}$:

$$\mathbf{u}^{n+1} = \mathbf{u}^n - \Delta t \nabla_f \cdot \mathbf{u}^n \mathbf{u}^n - \Delta t \nabla_f p$$

- or equivalently:

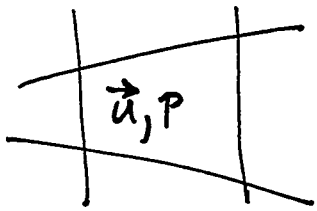
$$\begin{aligned} \mathbf{u}^{n+1} = \mathbf{u}^n & \\ & - \Delta t \nabla_f \cdot \mathbf{u}^n \mathbf{u}^n \\ & + \Delta t \nabla_f (\nabla_c \cdot \nabla_f)^{-1} \nabla_c \cdot \nabla_f \cdot \mathbf{u}^n \mathbf{u}^n \\ & - \nabla_f (\nabla_c \cdot \nabla_f)^{-1} \nabla_c \cdot \mathbf{u}^n \end{aligned}$$

- The cell–centered scheme has a similar flavor:

$$\mathbf{u}^* = \langle \mathbf{u}^n \rangle - \Delta t \nabla_f p$$

$$\mathbf{u}^{n+1} = \mathbf{u}^n - \Delta t \nabla_c \cdot \langle \mathbf{u}^n \rangle \mathbf{u}^* - \Delta t \nabla_f p$$

$$\nabla_c \cdot \mathbf{u}^* = 0$$



- We eliminate $\mathbf{u}^*$, and solve for p:

$$p = \frac{1}{\Delta t} (\nabla_c \cdot \nabla_f)^{-1} \nabla_c \cdot \langle \mathbf{u}^n \rangle$$

- Then backsubstitute for $\mathbf{u}^{n+1}$:

$$\mathbf{u}^{n+1} = \mathbf{u}^n - \Delta t \nabla_c \cdot \langle \mathbf{u}^n \rangle \mathbf{u}^* - \Delta t \nabla_c \langle p \rangle$$

- Which is equivalent to:

$$\begin{aligned} \mathbf{u}^{n+1} = \mathbf{u}^n & \\ & - \Delta t \nabla_c \cdot \langle \mathbf{u}^n \rangle \langle \mathbf{u}^n \rangle \\ & + \Delta t \nabla_c \cdot \langle \mathbf{u}^n \rangle \nabla_f (\nabla_c \cdot \nabla_f)^{-1} \nabla_c \cdot \langle \mathbf{u}^n \rangle \\ & - \nabla_c \langle (\nabla_c \cdot \nabla_f)^{-1} \nabla_c \cdot \langle \mathbf{u}^n \rangle \rangle \end{aligned}$$

- The reason this works is that the solenoidal velocity $\mathbf{u}^*$ is recognized as the flux of volume, and used accordingly.

Physical–Chemical Kinetics.

- Our goal is to account for phase change, heat exchange, and chemical–reactions in a fully coupled, implicit fashion.

- This yields the most robust integration, free of time–splitting errors connected with separation of these effects.

- One challenge is in handling the nonlinearities, in a way that guarantees physically–realizable (unique, equilibrium) solutions.

- Another challenge is to keep the accounting straight for energy conservation.

- Physical–Chemical reaction kinetic equations can be classified into three distinct functional forms:

  (1) Mass Action Law (Arrhenius gas, burning solid, catalysis):

$$\dot{\xi}_r = \prod [x_t^{n+1}]^{\nu'_{s,r}} k_{f,r} - \prod [x_t^{n+1}]^{\nu''_{s,r}} k_{b,r}$$

$$[x_s]^{\cdot} = \sum_r (\nu''_{s,r} - \nu'_{s,r}) \dot{\xi}_r$$

  (2) Mass–Saturation Limited (adsorption, desorption, pyrolysis):

$$\dot{y}_s = -(y_s^{n+1} - y_{sat}^n) k(p, T, a, \ldots)$$

  (3) Mass–Thermal–Saturation Limited (evaporation, condensation):

$$\dot{y}_s = -y_s^{n+1} (T_s^{n+1} - T_{sat}^n) k(p, T, T_{sat})$$

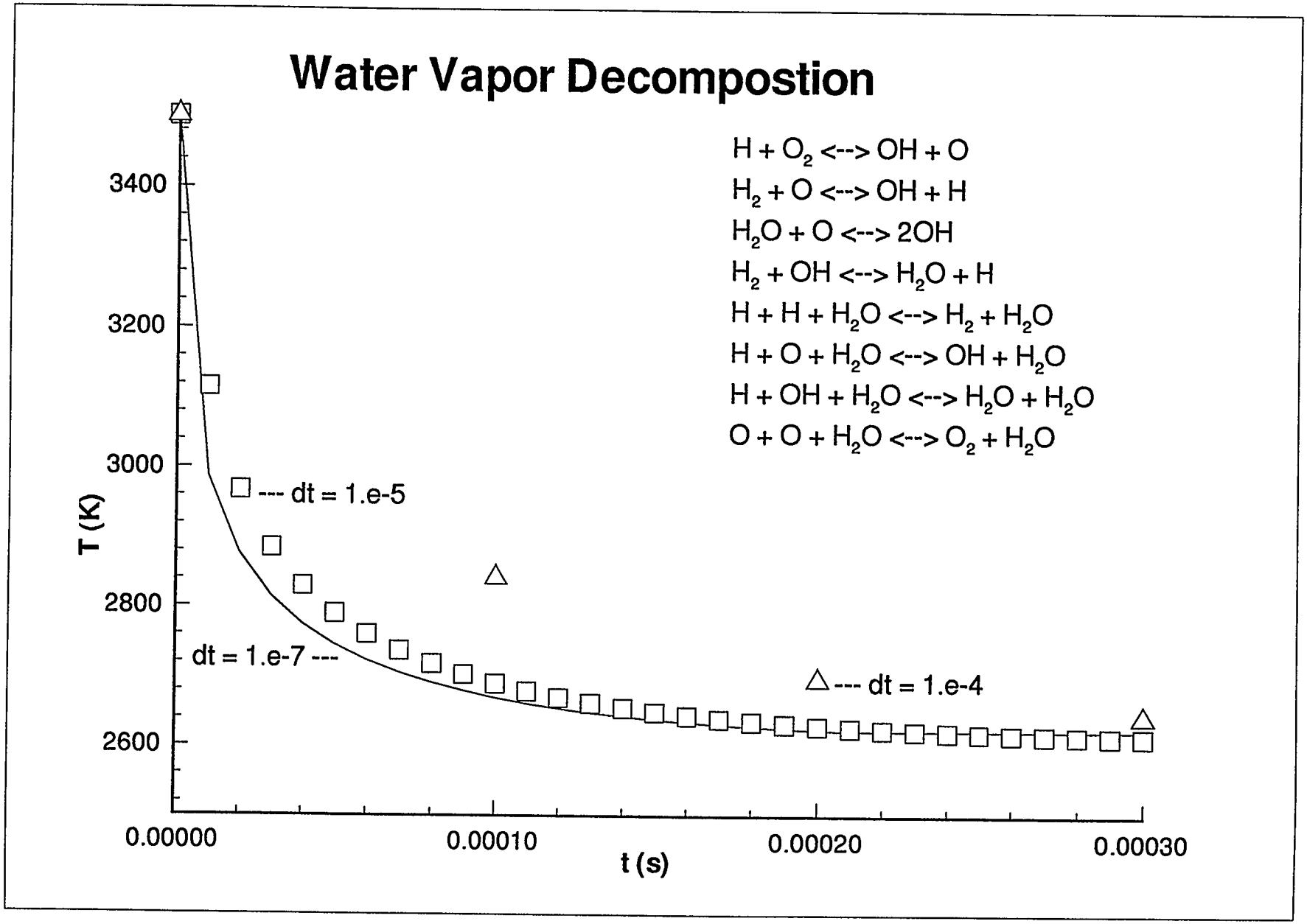
- Typically only a subset of reactions are stoichiometrically independent. Accordingly, only a subset of species can undergo independent changes in concentration.

- The abbreviated energy equations are:

$$\rho_k c_{p,k} \dot{T}_k = \theta_k \beta_k p \dot{p} + \sum_l \theta_k \theta_l R_{kl} (T_l^{n+1} - T_k^{n+1}) - \sum_{l \neq k} \frac{\dot{m}_k}{V} (h_l^* - h_k) + \sum_{r(k)} \dot{\xi}_r \Delta H_r$$

- Ramshaw and Chang devised a method for a single, gas–phase reaction mechanism that yields a time–accurate solution for small Δt, and the equlibrium solution for large Δt (J. Comput. Phys., **116**, 359–364, 1995).

- We have devised a scheme with the same properties. Results from a constant–volume, time–dependent, decompostion of water vapor follow.


Water Vapor Decompostion
H + O2 <--> OH + O
H2 + O <--> OH + H
H2O + O <--> 2OH
H2 + OH <--> H2O + H
H + H + H2O <--> H2 + H2O
H + O + H2O <--> OH + H2O
H + OH + H2O <--> H2O + H2O
O + O + H2O <--> O2 + H2O
3400
3200
3000
2800
2600
T (K)
--- dt = 1.e-5
dt = 1.e-7 ---
--- dt = 1.e-4
0.00000
0.00010
0.00020
0.00030
t (s)

A3.15

"Immersed Boundary Method"

- Introduced by Peskin for blood flow in the human heart, (J. Comput. Phys., **25**, 220–252, 1977).

- Extended to suspension flow by Sulsky and Brackbill, (J. Comput. Phys. **96**, 339–368, 1991).

- Currently being generalized for multiphase flow problems in CFDLIB.

- Uses many elements of the FLIP scheme made popular by Brackbill and Ruppel, (J. Comput. Phys. **65**, 314–343, 1986).

- The state vector is marched forward in time, in the Lagrangian frame relative to a finite mass of material.

- An underlying mesh of control volumes is used to assist in computing the changes along the Lagrangian trajectories.

- For example, consider the single–field incompressible case, for which the state vector is:

$$\{m_p,\, \mathbf{x}_p,\, \mathbf{u}_p,\, v_p\}^0$$

- The state vector advances according to:

$$m_p^{n+1} = m_p^n$$

$$\mathbf{x}_p^{n+1} = \mathbf{x}_p^n + \Delta t \sum_c \mathbf{u}_c^L S_{cp}^n$$

$$m_p^{n+1}\mathbf{u}_p^{n+1} = m_p^n \mathbf{u}_p^n - \sum_c V_c \rho_c^n (\mathbf{u}_c^L - \mathbf{u}_c^n) S_{cp}^n$$

$$v_p^{n+1} = v_p^n$$

$$0 = \boldsymbol{\nabla} \cdot \mathbf{u}_c^L$$

- Here $\sum_c (\ )_c S_{cp}^n$ represents a bilinear interpolation of data from mesh coordinates centered at $\mathbf{x}_c$, in volume V_c, to the point $\mathbf{x}_p^n$.

- The velocity in the mesh coordinate frame is defined:

$$\mathbf{u}_c^L = \mathbf{u}_c^n - \frac{\Delta t}{\rho_c^n} (\boldsymbol{\nabla} p)_c + \Delta t \mathbf{g}$$

- The "initial condition" is given by:

$$\mathbf{u}_c^n = \frac{\sum_p m_p^n \mathbf{u}_p^n S_{pc}^n}{\sum_p m_p^n S_{pc}^n} \equiv \frac{\text{expected momentum}}{\text{expected mass}}$$

and

$$\rho_c^n = \frac{\sum m_p^n S_{pc}^n}{\sum m_p^n v_p^n S_{pc}^n} \equiv \frac{\text{expected mass}}{\text{expected volume}}$$

- In this, $\sum_p (\ )_p S_{pc}^n$ represents the transfer of data from points $\mathbf{x}_p$ to mesh coordinates $\mathbf{x}_c$. As in the classical FLIP scheme, we use $S_{pc}^n = S_{cp}^n$.

- Results from the "Broken Dam Problem" follow.

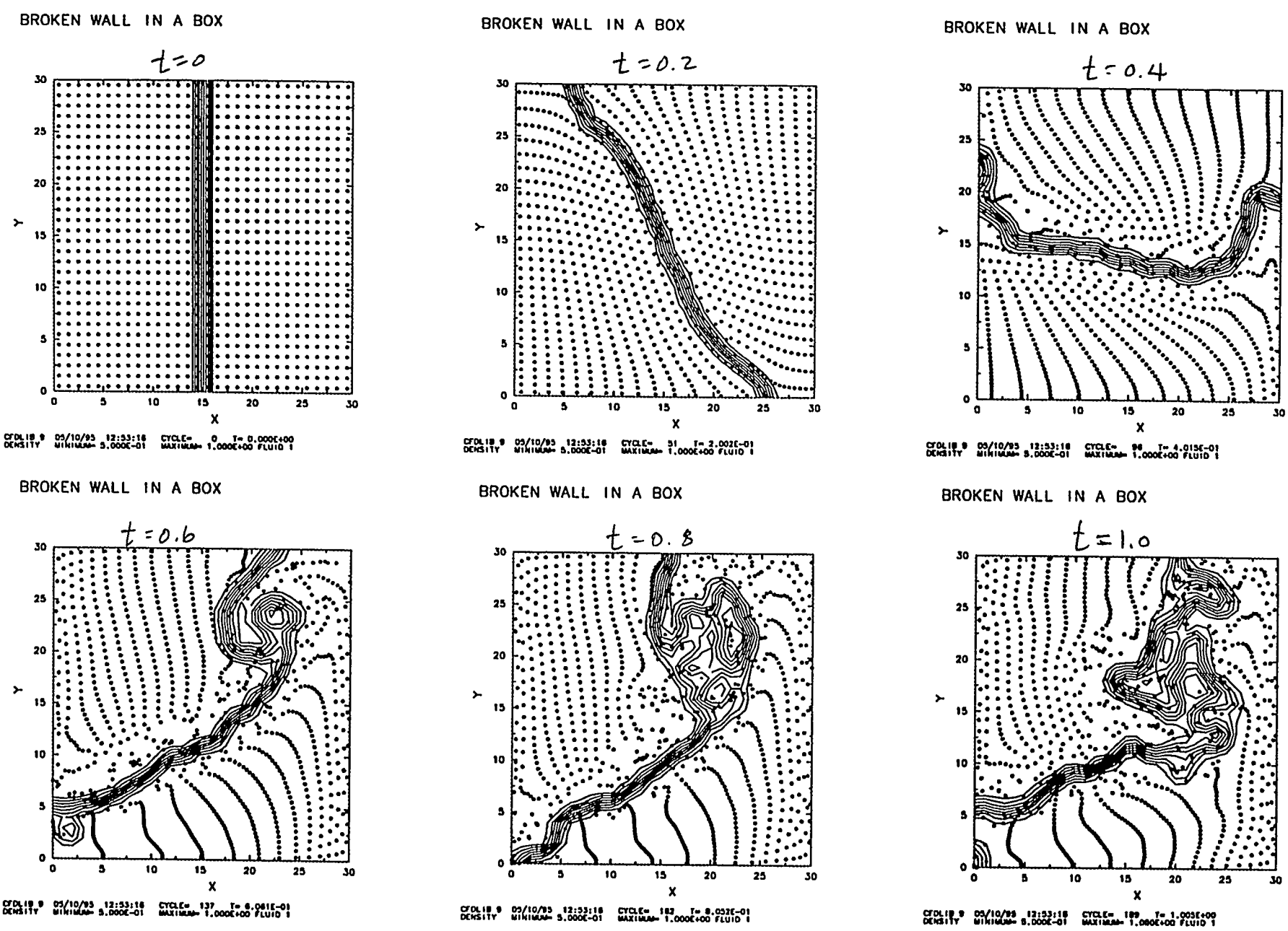


Figure 1. Single-Fluid, Lagrangian

43.24

Attachment 4
Review of CFDLIB/Current Theory
Brian VanderHeyden
LANL

Energy Conservation
Pressure Force Models
Current Turbulence Models

LA-UR-95-1723

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: **REVIEW OF CFDLIB/CURRENT THEORY—ENERGY CONSERVATION, MOMENTUM EXCHANGE MODELS, TURBULENCE MODELS**

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

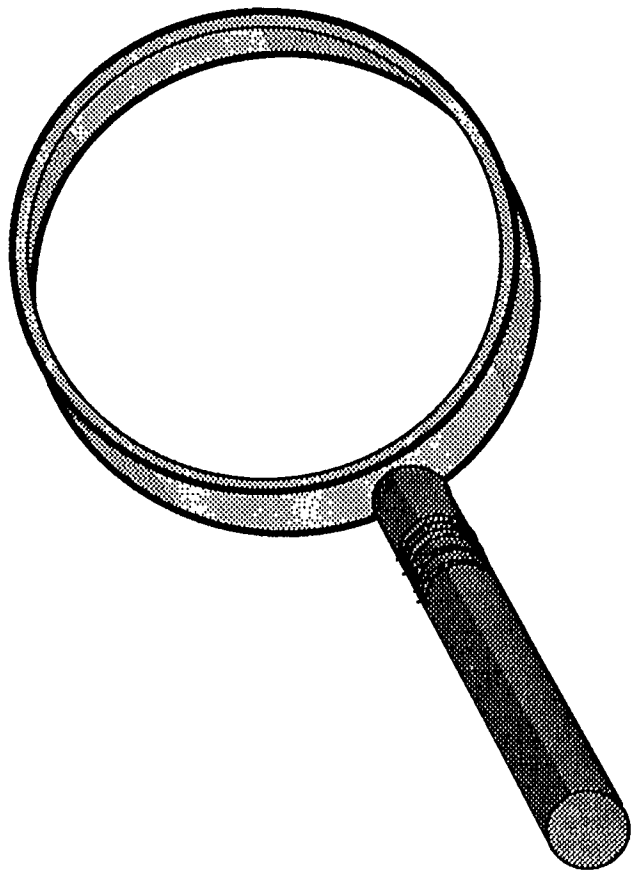
Los Alamos National Laboratory
Los Alamos, New Mexico 87545

