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**Reaction Engineering International and Pacific
Northwest Laboratory Staff Exchange: Addressing
Computational Fluid Dynamics Needs of the Chemical
Process Industry**

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MASTER

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Reaction Engineering International and Pacific Northwest Laboratory Staff Exchange: Addressing Computational Fluid Dynamic Needs of the Chemical Process Industry

Staff exchanges, such as the one described in this report, are intended to facilitate communications and collaboration among scientists and engineers at Department of Energy (DOE) laboratories, in U.S. industry, and academia,. Funding support for these exchanges is provided by the DOE, Office of Energy Research, Laboratory Technology Transfer Program. Funding levels for each exchange typically range from \$20,000 to \$40,000. The exchanges offer the opportunity for the laboratories to transfer technology and expertise to industry, gain a perspective to industry's problems, and develop the basis for further cooperative efforts through Cooperative Research and Development Agreements (CRADAs) or other mechanisms.

Information in this report on the staff exchange of the Pacific Northwest Laboratory (PNL) staff with Reaction Engineering International (REI) includes the significant accomplishments, significant problems, industry benefits realized, recommended follow-on work and potential benefit of that work and two appendices. Appendix A summarizes progress made on a jointly analyzed test problem and Appendix B is a letter from REI outlining follow-on work.

Purpose/Objectives

The objectives of this project were as follows:

- Work with REI to develop an understanding of the computational fluid dynamics (CFD) needs of the chemical process industry
- Assess the combined capabilities of the PNL and REI software analysis tools to address these needs
- Establish a strategy for a future programmatically funded, joint effort to develop a new CFD tool for the chemical process industry

Summary of Activities Performed

REI has a well-developed relationship with Dow Chemical and the first activity was for REI to get an initial list of CFD need from Dow's perspective. This list was refined during the course of this staff exchange. Then, to begin to assess our relative capabilities against these needs, PNL and REI staff conducted a parallel analysis of one problem. In the balance of this project, PNL and REI staff engaged in a dialogue with Dow and other participants to develop a strategy for a long term course of action for addressing chemical process industry needs.

Rushton Turbine Mixer Model

The CFD problem selected as having general interest to the chemical process industry was mixing in a stirred reactor. The particular design studied uses a rotating impeller and is known as a Rushton Turbine Mixer. PNL staff member Jim Fort spent a week at REI's offices in Salt Lake City, Utah to work with REI staff to apply PNL's TEMPEST code and REI's BANFF code to this problem. These separate analyses continued after this initial week at REI.

The rotating impeller of this mixer was approximated as a fixed set of blades in a rotating vessel because of both TEMPEST and BANFF's limitation to modeling moving surfaces. The results from the TEMPEST were substantially different from laboratory experiment results. The root cause of this problem was found to be the absence of several terms in the momentum equation that are induced by the Coriolis force. A summary of this work, including detailed modeling results and a proposed correction to this problem, is included in Appendix A.

Approach to Development of a New CFD Tool

The balance of the project was directed at assessing computational fluid dynamics (CFD) needs for the chemical industry and looking ahead to the feasibility of joint develop of a CFD software tool that would address these needs. This is an area of mutual technical interest and expertise for PNL and REI and the goal was to form an agenda for long-term, collaborative, programmatically-funded work.

To assess chemical industry needs, the plan was to work with REI to set up a workshop with CFD practitioners from a number of companies from that industry. Although the workshop had to be deferred to FY-96, contacts with Dow Chemical provided a detailed list of their company's needs that cannot presently be handled with available commercial and public-domain CFD tools. Dow's CFD issues are grouped into three technical areas and are being addressed by four Dow task forces (one for each technical area plus one for management/implementation). The charter of the technical area task forces is to assess in-house capabilities relative to state of the art externally (industry, national labs, academia). The issues are:

- Turbulent reacting flow
 - turbulent modeling
 - non-trivial number of reactants
- Multi-phase flow
 - reactions with crystallization
 - latex emulsion polymers
- Full simulation capability for polymer flows
 - 3-dimensional
 - free surfaces
 - time dependent
 - non-Newtonian/viscoelastic rheology

Contacts were also made with Dow Chemical to enlist their help and support in a CFD tool development program. Dow was interested, but participation was contingent on multiple company involvement and matching federal funding. Interaction with Nick Lombardo (PNL Advanced Processing Technology Initiative) and Steve Weiner (PNL chemical industry of the future initiative) identified potential federal funding agencies and helped develop a plan for the workshop, including names of potential chemical industry participants, and a strategy for collaborative program development. A strategy for follow-on work from REI's perspective is included as Appendix B.