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

A4.2

Review of CFDLIB / Current Theory

- Energy Conservation
- Pressure Force Models
- Turbulence Models



Energy Conservation

Choose $Q_o = \alpha_s \rho_o e_o$

where
- α_s material s selector
- ρ_o material density in V
- e_o internal energy per unit mass

Use $$\rho_o \dot{e}_o = -p_o \nabla \cdot \mathbf{u}_o + \frac{1}{2} tr(\tau_o \cdot \varepsilon_o) - \nabla \cdot \mathbf{q}_o$$

Insert in generalized conservation equation assuming $\rho_o e_o$ is a collisional invariant :

Energy Conservation

$\frac{\partial \rho_s e_s}{\partial t} + \nabla \bullet \rho_s e_s \mathbf{u}_s$	Rate of change in expected s energy at a point
$= \langle \rho_o e_o \dot{\alpha}_s \rangle$	net source of s internal energy due to s mass conversion
$-\nabla \bullet \langle \alpha_s \rho_o e_o \mathbf{u}_s' \rangle$	multiphase fluctuational transport of internal energy
$-\nabla \bullet \langle \alpha_s p_o \nabla \bullet \mathbf{u}_o \rangle$	work term
$+\frac{1}{2} \langle \alpha_s tr(\tau_o \bullet \varepsilon_o) \rangle$	average viscous dissipation
$-\nabla \bullet \langle \alpha_s \mathbf{q}_o \rangle$	thermal transport due to molecular conduction
$+\langle \mathbf{q}_o \bullet \nabla \alpha_s \rangle$	energy exchange due to molecular conduction

Work & Mass Exchange Terms

Mass conservation :

$$\frac{\partial \rho_s}{\partial t} + \nabla \cdot \rho_s \mathbf{u}_s = \frac{\dot{m}_s}{V}$$

Material Compressibility :

$$\beta_s = -\frac{1}{v_s}\left(\frac{\partial v_s}{\partial p}\right)_{T_s} = \frac{1}{\rho_{o_s} c^2_{s(T_s)}}$$

Specific Heat Relation :

$$C_{p_s} - C_{v_s} = \left[p + \left(\frac{\partial e_s}{\partial v_s}\right)_{T_s}\right]\left(\frac{\partial v_s}{\partial T_s}\right)_p$$

Temperature Equation

$$\rho_s \left\{ \frac{C_{p_s} + C_{v_s} \dfrac{1}{p}\left(\dfrac{\partial e_s}{\partial v_s}\right)_{T_s}}{1 + \dfrac{1}{p}\left(\dfrac{\partial e_s}{\partial v_s}\right)_{T_s}} \right\} \frac{dT_s}{dt} =$$

$$\frac{\dot{m}_s}{V}\left(h^* - h_s\right) + \qquad \text{enthalpy exchange}$$

$$\theta_s p \beta_s \frac{dp}{dt} + \qquad \text{compressible work}$$

$$-\nabla \bullet \left\langle \alpha_s \rho_o e_o \mathbf{u}_s' \right\rangle + \qquad \text{fluctuational transport}$$

$$-p\nabla \bullet \left\langle \alpha_s \mathbf{u}_s' \right\rangle + \qquad \text{fluctuational work}$$

$$-\left\langle p' \left(\frac{\partial \alpha_s}{\partial t} + \nabla \bullet \alpha_s \mathbf{u}_s' \right) \right\rangle \qquad \text{" " "}$$

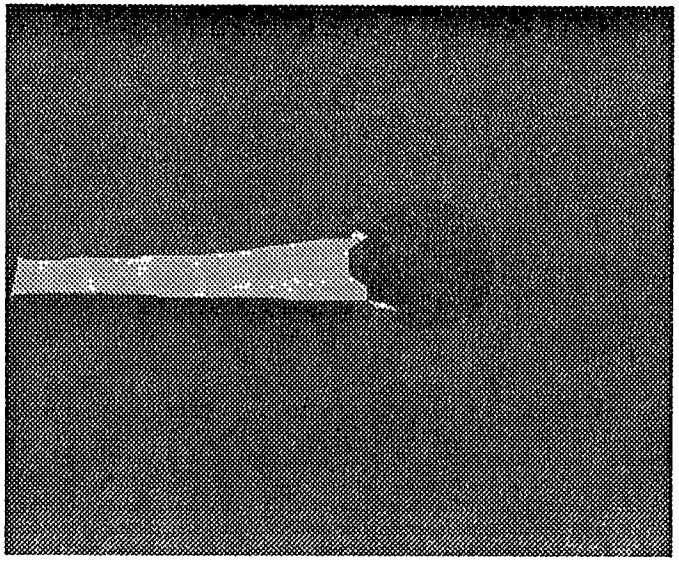
$$\frac{1}{2}\left\langle \alpha_s tr(\tau_o \bullet \varepsilon_o) \right\rangle + \qquad \text{average viscous dissipation}$$

$$-\nabla \bullet \left\langle \alpha_s \mathbf{q}_o \right\rangle + \qquad \text{molecular conduction}$$

$$\left\langle \mathbf{q}_o \bullet \nabla \alpha_s \right\rangle \qquad \text{energy exchange}$$

Energy Exchange

$$\langle \mathbf{q}_o \cdot \nabla \alpha_s \rangle = \sum_l \theta_s \theta_l R_{sl} (T_l - T_s)$$



where for a single sphere in a fluid

$$R_{sl} = \frac{6k_f}{d_p^2} Nu$$

where

$$Nu \approx 2 + 0.6 \,\mathrm{Re}^{0.5} \,\mathrm{Pr}^{0.33}$$

A4.8

Class Energy Equation

- Group species s(k) with identical mean velocities and temperatures into class k.
- Sum species s(k) transport equations to obtain class k equation.
- Group exchange terms as "intra" and "inter" class exchange.
- Use mixture thermodynamic/transport coefficients for each class as defined by sum over species equations:

$$\rho_k C_{p_k} = \sum_{s \in k} \rho_s C_{p_s} \qquad \theta_k \beta_k = \sum_{s \in k} \theta_s \beta_s$$

Class Energy Equation

- For simplicity, drop fluctuation, conduction and dissipation terms
- Assume calorically perfect materials

$$\rho_k C_{p_k} \frac{dT_k}{dt} = \theta_k \beta_k p \frac{dp}{dt} +$$

$$\sum_l \theta_k \theta_l R_{kl} \left(T_l - T_s \right) +$$

$$\sum_{l \neq k} \frac{\dot{m}_k}{V} \left(h_l^* - h_k \right) + \sum_{rxn \in k} \dot{\xi}_{rxn} \Delta H_{rxn}$$

Pressure Force Models

Expected Pressure Acceleration :

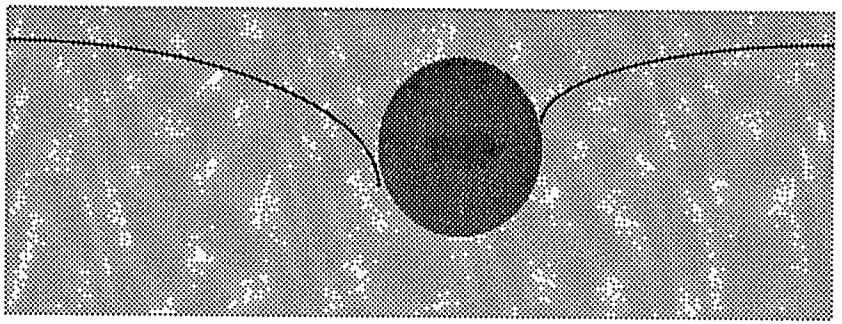
$$-\langle \alpha_k \nabla p_o \rangle = -\theta_k \nabla p \qquad \text{mean pressure force}$$

$$-\langle \nabla \alpha_k p_o' \rangle \qquad \text{conservative force}$$

$$+\langle p_o' \nabla \alpha_k \rangle \qquad \text{exchange force}$$

Decompose pressure deviations :

$$p_o' = p_{av}' + p_{dev}'$$



Then

$$-\nabla \langle \alpha_k p_{av}' \rangle \qquad \text{streaming force, close packing force}$$

$$+\langle p_{dev}' \nabla \alpha_k \rangle \qquad \text{exchange due to surface pressure deviations}$$

Types of Forces

Drag : $\left\langle p'_{dev} \nabla \alpha_k \right\rangle = \sum_l \theta_k \theta_l K_{kl} (\mathbf{u}_l - \mathbf{u}_k)$

Added Mass : $\left\langle p'_{dev} \nabla \alpha_k \right\rangle = \sum_l \theta_k \theta_l C_{kl} \left(\frac{d\mathbf{u}_l}{dt} - \frac{d\mathbf{u}_k}{dt} \right)$

Lift Force : $\left\langle p'_{dev} \nabla \alpha_k \right\rangle = \sum_l \theta_k \theta_l L_{kl} \left(\nabla \mathbf{u}_k - (\nabla \mathbf{u}_k)^{\mathrm{T}} \right) \cdot (\mathbf{u}_l - \mathbf{u}_k)$

Close Packing Force : $\nabla \left\langle \alpha_k p'_{av} \right\rangle = \nabla \left(\theta_k \rho_{o_k} c^2_{cp_k} f(\theta_k, \theta_{cp_k}) \right)$

Streaming force : $\nabla \left\langle \alpha_k p'_{av} \right\rangle = \nabla \left(\frac{1}{4} \rho_{o_f} U^2_{slip} \theta_p \right)$ for continuous fluid

A4.12

Some 2-Fluid Drag Models

Particle in Fluid :

$$K^{kl} = \frac{3\rho^f C_D}{4d_p}|\mathbf{u}_l - \mathbf{u}_k|$$

$$C_D = C_D^{\infty} + \frac{24}{\mathrm{Re}_p} + \frac{6}{\left(1+\sqrt{\mathrm{Re}_p}\right)}$$

$$\mathrm{Re}_p = \frac{|\mathbf{u}_l - \mathbf{u}_k| d_p}{\nu_f}$$

Particle - Particle :

$$K^{kl} = \frac{\rho_1\rho_2(d_1+d_2)^2}{d_1^3\rho_1 + d_2^3\rho_2}|\mathbf{u}_l - \mathbf{u}_k|$$

Ergun :

$$K_{kl} = \frac{150\mu_f\theta_s}{d_p^2\theta_f^2} + \frac{1.75\rho_f|\mathbf{u}_l - \mathbf{u}_k|}{d_p\theta_f}$$

Current Turbulence Implementation

- Multimaterial constant eddy viscosity
- Multimaterial Prandtl mixing length model
- Multimaterial k, k-epsilon

Current Turbulence Models

$$\rho_k \frac{d\mathbf{u}_k}{dt} = -\nabla \cdot \rho_k \mathbf{R}_k + \ldots \qquad \rho_k \mathbf{R}_k = \left\langle \alpha_k \rho_o \mathbf{u}_k' \mathbf{u}_k' \right\rangle \qquad \mathbf{R}_k = -\frac{2}{3} k_k + 2\nu_k \mathbf{S}_k$$

Boussinesq stress closure

$$k_k = \frac{1}{2} tr(\mathbf{R}_k) \;; \qquad \mathbf{S}_k = \frac{1}{2}\left(\nabla \mathbf{u}_k + (\nabla \mathbf{u}_k)^T\right) - \frac{1}{3} \nabla \cdot \mathbf{u}_k \mathbf{I}$$

ν_k = constant — constant eddy viscosity model

$$\nu_k = \ell_k^2 \sqrt{tr(\mathbf{S}_k \cdot \mathbf{S}_k)}$$ — Prandtl mixing length model

$$\nu_k = \ell_k \sqrt{k_k}$$ — One - equation model

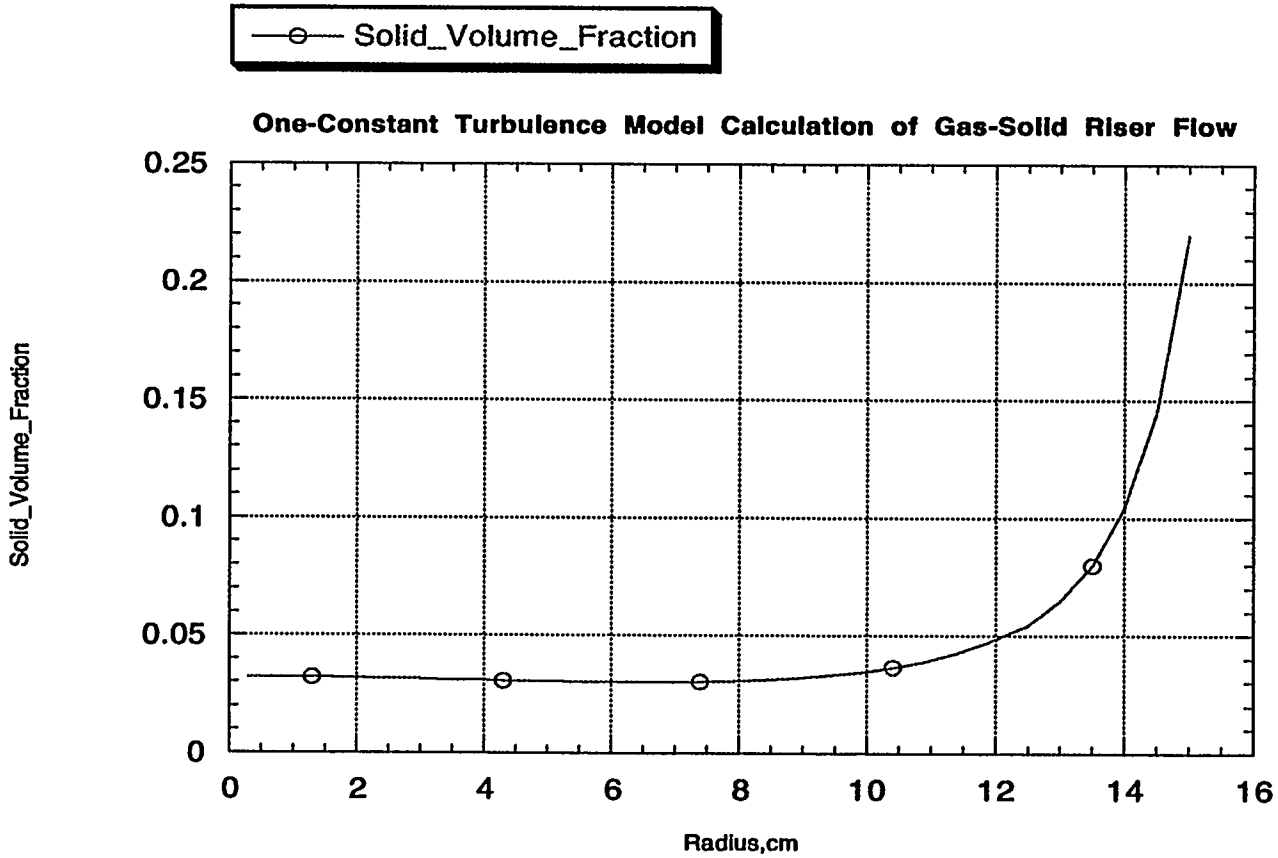
$$\rho_k \frac{dk_k}{dt} = \nabla \cdot (\rho_k \nu_k \nabla k_k) + \rho_k \nu_k tr(\mathbf{S}_k \cdot \nabla \mathbf{u}_k) - \varepsilon_k \qquad \varepsilon_k = \rho_k \frac{(k_k)^{\frac{3}{2}}}{\ell_k}$$

$$\nu_k = 0.09 \frac{k_k^2}{\varepsilon_k}$$ — "$k - epsilon$"

$$\rho_k \frac{d\varepsilon_k}{dt} = 0.77 \nabla \cdot (\rho_k \nu_k \nabla \varepsilon_k) + 1.44 \frac{\varepsilon_k}{k_k} \rho_k \nu_k tr(\mathbf{S}_k \cdot \nabla \mathbf{u}_k) - 1.92 \frac{\varepsilon_k^2}{k_k}$$

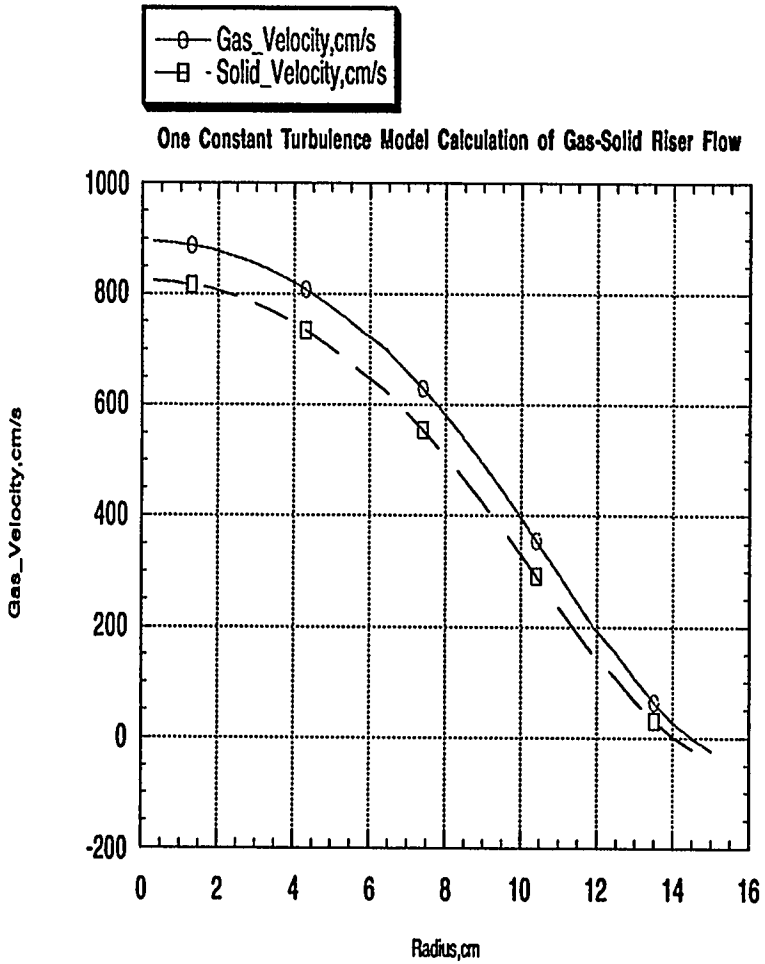
One-Equation Model Calculation of Developed Gas-Solid Riser Flow

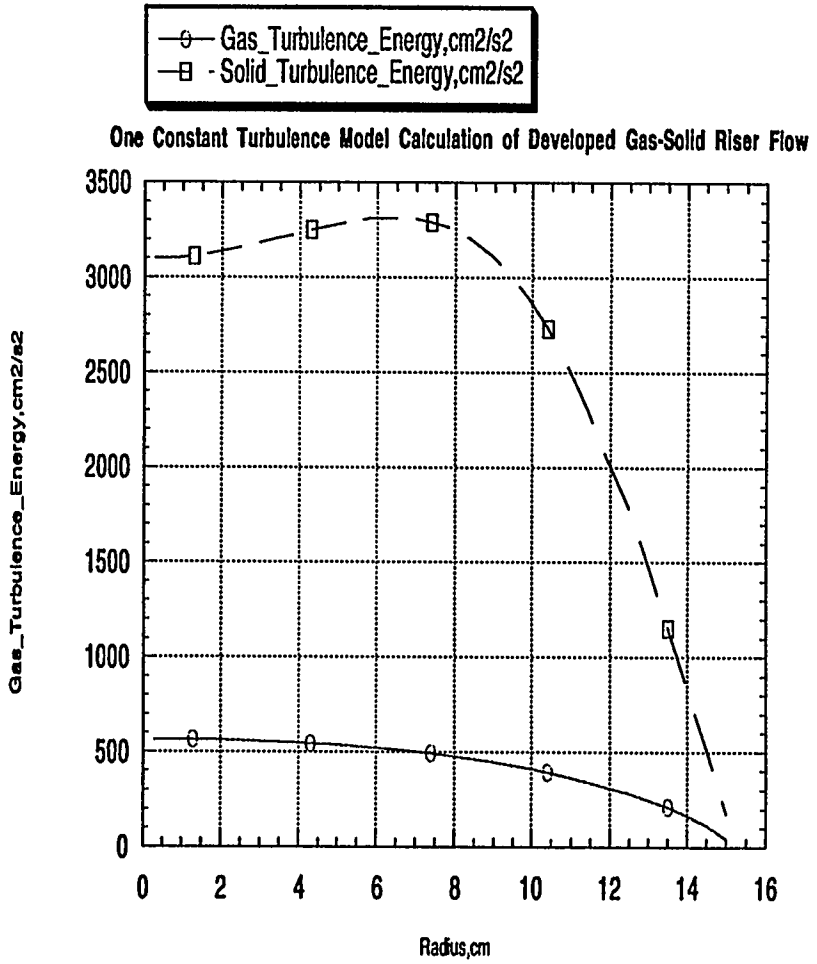
- 100 micron particles; 1,2 cm turbulent length scales



A7.lb

One-Equation Model Calculation of Develped Gas-Solid Riser Flow





(2D) || Print || 17 May 1995 || tb+am/tecfl99.plt || v07 (1=liq, 2=gas) 10 x 1 2 d bubble col

CHEN 2D BUBBLE COLUMN SIMLUATIONS

DRAG

DRAG
ADDED MASS

DRAG

TURBULENCE

DRAG
ADDED MASS
TURBULENCE

Attachment 5
Review of CFDLIB/Current Theory
Nely Padial
LANL

Parallel Implementation and Results

LA-UR-95-1726

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: **CFDLIB AND PARALLEL COMPUTATION**

AUTHOR(S): Nely T. Padial , 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

A5.2

CFDLIB and Parallel Computation

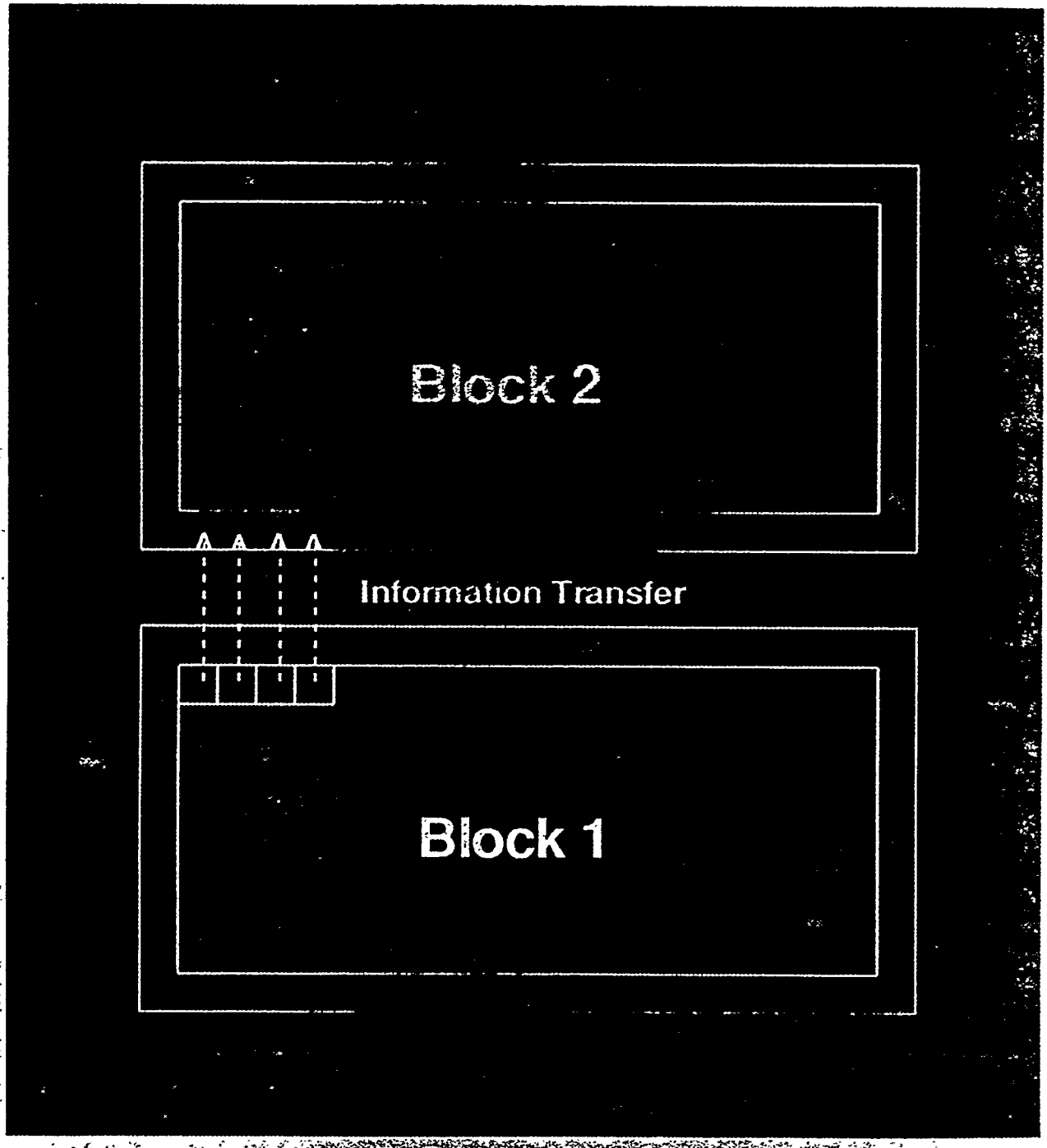
1- Parallel Problems

2- a. Massive Parallel Processing (MPP)

b. Virtual Machines

3- Terminology:

Configuration
Host
Task
Spawn a task



A5.4

Efficiency

1- Computation in each processor.

2- Communication among processors or hosts:

a- PVM (UNCOL)
b- MPI
c- Cray High Speed Data Transfer (SHMEM, F--)

Parallelization of CFDLIB:

1- Apportioning the work:

a. PE = 0 : I/O; Calculations common to all blocks.

b. PE > 0 : iblk = mytask,nblks,nupro

Example: 15 blocks, 4 tasks (0,1,2,3)

PE1 with iblk = 1,15,3 (1,4,7,10,13)

PE2 with iblk = 2,15,3 (2,5,8,11,14)

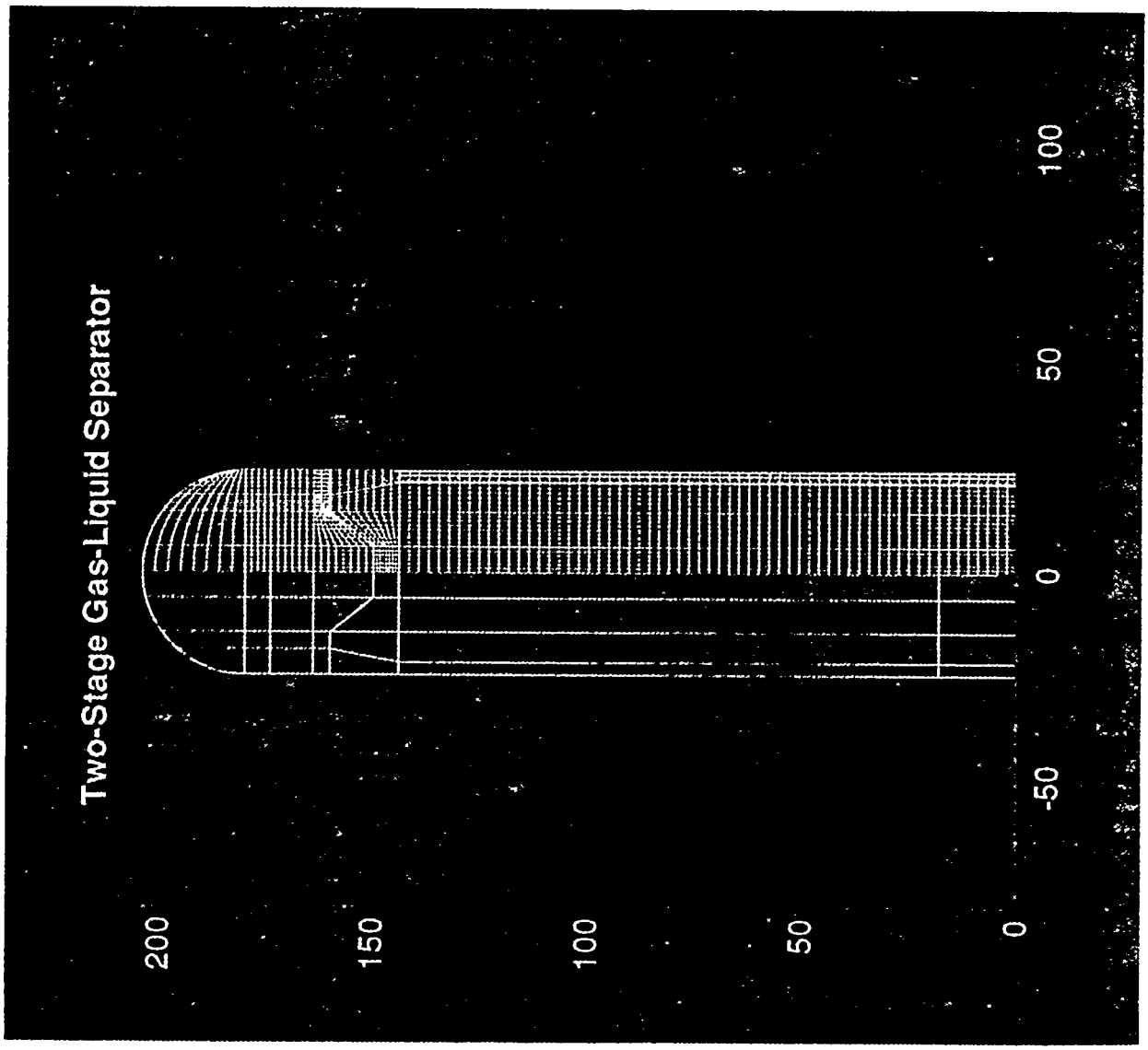
PE3 with iblk = 3,15,3 (3,6,9,12,15)

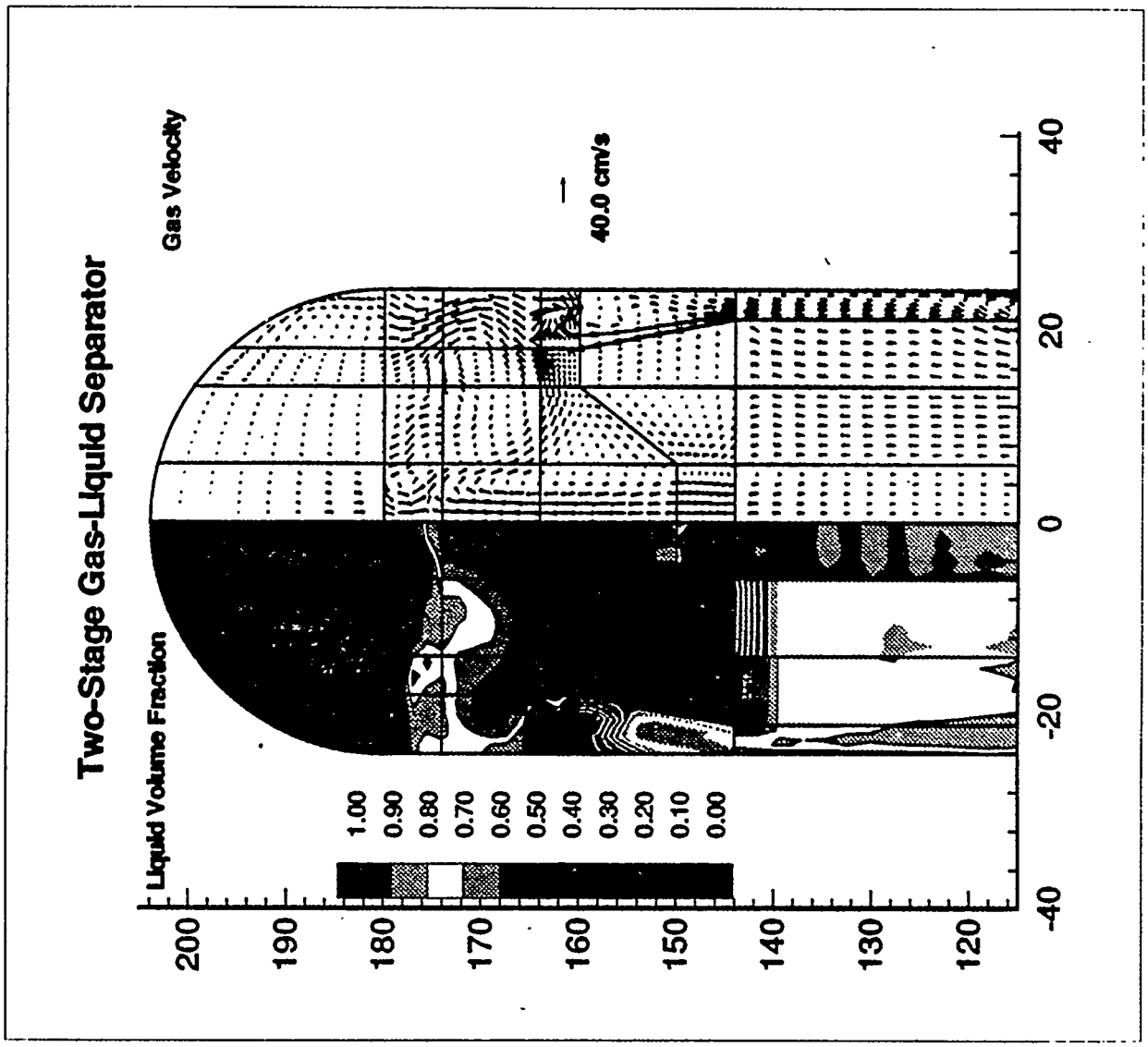
2. Rewriting the subroutines:

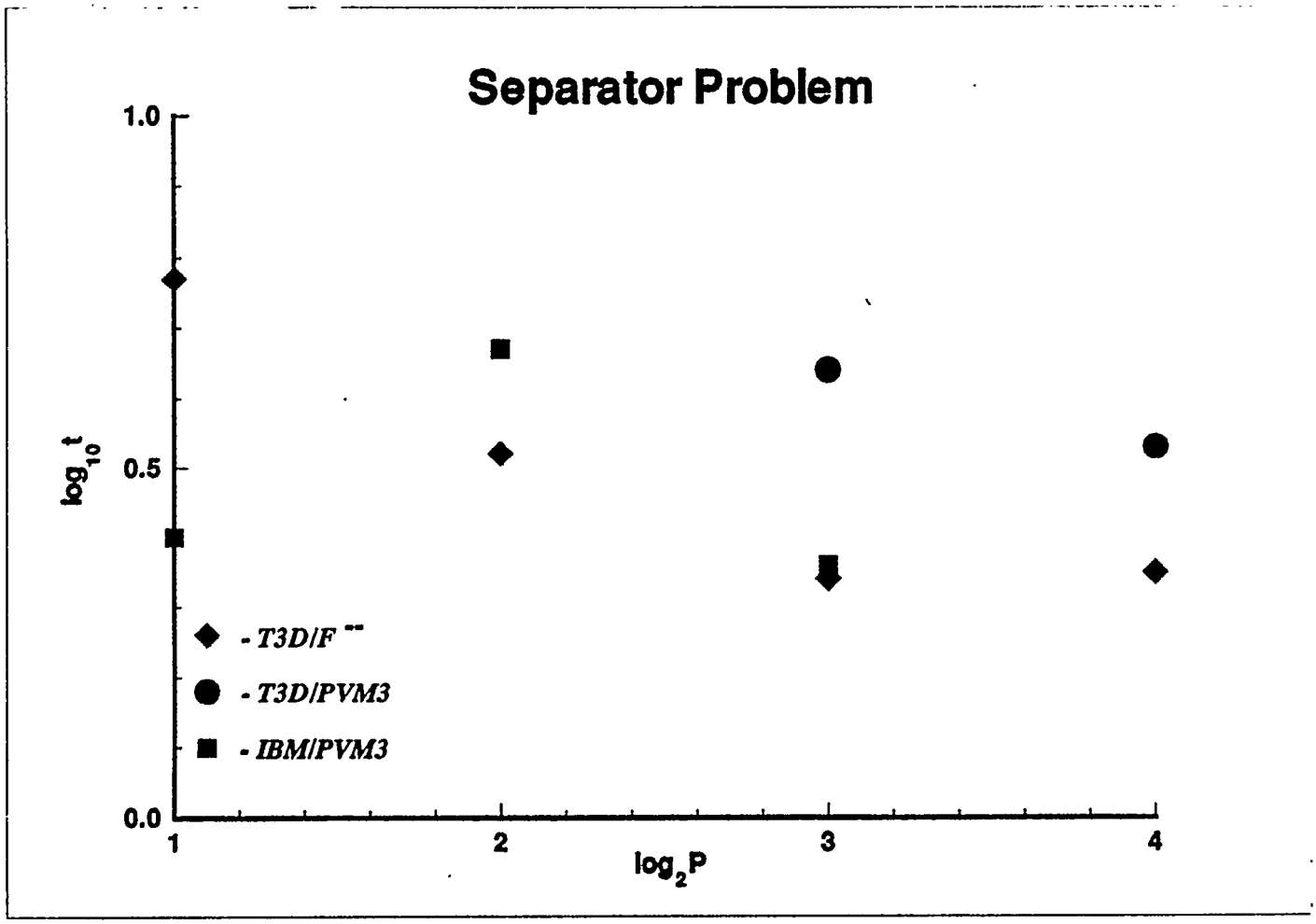
a. Routines dealing with calculations in each block need not to be changed (LIBSRC).

b. Drivers that send work to the various processors had to be changed a little.

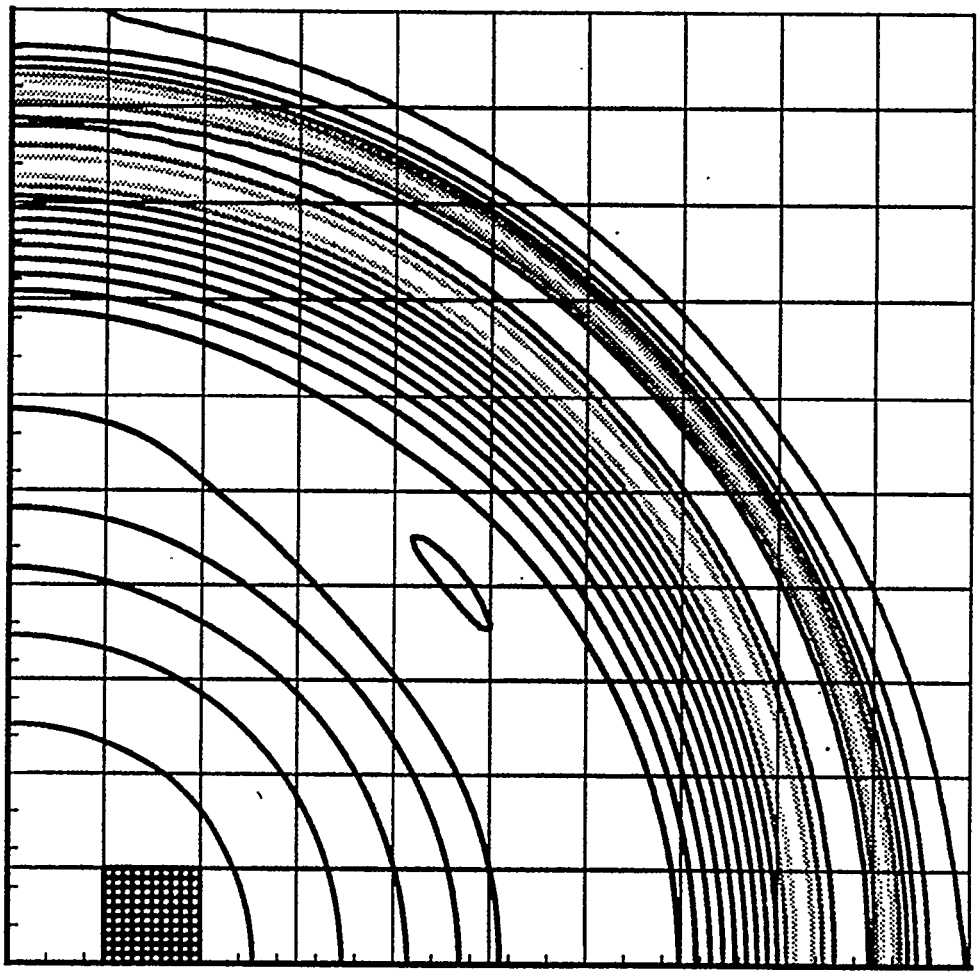
c. Communication routines were rewritten.


Two-Stage Gas-Liquid Separator
200
150
100
50
0
-50
0
50
100

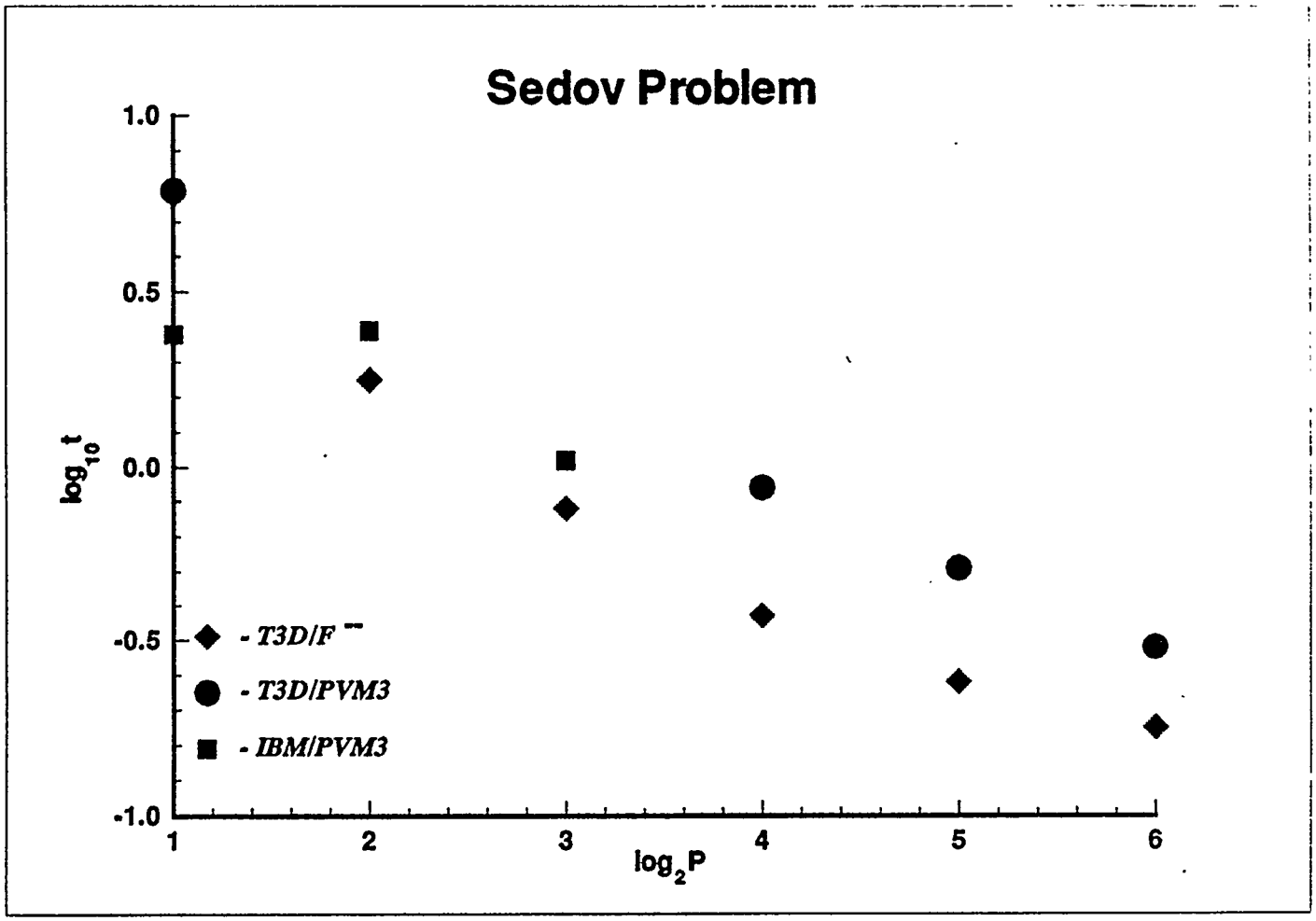

Two-Stage Gas-Liquid Separator
Gas Velocity
40.0 cm/s
Liquid Volume Fraction
1.00
0.90
0.80
0.70
0.60
0.50
0.40
0.30
0.20
0.10
0.00
200
190
180
170
160
150
140
130
120
-40
-20
0
20
40


Separator Problem
1.0
0.5
0.0
$\log_{10} t$
1
2
3
4
$\log_2 P$
- T3D/F --
- T3D/PVM3
- IBM/PVM3

100 Blocks Blast Wave



Pressure Contour

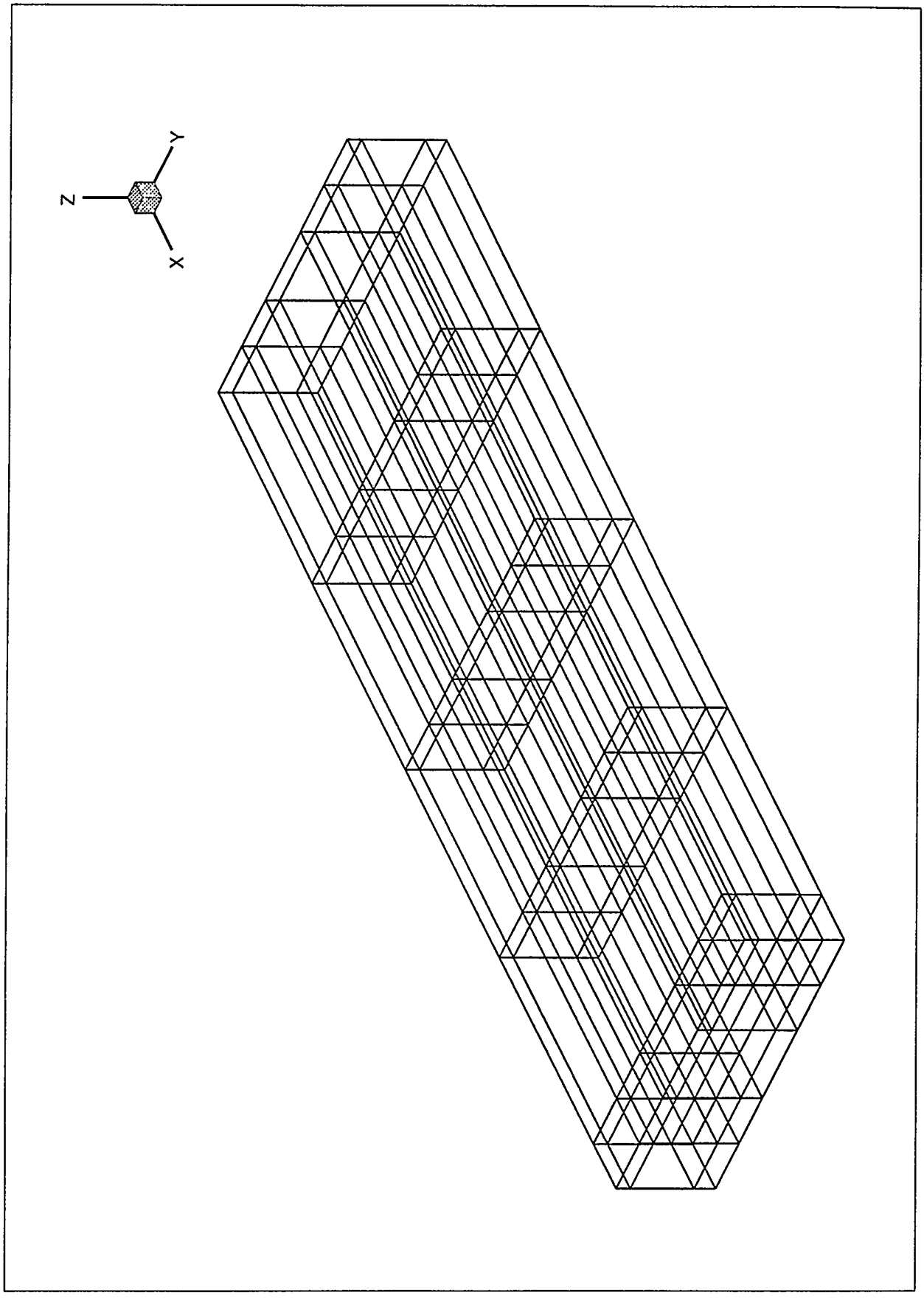

Sedov Problem
1.0
0.5
0.0
-0.5
-1.0
log10 t
- T3D/F --
- T3D/PVM3
- IBM/PVM3
1
2
3
4
5
6
log2P

```
      subroutine bcomcc (w,ncm2,nadd)

c=======================================================================
c     This routine performs inter-block communication for cell-centered
c     array w.
c     Called by:  HYDROICE   NEWPROB
c     Calls:      SECOND
c=======================================================================
      implicit double precision (a-h,o-z)
      include 'comdeck'
      include 'uncol_comm.h'
      include 'uncol_header.h'
      dimension w(*)
      dimension wsen(200,4,nbp1), wrec(200,4,nbp1)
c=======================================================================
      tin             = second (noprint)
      do 50 jdmx      = 1,ncm2
        do 40 iblk    = minic,nblks,nupro
          ibpp        = ibp(iblk)
          mobj        = mob(iblk)*ncm2 + (jdmx-1)*msz(iblk)
          do 20 ib    = 1,4
            if (nbc(1,ib,iblk) .ne. 0) then
              i1      = i1bc(ib,iblk)+idelbc(ib,iblk)+i3bc(ib,iblk)
              i2      = i2bc(ib,iblk)+idelbc(ib,iblk)-i3bc(ib,iblk)*2
              is      = 0
              do ic   = i1,i2,i3bc(ib,iblk)
                is    = is + 1
                wsen(is,ib,ibpp)  = w(ic+mobj)
              enddo
              ism     = is
              jblk    = nbc(1,ib,iblk)
              jbpp    = (jblk-1)/nupro + 1
              ntask   = jblk - (jbpp-1)*nupro - mcmad
              msgtag  = iblk + 100000*ib + 400000*jdmx + nadd
              if (my_task .ne. ntask) then
                call snd_real_msg (ntask,msgtag,wsen(1,ib,ibpp),200)
              else
                jb      = nbc(2,ib,iblk)
                do is   = 1,ism
                  wrec(is,jb,jbpp) = wsen(is,ib,ibpp)
                enddo
              endif
            endif
 20       continue
 40     continue

        do 42 jblk    = minic,nblks,nupro
          jbpp        = ibp(jblk)
          mobj        = mob(jblk)*ncm2 + (jdmx-1)*msz(jblk)
          do 22 jb    = 1,4
            if (nbc(1,jb,jblk) .ne. 0) then
              if (jb.eq.nbc(2,jb,jblk) .or. jb+nbc(2,jb,jblk).eq.5) then
                i2    = i1bc(jb,jblk)+i3bc(jb,jblk)
                i1    = i2bc(jb,jblk)-i3bc(jb,jblk)*2
                i3    =-i3bc(jb,jblk)
              else
                i1    = i1bc(jb,jblk)+i3bc(jb,jblk)
                i2    = i2bc(jb,jblk)-i3bc(jb,jblk)*2
                i3    = i3bc(jb,jblk)
              endif
              iblk    = nbc(1,jb,jblk)
              ibpp    = (iblk-1)/nupro + 1
              itask   = iblk - (ibpp-1)*nupro - mcmad
              msgtag  = iblk + 100000*nbc(2,jb,jblk) + 400000*jdmx
     &                  + nadd
              if (my_task .ne. itask)
     &        call rcv_real_msg (itask,msgtag,wrec(1,jb,jbpp),200)
              is      = 0
              do ic   = i1,i2,i3
                is    = is + 1
                w(ic+mobj) = wrec(is,jb,jbpp)
              enddo
            endif
 22     continue
 42   continue
 50   continue
c=======================================================================
      tout    = second (noprint)
      sec(3)  = sec(3)  + tout - tin
      end
```

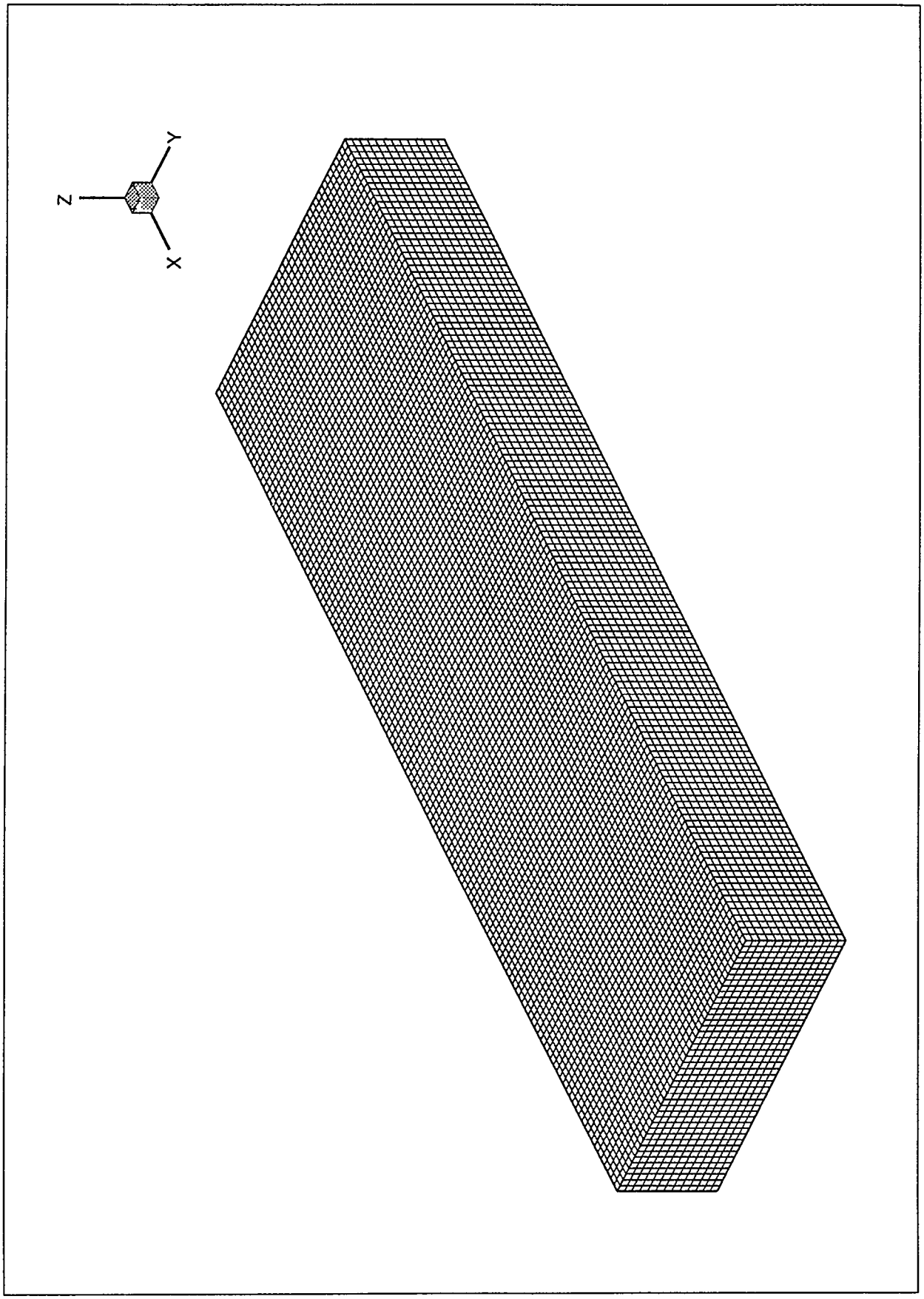
A5.13

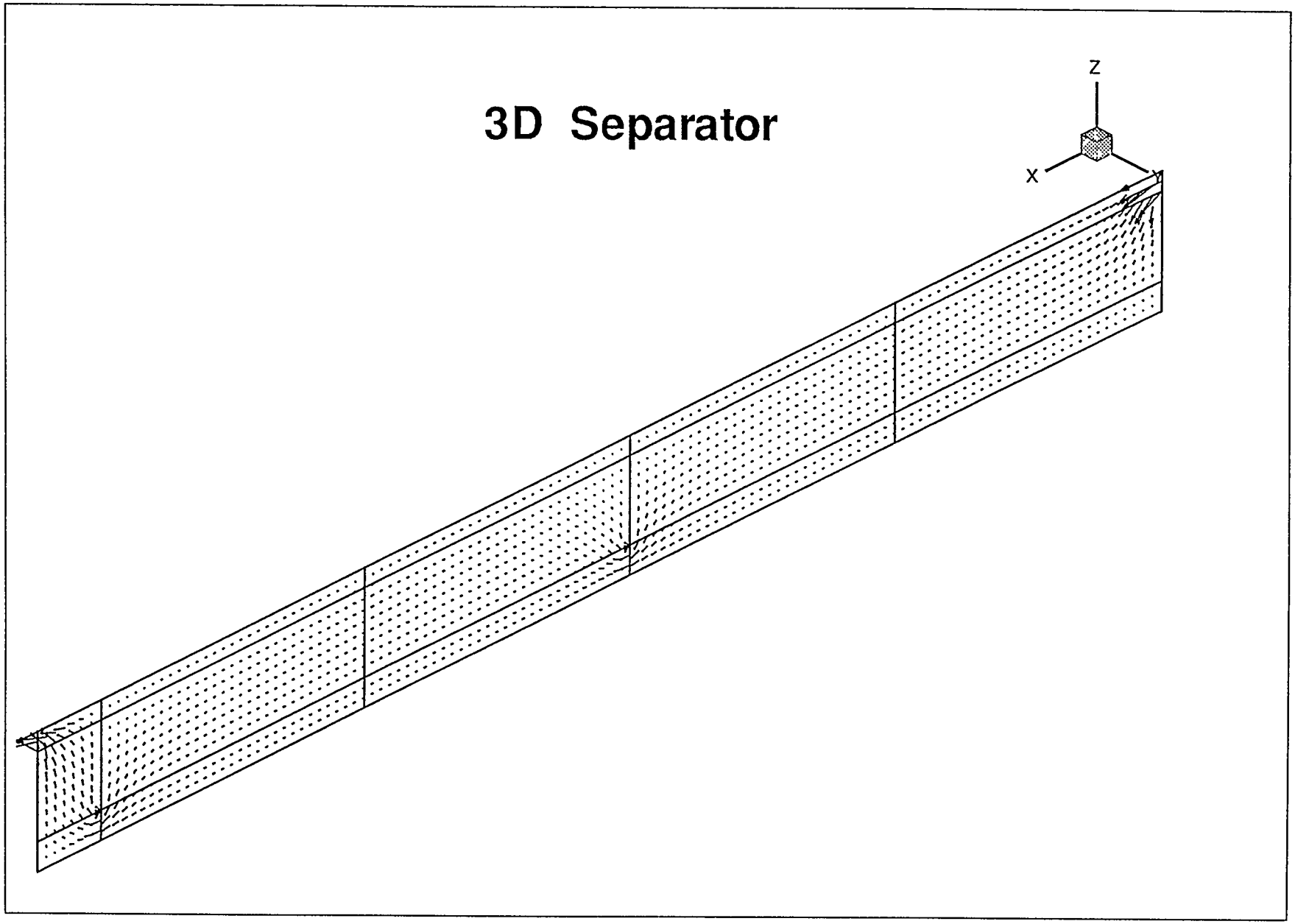
```
      subroutine bcomcc (w,ncm2,nadd)

c=======================================================================
c     This routine performs inter-block communication for cell-centered
c     array w.

c     Called by:  HYDROICE   NEWPROB
c     Calls:      SECOND
c=======================================================================
      implicit double precision (a-h,o-z)
      include 'comdeck'
      include 'uncol_comm.h'
      include 'uncol_header.h'
      pointer (iptr,r_w)
      dimension w(*)
      dimension r_w(*)
c=======================================================================
      tin              = second (noprint)

      call ring_sync (1,nupro)
      do 50 jdmx       = 1,ncm2
        do 40 iblk     = minic,nblks,nupro
          mobj         = mob(iblk)*ncm2 + (jdmx-1)*msz(iblk)
          do 20 ib     = 1,4
            if (nbc(1,ib,iblk) .ne. 0) then
              jblk     = nbc(1,ib,iblk)
              jb       = nbc(2,ib,iblk)
              jbpp     = (jblk-1)/nupro + 1
              ntask    = jblk - (jbpp-1)*nupro - mcmad
              nobj     = mob(jblk)*ncm2 + (jdmx-1)*msz(jblk)
              iptr     = mpp_annex (w,itskmp(ntask),21,4)
              if (jb.eq.nbc(2,jb,jblk) .or. jb+nbc(2,jb,jblk).eq.5) then
                j2     = i1bc(jb,jblk)+i3bc(jb,jblk)
                j1     = i2bc(jb,jblk)-i3bc(jb,jblk)*2
                j3     =-i3bc(jb,jblk)
              else
                j1     = i1bc(jb,jblk)+i3bc(jb,jblk)
                j2     = i2bc(jb,jblk)-i3bc(jb,jblk)*2
                j3     = i3bc(jb,jblk)
              endif
              i1       = i1bc(ib,iblk)+idelbc(ib,iblk)+i3bc(ib,iblk)
              i2       = i2bc(ib,iblk)+idelbc(ib,iblk)-i3bc(ib,iblk)*2
              nobj1    = nobj + j1 - j3
              do ic    = i1,i2,i3bc(ib,iblk)
                nobj1 = nobj1 + j3
                r_w(nobj1)     = w(ic+mobj)
              enddo
            endif
   20     continue
   40   continue
   50 continue

      call mem_quiet ()
      call ring_sync (1,nupro)

c=======================================================================
      tout     = second (noprint)
      sec(3)   = sec(3)  + tout - tin
      end
```

A5.14

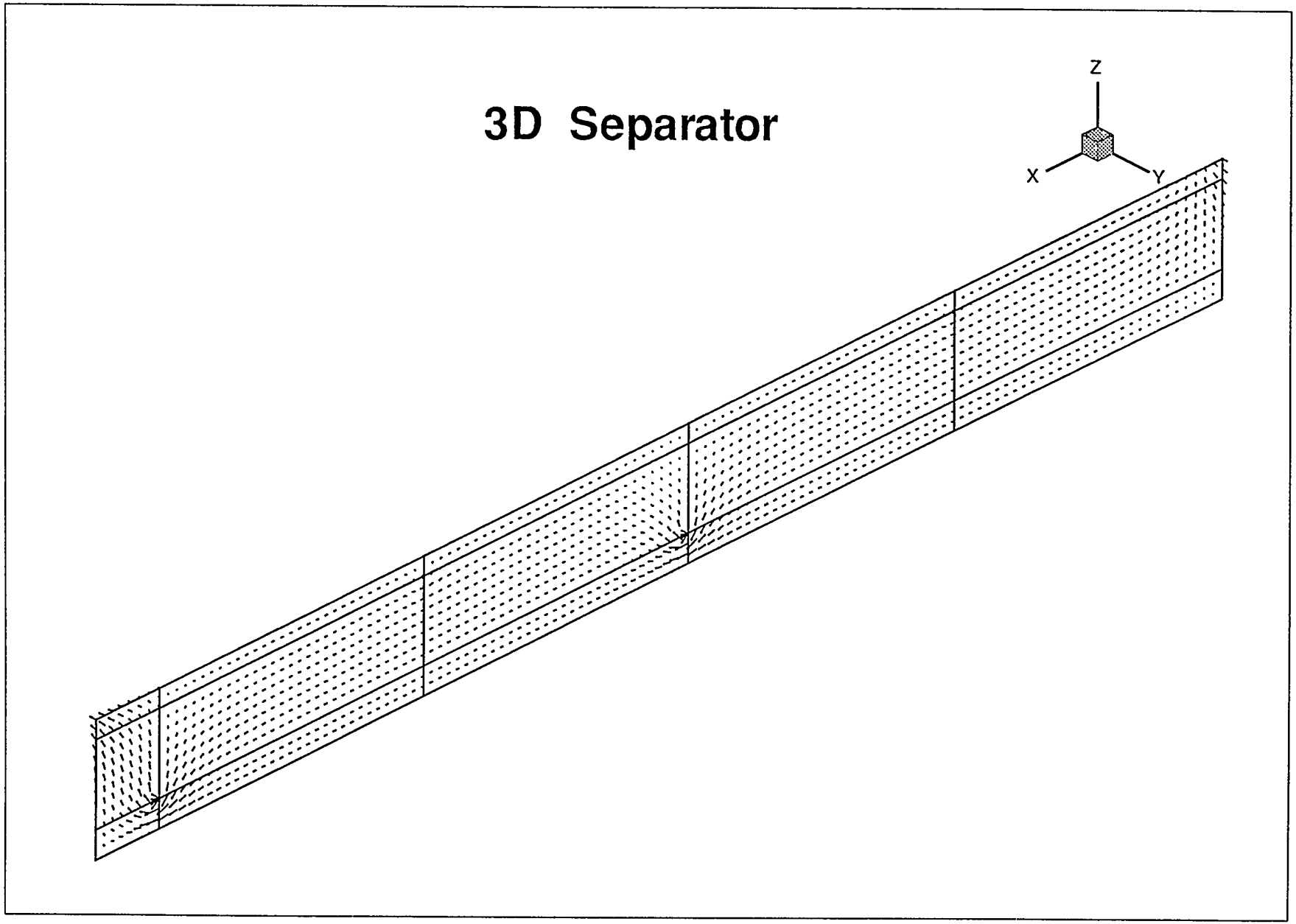


A5.15


Y
Z
X



A5.17


3D Separator
Z
X
Y

3D Separator

$t_{ymp} = 226.0$ μs/cell/cycle

T3D

$t_{32} = 125.1$ μs/cell/cycle

$t_{64} = 76.5$ μs/cell/cycle

Attachment 6
Telluride/Pagosa
Doug Kothe
LANL

EXPERIENCES IN HIGH-PERFORMANCE COMPUTING: THE *TELLURIDE* AND *PAGOSA* PROJECTS

Douglas B. Kothe

Theoretical Division
Fluid Dynamics Group T-3
MS-B216
Los Alamos National Laboratory
Los Alamos, NM 87545

E-mail: *dbk@mizzou.lanl.gov*
Group Home Page: *http://gnarly.lanl.gov/Home.html*
Personal Home Page: *http://info-server.lanl.gov:52271/?-l+097301*

A92

PARALLEL COMPUTING

- **Cooperative effort of many individual processors, each working on its own portion of the problem in parallel with the others**
- **Results are communicated between processors when necessary**
- **Two principal parallel computing strategies:**
  - *Data Parallel* (SIMD): processors perform their operations in lockstep under the control of a master processor
  - *Explicit Message Passing* (SPMD, MIMD): processors operate independently using potentially different instructions, with work coordinated via explicit message passing of messages
- **Data parallel machines: CM-200, CM-5**
- **Message passing machines: nCUBE2, Cray T3D, Paragon, clusters**
- **Hybrid machines: CM-5**

DATA PARALLEL VERSUS MESSAGE PASSING

- **Benefits of the data parallel approach:**
  - High potential concurrency (proportional to quantity of data)
  - Potential for high performance
  - Easy to construct data parallel applications
  - Data layout is performed by compiler
  - High-level language support
  - Compiler-determined machine-usage decisions
- **Benefits of the message passing approach:**
  - More portable code
  - Enables communicaton of data between any 2 processors
  - More suitable for complex geometries using unstructured data
  - Allows explicit control over data and task partitioning
  - Allows explicit control over communication and sychronization
  - Better performance?

A6.4

TELLURIDE: A MODERN CASTING SIMULATION TOOL

- *High-Performance*: designed to meet the TFlop/TByte requirements necessary for reliable modeling of fine-scale microstructural features
- *Leveraged*: built upon successful framework established by our recent DOE/DP simulation tools (PAGOSA)
- *High-Fidelity*: incorporates state-of-the-art high-resolution finite-volume algorithms
- *Realistic*: integrates all relevant processes of fluid flow, heat flow, solidification, species diffusion, and interface dynamics in complex 3-D mold/part geometries
- *Flexible, Portable, and Modular*: adapts to the changing needs of users, executes on high-performance computing platforms, and is designed with reusable software
- *User-Friendly*: housed inside a modern graphical user interface
- *Object-Oriented*: built with high-level language (F90, C++) constructs
- *Accountable*: will be validated with Industry and National Lab data
- *An integral component of LAMMP*

A6.5

FUNCTIONAL ADVANCES IN CASTING SIMULATION WITH TELLURIDE

- **Address effects of mold filling with greater fidelity**
  - *Faithful representation of complex mold/part geometries* via unstructured grids
  - *Accurate models for interface kinematics and dynamics* enable better prediction of post-fill temperature, velocity, and porosity distribution
- **Address fine-scale microstructural effects of solidification and melt convection with high-resolution simulations and improved physical models**
  - Resolved casting simulations: *TFlop/TByte requirements*!
  - *Parallel algorithms* for modern MPP platforms are required
  - High resolution enables *better prediction* of gate/riser location, mold boundary heat transfer, part shrinkage, residual stresses
  - High resolution enables *improved models* for solidification growth and propagation, solute redistribution, melt convection

MOTIVATION AND RATIONALE FOR DEVELOPMENT OF A NEW CASTING SIMULATION TOOL

- Resolved casting simulations demand high performance computing
- Opportunity to incorporate more detailed microstructural models
- LANL expertise in development and application of high resolution numerical methods provides a sound basis:
  - 3-D conformal and unstructured meshing of complex geometries
  - Robust and accurate hydrodynamic algorithms
  - High order schemes for material movement
  - Accurate and reliable methods for tracking fluid interfaces and solidification fronts
  - Robust and efficient linear equation solvers
  - Physically-based models for surface tension, phase change, solidification, etc.
  - Parallel algorithm development
  - Microstructural theory model development

A6.7

INFLUENCE OF MELT CONVECTION ON MICROSTRUCTURE

- **Melt convection patterns (fluid flow) result in large scale solute transport**
- **Potentially large microstructural impact**
  - Compositional differences over the entire casting (macrosegregation)
  - Acceleration of columnar-to-equiaxed transition
  - Dendrite fragmentation, clustering, and collision
  - Reduction of solute boundary layer
  - Frequently promotes fine-scale microstructure
- **Recently received considerable attention, but remains poorly understood**
- **Numerical modeling of melt convection is in need of improvement**
  - Collaborating with academia on a promising volume-averaged multi-field model

TELLURIDE: Physical Model

- Hydrodynamics
- Interface kinematics: volume tracking
- Interface dynamics: surface tension, phase change
- Momentum diffusion
- Thermal transport
- Solidification model
- Species (solute) diffusion
- Strength model
- Geometry: generalized unstructured hexahedra
- Portable to all modern computing platforms
- MP paradigm: explicit message passing

AL.9

TELLURIDE: Hydrodynamic Algorithm

- **Solve Navier-Stokes equations with an approximate projection method**
  - Introduced by J. Bell (LLNL)
  - Refined recently by W. Rider (LANL)
- **Control volume method, with all fluid variables collocated at cell centers**
- **Godunov-like upwind advection scheme**
- **Computational domain: generalized unstructured hexahedra**
- **Second order accuracy in time and space**
- **Linear equation solvers: Krylov-subspace schemes (PCG, GMRES, TFQMR)**
- **Written from scratch in F90 (selected algorithms being explored in C++)**
- **Build upon framework proven successful in RIPPLE and PAGOSA**

AC, 1D

F90 OFFERS MANY NEW FEATURES THAT ARE WELL-SUITED FOR HIGH-PERFORMANCE SCIENTIFIC COMPUTING

- **F77 is a subset**
- **New free source form**
- **Array processing**
  - Important for vector and parallel computers
  - Enables concise constructs
- **A multitude of new intrinsic functions that act on whole arrays**
- **Derived types, modules, and generic functions (operator overloading)**
  - Enables *data abstraction*, *language extension*, and many of the features required for *object-oriented programming*
- **Pointers and dynamic data structures**
- **Parameterized data types**
  - Solves the portability problems inherent in F77
- **Recursion, numerical inquiry and manipulation functions**
- **Consult URL *http://lenti.med.umn.edu/~mwd/f90-faq.html* for F90 info**

A6.11

F90 DERIVED TYPES: A POWERFUL TOOL FOR ENCAPSULATING RELATED DATA

```
MODULE MESH_MODULE

use base_module

type MESH_CONNECTIVITY

c     ...Cell vertex numbers; cell and
c        face number across each face
integer (kind = INT_TYPE), dimension(nfc) :: Ngbr_cell
integer (kind = INT_TYPE), dimension(nfc) :: Ngbr_face
integer (kind = INT_TYPE), dimension(nvc) :: Ngbr_vrtx

c     ...Face numbers associated with each sweep direction
integer (kind = INT_TYPE), dimension(ndim) :: Face_dir

c     ...Cell PE number, neighboring cell PE number across each face
integer (kind = INT_TYPE) :: Pe
integer (kind = INT_TYPE), dimension(nfc) :: Ngbr_pe

c     ...BC at each face
integer (kind = INT_TYPE), dimension(nfc) :: Bc_vel  ! velocity
integer (kind = INT_TYPE), dimension(nfc) :: Bc_prs  ! pressure
integer (kind = INT_TYPE), dimension(nfc) :: Bc_temp ! temp

end type MESH_CONNECTIVITY

end module mesh_module
```

```
MODULE MATL_MODULE

use base_module

type MATERIAL

c     ...Material identifier
integer (kind = INT_TYPE) :: Id

c     ...Volume fraction
real (kind = REAL_TYPE) :: Vof

c     ...Density
real (kind = REAL_TYPE) :: Rho

c     ...Enthalpy
real (kind = REAL_TYPE) :: Enthalpy

c     ...Conductivity
real (kind = REAL_TYPE) :: K

c     ...Constant pressure specific heat
real (kind = REAL_TYPE) :: Cp

end type MATERIAL

end module matl_module
```

- **New physical models: add new attributes to previously defined modules**
- **Only module files change with new physics: rest of source is untouched**
- **Module size and content: determined dynamically at runtime**
- **Similar to C structures and C++ classes**

AL.12

TELLURIDE F90 EXAMPLE: COMPUTE CELL VOLUMES

```
      SUBROUTINE CELL_VOLUME (Cell, Mesh, Vertex)

      use geom_module
      use mesh_module
      use vertex_module

      implicit none

#include "parameter.h"
#include "constants.h"

c-------------------------------------------------------------------------------
c     ...Global scalars & arrays
c-------------------------------------------------------------------------------

      type (MESH_CONNECTIVITY), dimension(ncells), intent (IN) :: Mesh
      type (VERTEX_DATA), dimension(nnodes), intent (IN) :: Vertex
      type (CELL_GEOMETRY), dimension(ncells), intent (OUT) :: Cell

c-------------------------------------------------------------------------------
c     ...Local scalars & arrays
c-------------------------------------------------------------------------------

      integer (kind = INT_TYPE) f, v1, v2, v3, v4, v5, v6
      real (kind = REAL_TYPE), dimension (nvc,ncells) :: Xn, Yn, Zn
      real (kind = REAL_TYPE), dimension (ncells) :: X1, Y1, Z1,
     &                                               X2, Y2, Z2, X3, Y3, Z3

c-------------------------------------------------------------------------------

c     ...Gather node coordinates into
c        local temporaries Xn, Yn, and Zn

      call v2c_real_v_all (Xn, Vertex%X, Mesh)
      call v2c_real_v_all (Yn, Vertex%Y, Mesh)
      call v2c_real_v_all (Zn, Vertex%Z, Mesh)
```

```
c     ...Loop over faces, accumulating the cell volume

      do f = 1,nfc
        select case (f)
          case (1) ! Side 1 (vertices 4-8-7-3)
            v1 = 8
            v2 = 4
            v3 = 7
            v4 = 8
            v5 = 3
            v6 = 4
            .
            . (other sides)
            .

        end select

        X1 = Xn(v1,:) + Xn(v2,:)
        Y1 = Yn(v1,:) + Yn(v2,:)
        Z1 = Zn(v1,:) + Zn(v2,:)
        X2 = Xn(v3,:) + Xn(v4,:)
        Y2 = Yn(v3,:) + Yn(v4,:)
        Z2 = Zn(v3,:) + Zn(v4,:)
        X3 = Xn(v5,:) + Xn(v6,:)
        Y3 = Yn(v5,:) + Yn(v6,:)
        Z3 = Zn(v5,:) + Zn(v6,:)

        Cell%Volume = Cell%Volume
     &              + X1*(Y2*Z3 - Y3*Z2)
     &              + Y1*(X3*Z2 - X2*Z3)
     &              + Z1*(X2*Y3 - X3*Y2)
      end do

      Cell%Volume = twelfth*Cell%Volume

      end subroutine cell_volume
```

A6.13

TELLURIDE F90 EXAMPLE: GATHER VERTEX DATA TO CELLS

```
      SUBROUTINE V2C_REAL_V_ALL (Dest, Src, Mesh)

      use mesh_module

      implicit none

#include "parameter.h"
#include "constants.h"

c-------------------------------------------------------------------------------
c     ...Global scalars & arrays
c-------------------------------------------------------------------------------

      type (MESH_CONNECTIVITY), dimension(ncells), intent (IN) :: Mesh
      real (kind = REAL_TYPE), dimension (nnodes), intent(IN) :: Src
      real (kind = REAL_TYPE), dimension (nvc,ncells), intent(OUT) :: Dest

c-------------------------------------------------------------------------------
c     ...Local scalars & arrays
c-------------------------------------------------------------------------------

      integer (kind = INT_TYPE) :: v
      integer (kind = INT_TYPE), dimension(ncells) :: Neighbor

c-------------------------------------------------------------------------------

      Dest = zero

c     ...Loop over vertices
      do v = 1,nvc

        Neighbor = Mesh%Ngbr_vrtx(v)
        Dest(v,:) = Src(Neighbor)

      end do

      end subroutine v2c_real_v_all
```

The communication is isolated here in the indirect addressing

Message passing (MPI) routines will be called here on multiprocessor systems

A6.14

BUILDING EFFICIENT, PORTABLE CODE

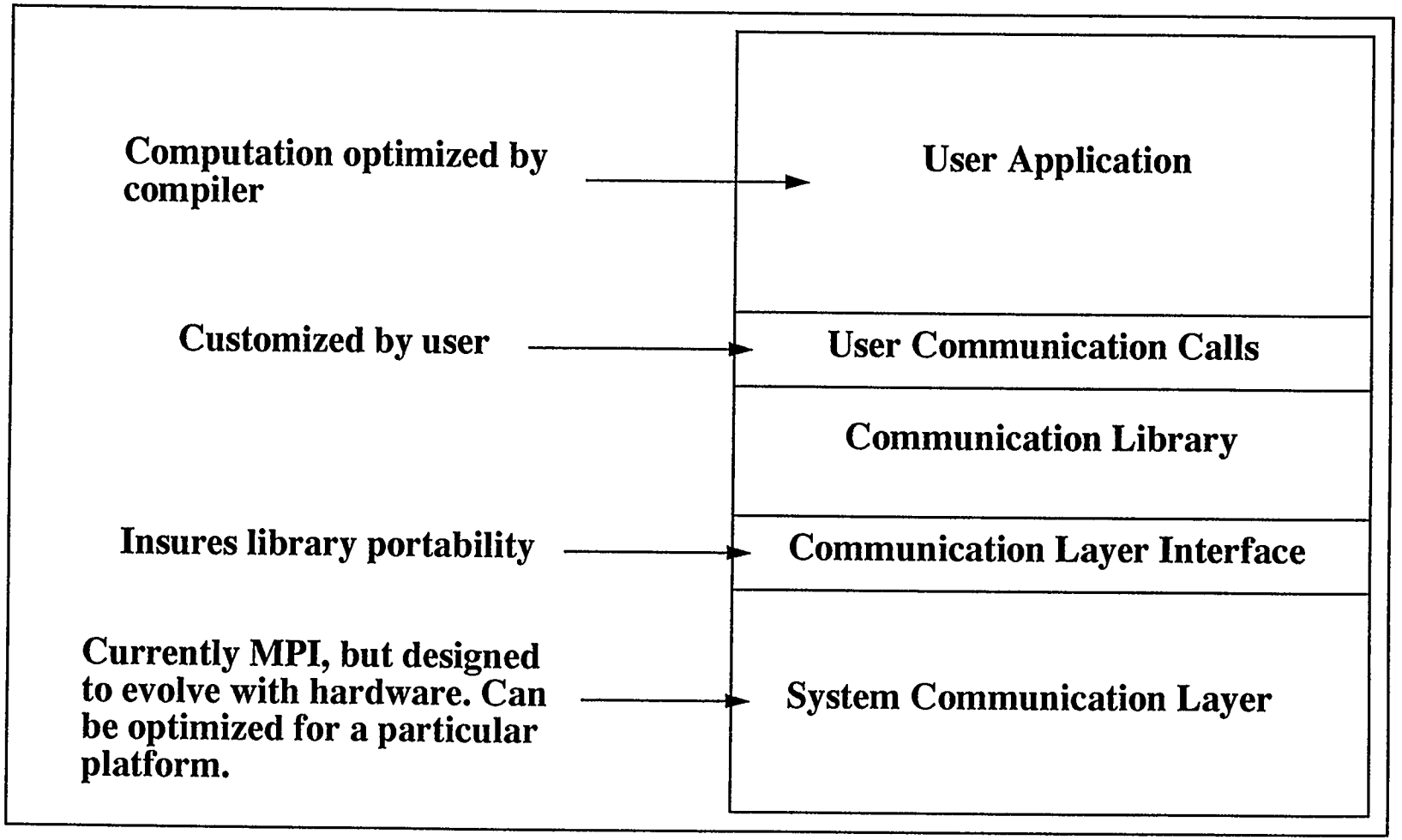
- **Current state of computing:**
  - Computation hardware is similar on all systems (RISC + cache)
  - Good single-PE compilers
  - Communication hardware varies between systems and is evolving rapidly
- **Software design goals:**
  - Exploit compilers as much as possible
  - Isolate communication in a few routines
  - Data parallel paradigm is good for physics, but not yet portable
  - Need flexibility of message passing in performing certain functions
- **Solution: F90 with MPI-based communication library**
- **Benefits:**
  - Easy to maintain and develop
  - Portable, ready for future hardware evolution (e.g., SMPs)
  - Easily optimized for a particular system

AL.15

SOFTWARE PARALLELIZATION STRATEGY

- **For MPPs or heterogeneous clusters:**
  - Partition the mesh into sub-meshes with proven domain decomposition methods
  - Allocate one or more submeshes to each processing element (PE)
  - Load balance by partitioning dynamically (if necessary)
- **Exploit data parallel paradigm for sub-mesh data residing on individual PEs**
  - Use advanced F90 features *extensively*
  - Source code is *clean, concise, readable, easy-to-maintain, and portable!*
- **Physics modules are separate from low-level architecture-specific constructs**
  - Cell-to-cell communication is implemented with "black-box" *gather/scatter functions* that reside in a separate communication library
  - Architecture-specific details remain hidden in the communication and I/O libraries: *physics modules do not change across platforms*

DESIGN STRATEGY: SOFTWARE LAYERS



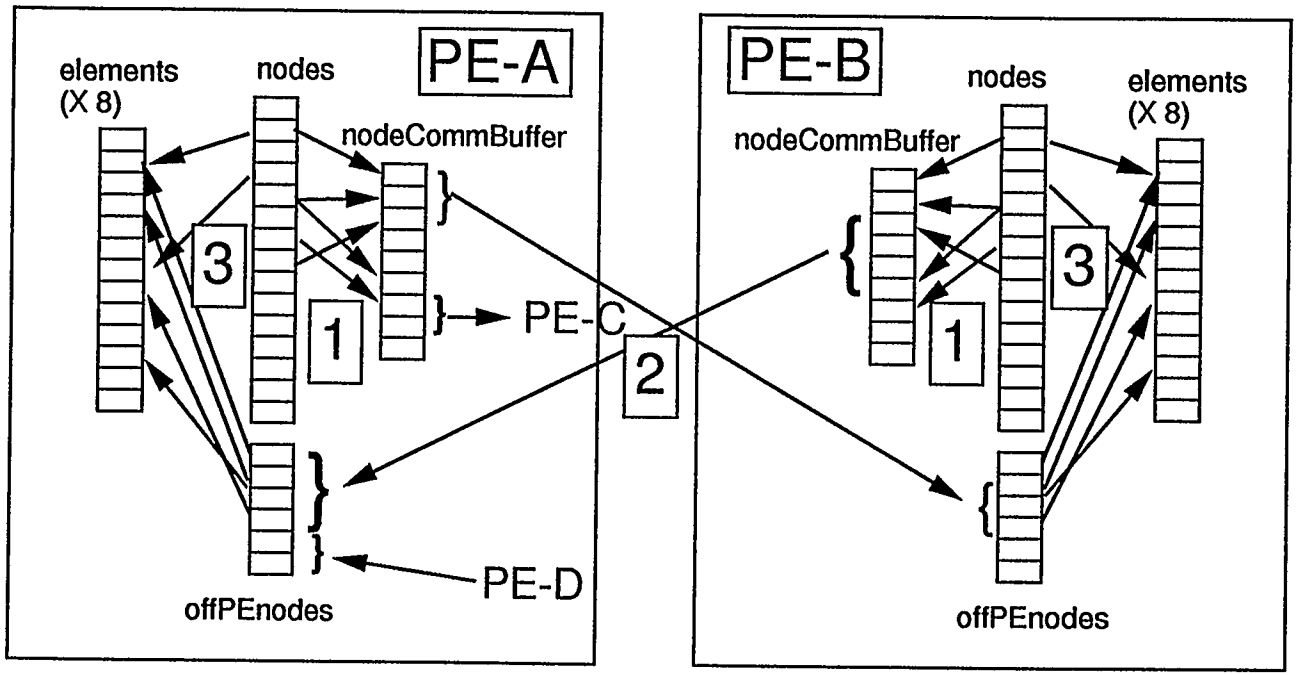
A6.17

PARALLEL COMMUNICATION LIBRARY FOR UNSTRUCTURED GRID SIMULATION TOOLS

- **Developed in collaboration with a parallel software expert (Robert Ferrell)**
- **Designed for:**
  - Parallelization of workstation clusters and SMPs through message passing
  - Any MPP that supports message passing (CM5, Cray-T3D, Paragon)
- **A handful of MPI routines currently handle all message passing functions**
- **Portability depends upon availability of MPI**
  - Currently an accepted standard, available as freeware for all UNIX platforms
  - Being optimized and integrated into the IBM operating system
- **Used by developers of physics models and numerical algorithms as a black box**
- **Should plug into unstructured grid simulation tools with little modification**
  - Written in C; callable from Fortran, C, or C++

AL.18

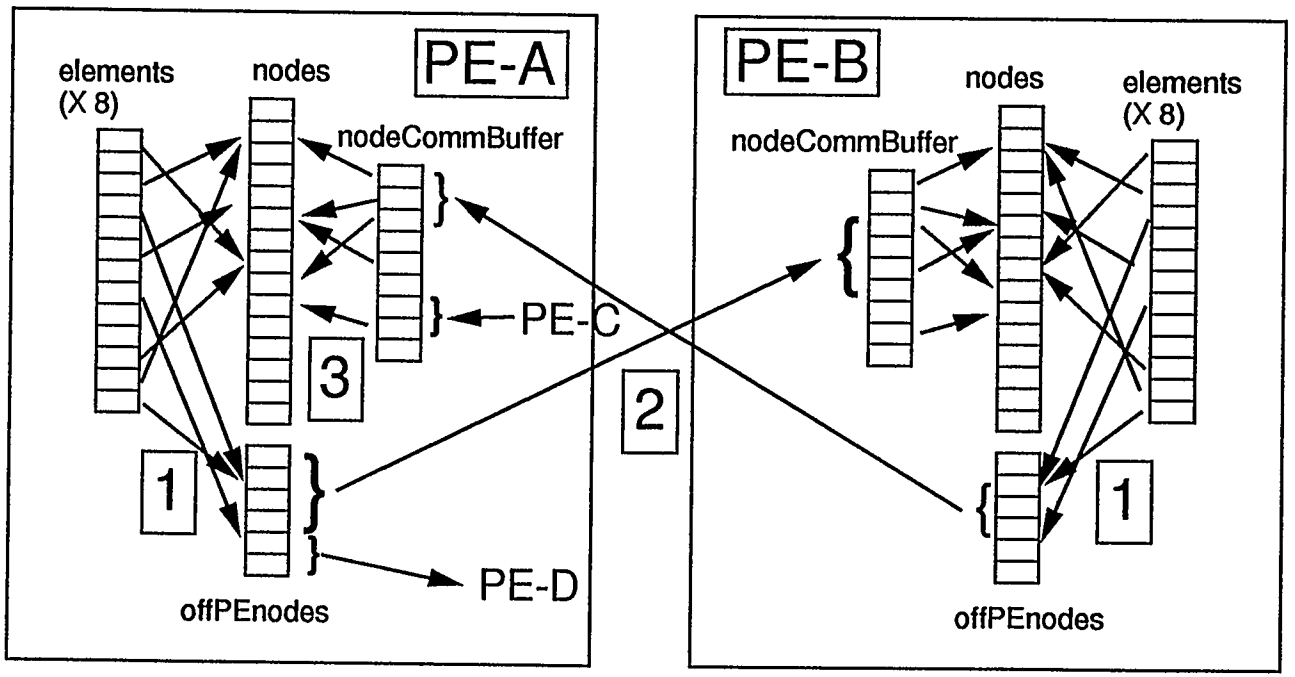
GATHER DATA FROM NODES TO ELEMENTS



Step 1: Load node data that must go off-PE into a communication buffer (nodeCommBuffer)
Step 2: Send data in communication buffer to buffers in destination PEs (offPEnodes)
Step 3: Gather node data to elements from on-PE (nodes) and off-PE (offPEnodes) buffers

46.19

SCATTER DATA FROM ELEMENTS TO NODES



Step 1: Scatter element data to on-PE nodes (nodes) and off-PE buffers (offPEnodes)
Step 2: Send data in off-PE buffer to communication buffer in destination PEs (nodeCommBuffer)
Step 3: Scatter element data in communication buffer (nodeCommBuffer) to nodes (nodes)

A6.2.0

TELLURIDE: GRAPHICAL USER INTERFACE (GUI)

- **A powerful interface for users *and* developers**
- **Developed with a "GUI-builder" known as Tcl/Tk**
- **GUI-builders decrease GUI development time**
- **Tcl/Tk is**
  - Based on a simple scripting language
  - Freeware - ideal for portable code
  - Fast becoming a "standard"
- **GUIs must be a part of modern simulation tools because they**
  - Decrease software development time and increase user productivity
  - Aid in widespread dissemination, use, and acceptance of the software
- **Consult WWW site `http://gnarly.lanl.gov/Home.html`**

A4.21

TELLURIDE STATUS

- **Design of a modern, flexible data structure**
  - Ideal for meshes that do not possess regular connectivity
  - Fully parallelized - supports arbitrary partitioning for multiple processors
- **A unique and accurate interface tracking method is in place**
  - Designed for complex 3-D geometries
  - More reliable mold-filling simulations will soon be possible
  - Convected solidification fronts will be highly resolved
- **A robust heat flow model is in place**
  - Utilizes a state-of-the-art, parallelized linear equation solver library
  - A unique, fully second-order finite-volume algorithm will improve results
- **Reliable fixed-grid enthalpy-based solidification models are being implemented**

AG.22

TELLURIDE STATUS

- **Portability issues have been addressed**
- **Gather/scatter communication library is currently being written**
  - Enables portable parallel execution based on the explicit message-passing paradigm
- **Integration of principal hydrodynamic algorithm components**
  - Three main phases per cycle: Remap, Corrector, and Projection
  - Remap phase: currently being implemented
  - Corrector/Projection phases: before end of FY95
- **Versatile and modern linear equation solver library**
  - New F90 library based on Krylov-subspace methods
  - Designed and well-suited for unstructured meshes
- **Important collaborations have been established industry and academia**

A6.23

PAGOSA HISTORY

- **Began as a research project in October 1989:**
  - Can modern CFD algorithms perform efficiently on parallel architectures?
  - What new methods and algorithms must be developed for parallel machines?
  - Can the increase CPU speed and memory capacity afforded by parallel computers be fully utilized?
- **Goal: quantitative accuracy and predictive capability of 3-D flows and high-rate deformation in real geometries**

A6.24

PAGOSA PHYSICS

- Compressible, 3-D hydrodynamics
- One-point turbulence models
- Elastic-plastic material deformation
- Material flow stress constitutive models
- Material damage models
- Analytic and tabular EOS for pure materials
- Pressure relaxation models for EOS of mixtures of materials
- Reactive HE burn models
- The kitchen sink

A6.25

PAGOSA NUMERICAL MODEL

- **3-D computational domain partitioned in Cartesian geometry into logically-connected orthogonal hexahedra**
- **Continuum mechanical conservation laws are solved with finite-difference approximations in the Eulerian frame**
- **Simulation is marched forward in time with a computational cycle comprised of two phases:**
  - *Lagrangian phase:* explicit predictor-corrector time integration
  - *Advection phase*: third-order, directionally-split upwind scheme of van Leer
- **Material interfaces are resolved accurately with a PLIC volume-tracking algorithm**
- **Written in data parallel fashion with CMF (Connection Machine Fortran)**

A6.26

EVOLUTION OF INTERFACIAL FLOW MODELING AT LOS ALAMOS

- **1960s:**
  - PIC method: particles represent fluid
  - MAC method: particles represent interfaces (SMAC)
  - Lagrangian method: mesh follows interfaces (LINC)
- **1970s:**
  - VOF method: volume fractions represent interfaces (SOLA-VOF)
- **1980s:**
  - Dramatic improvement of VOF methods (NASA SOLA-VOF, NASA VOF2D NASA VOF3D, CAVEAT, MESA2D, MESA3D, RIPPLE, ...)
  - Dramatic improvement of PIC methods (FLIP code family)
- **1990s:**
  - Three-dimensional VOF and PIC capabilities made readily available (PAGOSA, TELLURIDE, CAVEAT3D, CIC-3 suit of AMR codes, CELESTE3D)

A6.27

INTERFACIAL FLOW MODELING WITH VOF: IMPROVEMENTS SINCE "SOLA-VOF"

- Volume tracking is much more accurate
- Much improved surface tension model (CSF)
- Linear equation solvers are much faster and more robust
- Montonic, high order (2nd - 4th) advection algorithms
- Better resolution of flow transients (2nd order accuracy in time)
- Much improved projection methods
- Algorithms: typically finite volume, therefore amenable to body-fitted meshes
- Three-dimensional capabilities are the norm rather than the exception
- Portable, parallelized software

A6.28

FOR MORE INFO . . .

1. C. Zemach, D.B. Kothe, and T. Chaumauzeau, **Three-Dimensional Volume-Tracking of Fluid Interfaces on Generalized Hexahedral Meshes**, document in preparation.
2. D.B. Kothe and W.J. Rider, **Stretching and Tearing Interface Tracking Methods**, Technical Report AIAA 95-1717, to be presented at the 12th AIAA CFD Conference June 19-22, San Diego, CA (1995).
3. D.B. Kothe and W.J. Rider, **Comments on Modeling Interfacial Flows with Volume-of-Fluid Methods**, submitted to J. Comput. Phys. (1995).
4. W.J. Rider, D.B. Kothe, S.J. Mosso, J.H. Cerutti, and J.I. Hochstein, **Accurate Solution Algorithms for Incompressible Multiphase Flows**, Technical Report AIAA 95-0699, presented at the 33rd Aerospace Sciences Meeting and Exhibit, January 9-12, Reno, NV (1995).
5. J.I. Hochstein, T.A. Fletcher, and D.B. Kothe, **A Computational Model for Solidifying Flows**, Technical Report AIAA 95-0503, presented at the 33rd Aerospace Sciences Meeting and Exhibit, January 9-12, Reno, NV (1995).
6. D.B. Kothe, et al., **PAGOSA: A Massively-Parallel, Multi-Material Hydrodynamics Model for Three-Dimensional High-Speed Flow and High-Rate Material Deformation**, in proceedings of the 1993 SCS Simulation Multiconference: High Performance Computing, March 29--April 1 (1993).
7. D.B. Kothe and R.C. Mjolsness, **RIPPLE: A New Model for Incompressible Flows with Free Surfaces**, AIAA Journal **30**, 2694--2700 (1992).
8. J.U. Brackbill, D.B. Kothe, and C. Zemach, **A Continuum Method for Modeling Surface Tension**, J. Comput. Phys. **100**, 335--354 (1992).
9. J.U. Brackbill, D.B. Kothe, and H.M. Ruppel, **FLIP: A Low-Dissipation, Particle-in-Cell Method for Fluid Flow**, Comput. Phys. Commun. **48**, 25--38 (1988).

A6.29

Attachment 7
Multiphase Reynolds Stress Transport Modeling
Brian VanderHeyden
LANL

LA-UR-95-1725

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: **MULTIPHASE REYNOLDS STRESS TRANSPORT MODELING**

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

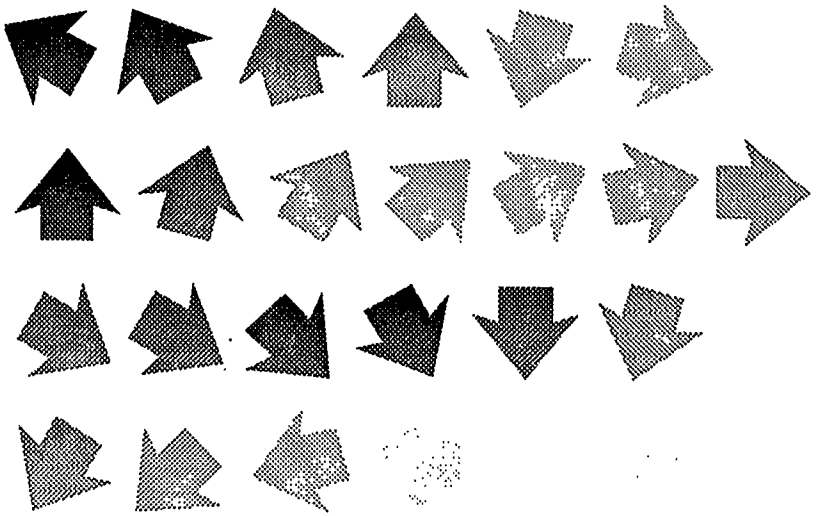
Los Alamos National Laboratory
Los Alamos, New Mexico 87545

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

A7.2

Multiphase Reynolds Stress Transport Modeling

- Exact Transport Equation
- Multiphase exchange and production
- Generalized multiphase Boussinesq closure



Multiphase Reynolds Stress

$$\rho_k \frac{d\mathbf{u}_k}{dt} = -\nabla \cdot \rho_k \mathbf{R}_k + \ldots \qquad \rho_k \mathbf{R}_k = \left\langle \alpha_k \rho_o \mathbf{u}_k' \mathbf{u}_k' \right\rangle$$

Select $Q_o = \alpha_k \rho_o \mathbf{u}_o \mathbf{u}_o$

Use micro and macro mass and momentum conservation equations

Insert in generalized conservation equation assuming non - collisional invariance :

$$\frac{d\mathbf{R}^k}{dt} = \frac{1}{\rho^k} \nabla \bullet \mathbf{D}^k + \mathbf{P}^k + \Phi^k - \varepsilon^k - \mathbf{M}^k + \mathbf{E}^k + \mathbf{C}^k + \mathbf{CP}^k - 2\left(\Omega \times \mathbf{R}^k + \mathbf{R}^k \times \Omega\right)$$

Single-Phase-Like Terms

$$P_{ij}^k = -R_{ik}^k \frac{\partial u_j^k}{\partial x_k} - R_{jk}^k \frac{\partial u_i^k}{\partial x_k}$$

mean flow gradient production

$$D_{ijk}^k = -\left\langle \alpha^k \begin{bmatrix} \rho_o c_i^k c_j^k c_k^k \\ -\left(p' \delta_{ik} + \tau_{oik}\right) c_j^k \\ -\left(p' \delta_{jk} + \tau_{ojk}\right) c_i^k \end{bmatrix} \right\rangle$$

diffusion flux

$$\Phi_{ij}^k = \left\langle \alpha^k p' \left(\frac{\partial c_i^k}{\partial x_j} + \frac{\partial c_j^k}{\partial x_i} \right) \right\rangle / \rho^k$$

pressure strain

$$\varepsilon_{ij}^k = \left\langle \alpha^k \left(\tau_{ojk} \frac{\partial c_i^k}{\partial x_k} + \tau_{oik} \frac{\partial c_j^k}{\partial x_k} \right) \right\rangle / \rho^k$$

dissipation

$$CP_{ij}^k = -\left\langle \alpha^k c_{(i}^k \right\rangle \frac{\partial p}{\partial x_{j)}}$$

compressibility production

Pure Multiphase Terms

$$M_{ij}^k = \left\langle \begin{bmatrix} \left(-p' \delta_{ik} + \tau_{oik}\right) c_j^k \\ +\left(-p' \delta_{jk} + \tau_{ojk}\right) c_i^k \end{bmatrix} \frac{\partial \alpha^k}{\partial x_k} \right\rangle / \rho^k$$

slip production, exchange

$$\mathrm{E}_{ij}^k = \left\langle \frac{d\alpha^k}{dt} \rho_o c_i^k c_j^k \right\rangle / \rho^k - R_{ij}^k \left\langle \frac{d\alpha^k}{dt} \rho_o \right\rangle / \rho^k$$

mass exchange source

$$\mathrm{C}_{ij}^k = \int \alpha^k u_{oi} u_{oj} \frac{Df}{Dt} d\Gamma_o / \rho^k$$

collision source

Multiphase Production & Exchange

$$M_{mm}^{f} = -2\theta^{f}\theta^{p}K^{pf}\left\{\begin{array}{l} w^{f}\left(\dfrac{C^{pf}}{\eta^{pf}}k^{p} - k^{f}\right) + \\ w^{p}\left(k^{p} - C^{pf}k^{f}\right) \end{array}\right\} - 2w^{p}\theta^{f}\theta^{p}K^{pf}U^{2}$$

$$M_{mm}^{p} = +2\theta^{f}\theta^{p}K^{pf}\left\{\begin{array}{l} w^{f}\left(\dfrac{C^{pf}}{\eta^{pf}}k^{p} - k^{f}\right) + \\ w^{p}\left(k^{p} - C^{pf}k^{f}\right) \end{array}\right\} - 2w^{f}\theta^{f}\theta^{p}K^{pf}U^{2}$$

Generalized Multiphase Boussinesq Closure

- Examine homogeneous limit
- Invert tensor algebraic equation
- Obtain true tensorial form of stress
- Obtain dependence of eddy viscosity on slip velocity

Attachment 8
Spectral Models, Symmetry and Engineering Turbulence Closures
Tim Clark
LANL

LA-UR-95-1751

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: **SPECTRAL MODELS, SYMMETRY AND ENGINEERING TURBULENCE CLOSURES**

AUTHOR(S): Tim(othy) Clark, T-3
Leaf Turner, T-3
Charles Zemach, 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 National Laboratory
Los Alamos, New Mexico 87545

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

A8.2

Spectral Models, Symmetry and Engineering Turbulence Closures

Tim Clark

Leaf Turner

Charles Zemach

Los Alamos National Laboratory
Group T-3

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

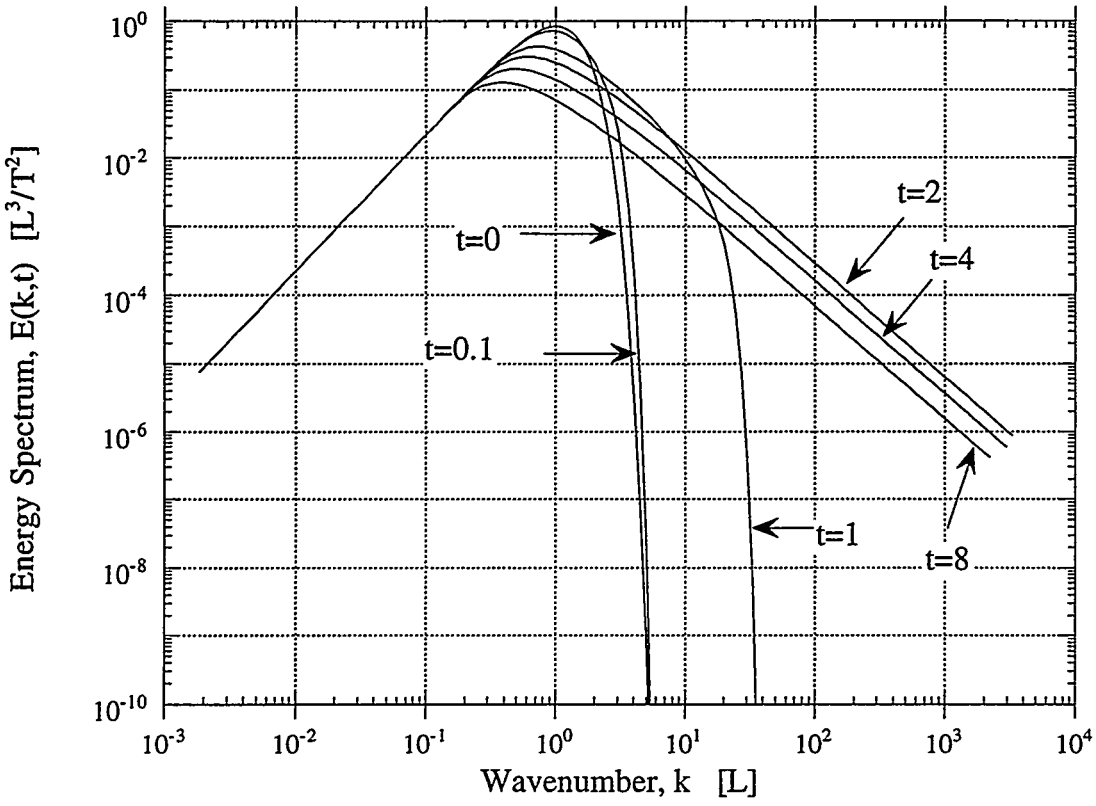
$$K(t) = K_0 \,(1 + t/t_0)^{-\gamma_K}, \;\; L(t) = L_0 (1 + t/t_0)^{\gamma},$$

and

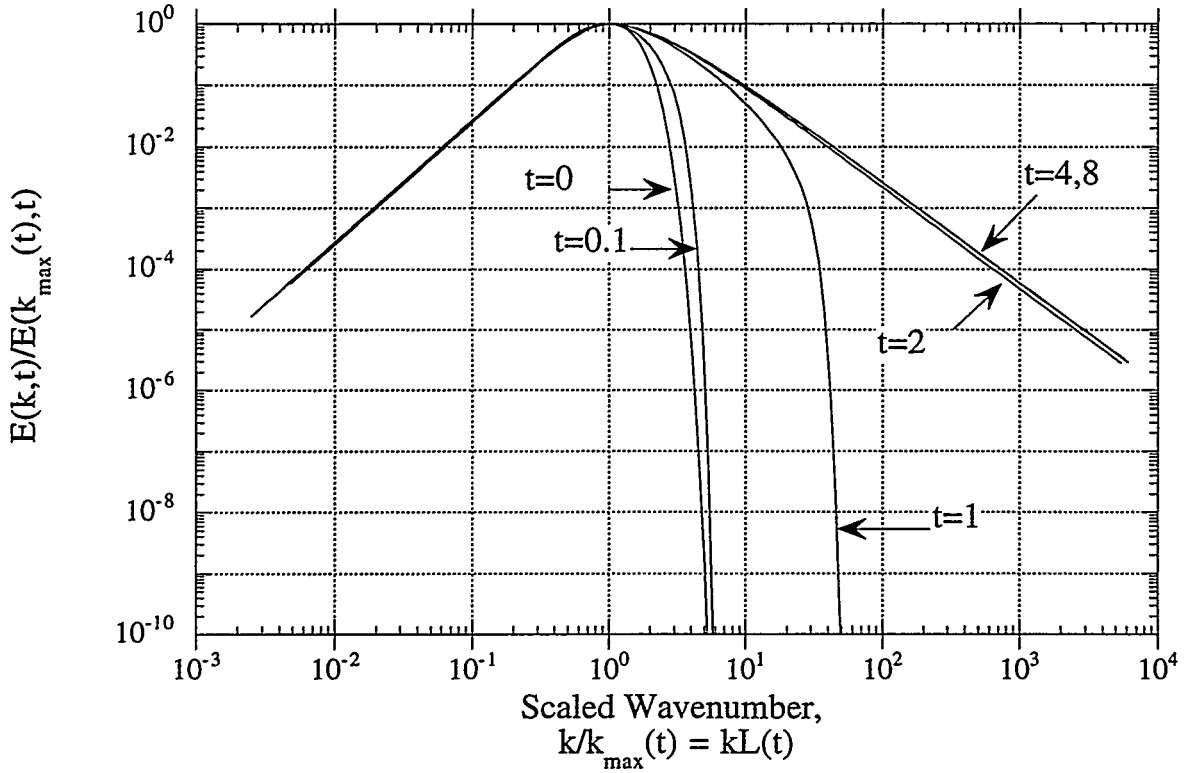
$$\gamma_K = 2 - 2\gamma.$$

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)

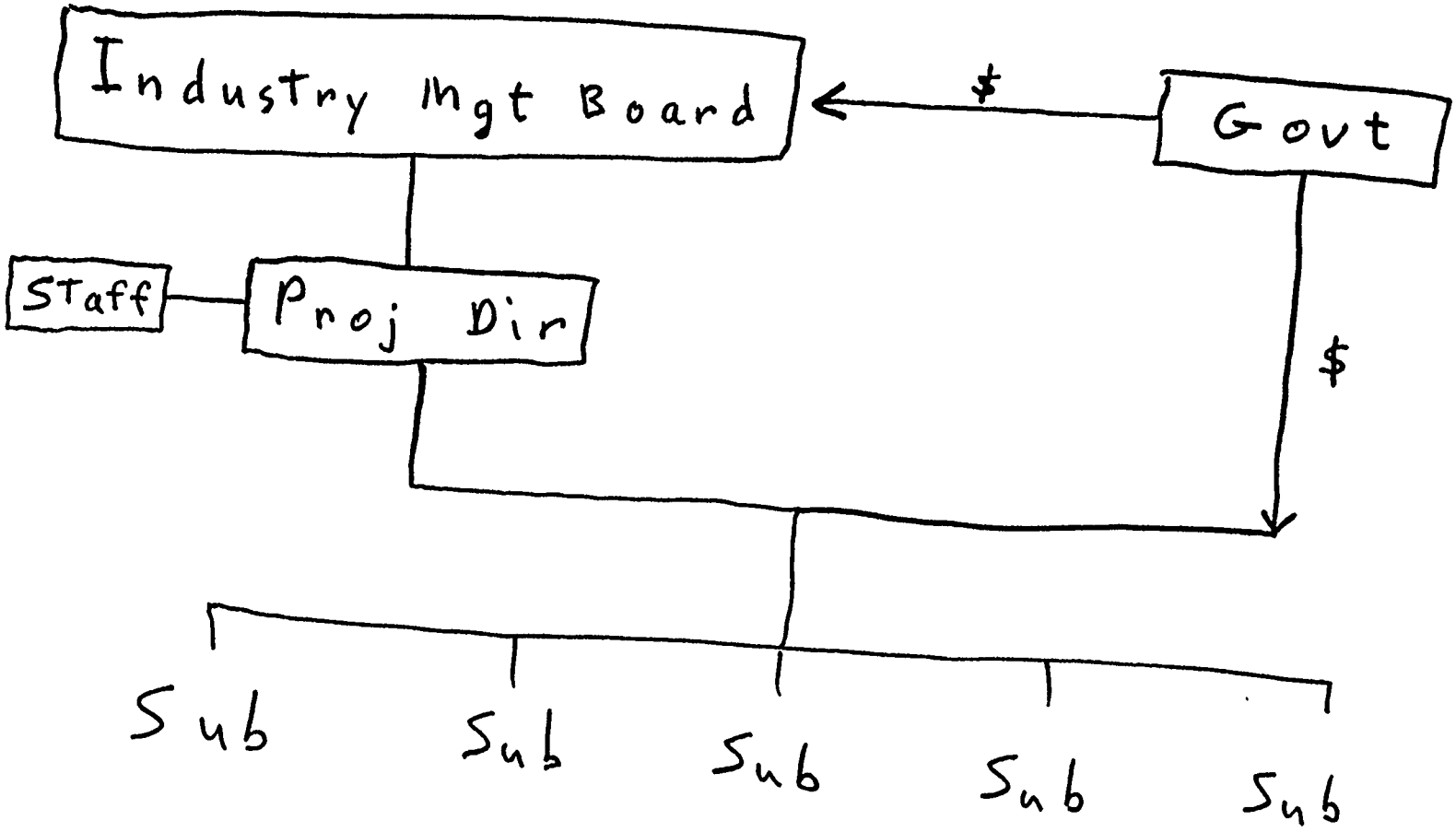
Premise

- 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.

Authors:

Dr. Joseph D. Smith
Engineering Research & Process Development Lab
The Dow Chemical Company
Building 734
Midland, MI 48667
Phone 517-638-7982

Dr. Tyler B. Thompson
Cooperative Research
The Dow Chemical Company
Building 1801
Midland, MI 48674
Phone 517-636-0330

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

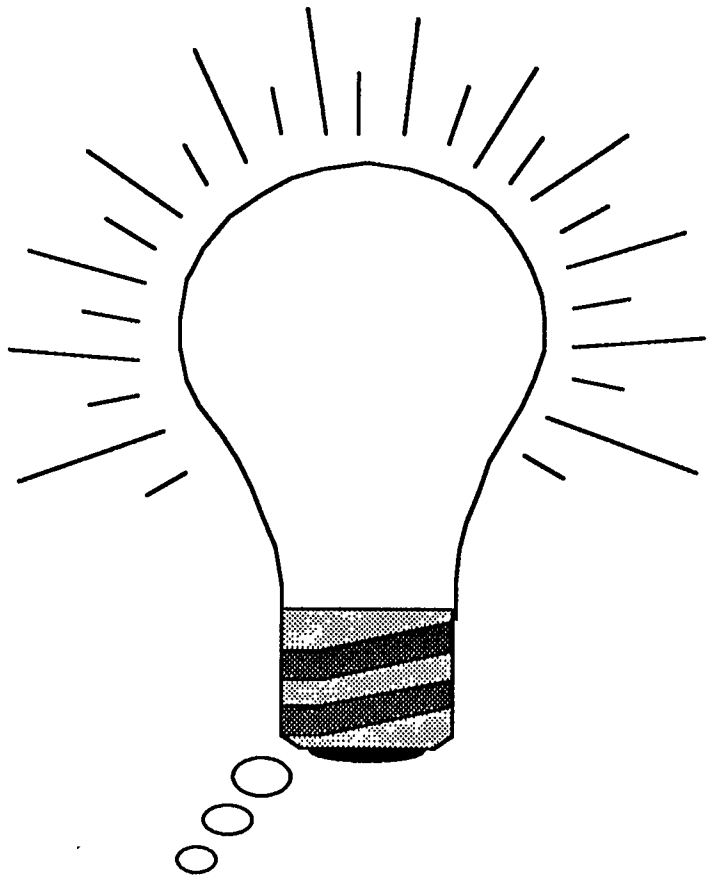
Los Alamos National Laboratory
Los Alamos, New Mexico 87545

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

A12.2

Brainstorm / Discussion on Consortium / Center of Excellence

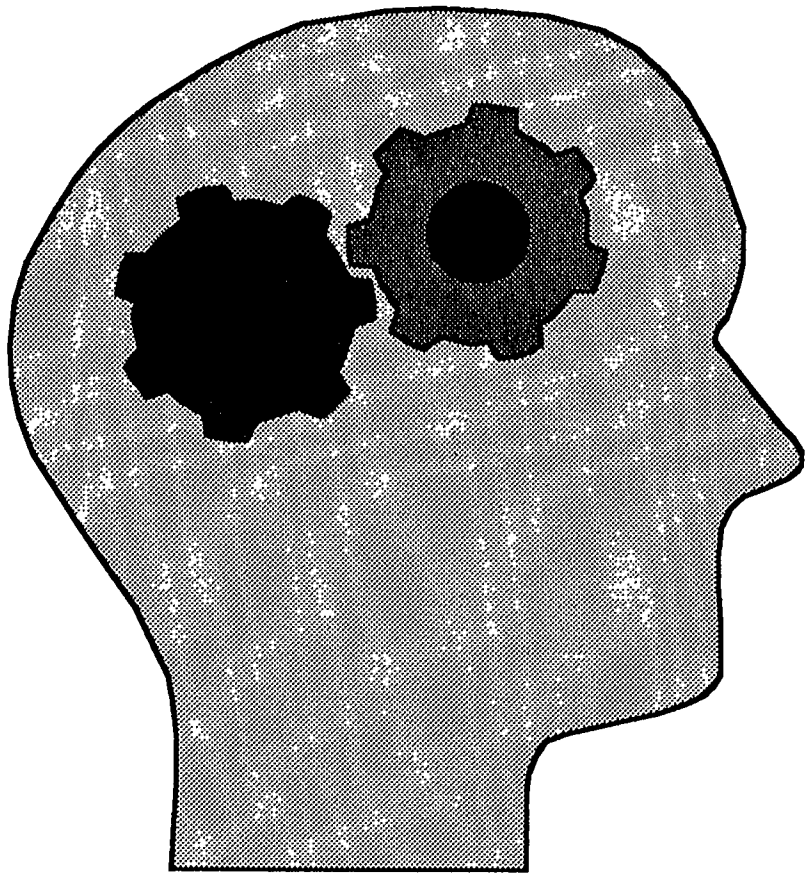
- Needs
- Potential Consortium/Center of Excellence



A12.3

Needs - Theory

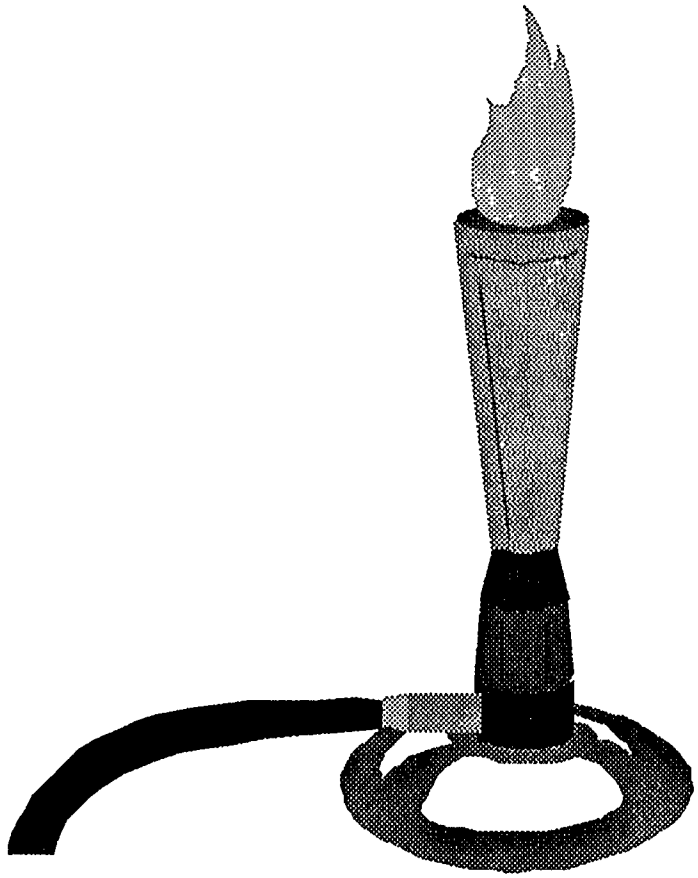
- Multiphase Turbulence
- Exchange
- Granular stresses
- Electromagnetic fields
- Radiation Transport



A12.4

Needs-Experiment

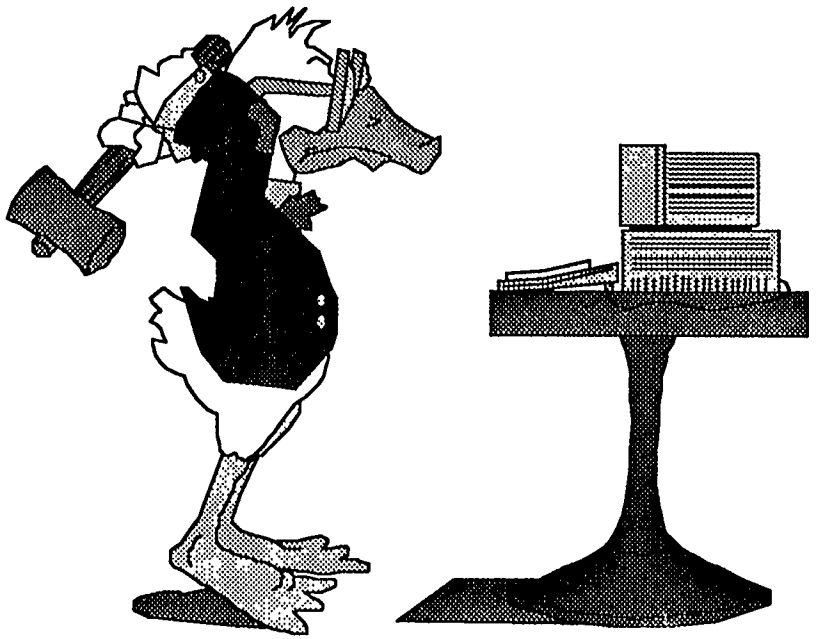
- Tomography
- Probes
- Turbulence
- Multifluid exchange



A12.5

Needs-Numerical Methods

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



A12.6

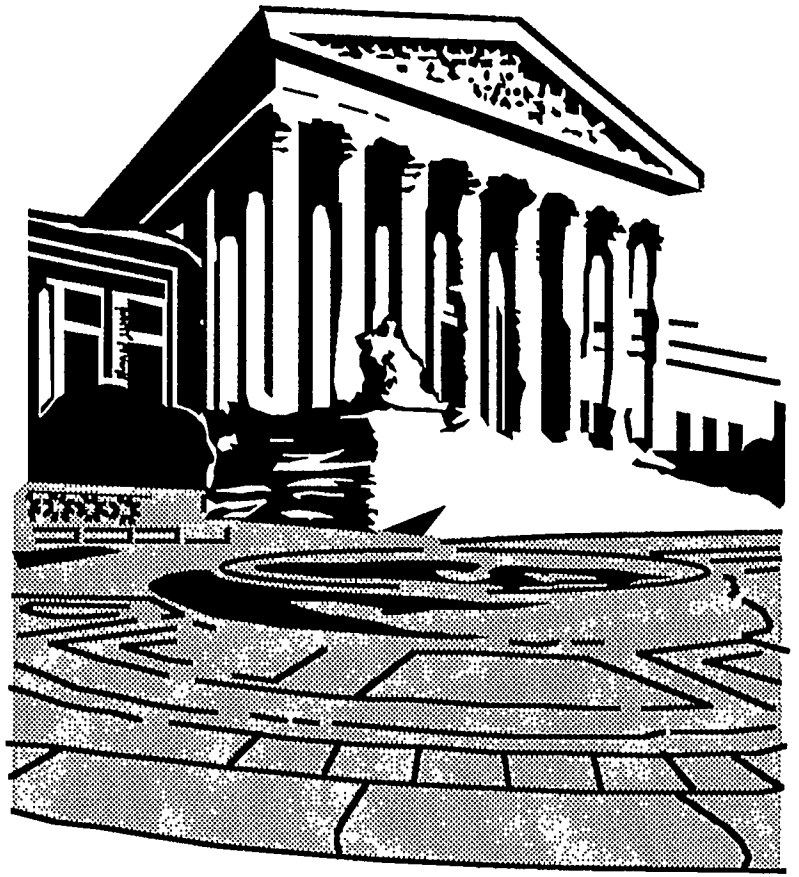
Needs-Generic Simulations

- 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