Significant Accomplishments

The most significant accomplishment for this project was to develop a relationship with a industrial partner, with strengths that are complimentary to PNL's that has the strong potential to result in future programmatically funded work. In addition, improvements were made to the PNL TEMPEST simulation model and the REI BANFF code which should increase their value in meeting the Computational Fluid Dynamics needs of the chemical industry.

Significant Problems

PNL and REI encountered similar difficulties in modeling the Rushton Turbine Mixer, however a correction would work in both codes was identified.

Industry Benefits Realized

Through our new relationship, REI now has established contact at PNL that can help tap PNL and other federal laboratory strengths to address their client's problems.

Recommended Follow-On Work

In FY96, work with REI to conduct a workshop with chemical process industry CFD practitioners to identify industry wide needs in this area. From priorities identified in this workshop, formulate a jointly-funded (industry and government) development program to address these needs. Identify government sponsors (DOE-OIT and NIST-ATF are currently viewed as possibilities) and enlist industrial membership support.

Potential Benefits from Pursuing Follow-On Work

Benefit in the follow-on work shifts to the U.S. chemical process industry, as they will be provided with a tool that improves their competitiveness. PNL and REI also benefit by utilizing their unique skills and by long-term funded programs.

Appendix A

Progress Report on Rushton Turbine Mixer

Memo

TO: Brad Adams (Reaction Engineering International)
FROM: Jim Fort *JS*
DATE: February 21, 1994
RE: Rushton Turbine Mixer Model - Progress to Date
CC: Inn Choi, Don Trent, Erik Pearson

Because of the common limitations in modeling moving surfaces in TEMPEST and BANFF, our initial approach to this problem was to approximate the rotating impeller as a fixed set of blades in a rotating vessel. Our assumption was that the induced centrifugal and Coriolis forces would be small and that the flow field would be reasonably well represented for the actual problem. Our approximation amounts to a transformation of coordinates from a stationary to rotating reference frame, and I have sent you derivations of correction terms to make this rigorously correct (Attachment 1 - note sign changes from draft I sent earlier). These corrections have not yet been included in TEMPEST.

The results I am getting with TEMPEST are grossly different than in Stoots' experiment¹ and I suspect that the cause is the induced forces in our rotating model (i.e. our approximation is invalid and we are really simulating a different problem). Using the results of my simulation, I have completed an order of magnitude analysis of terms in the r -momentum equation (Equation 15 in Attachment 1). Results of this analysis show that the correction terms are significant and should be included in our analyses.

The detailed results of the order of magnitude analysis are given in Attachment 2 in the form of colored contour plots in the plane of the impeller blade. In the current simulation, the affect of the rotating reference frame shows up first in the term u_θ^2/r , which is balanced by like increases in the pressure gradient term $(1/\rho) \partial p / \partial r$. If an increased hydrostatic head were the only affect, our simulation of this uniform density flow would be satisfactory as-is. However, Coriolis forces are also induced. And although the magnitude of the Coriolis force term ($2u_\theta\omega$) was found to be comparable to that of the centrifugal terms, a more useful comparison is the sum of the correction and centrifugal force terms ($2u_\theta\omega - u_\theta^2/r - r\omega^2$) with the advective terms in the equation. They were found to be of the same order of magnitude, with $(u_\theta/r) \partial u_r / \partial \theta$ being the dominant advective term.

I have already FAXed you details of the TEMPEST model (grid, boundary and initial conditions) and vector plots giving the resulting flow field, but have included them again as Attachment 3 for the record. The flow field is given at 2.4s, and appears to be steady when compared to earlier solutions. This solution time was achieved in about 55 hrs on an IBM/RS6000-560.

1. Stoots, Carl Marcel, *The Velocity Field Relative to a Rushton Turbine Blade*, Ph.D. Dissertation, University of Maryland, 1989.

Attachment 1

Memo

TO: Don Trent
FROM: Jim Fort *jni*
DATE: February 21, 1994
RE: Coordinate Transformation from Stationary to Rotating Reference Frame
CC: Perry Meyer, Loren Eyler

A coordinate transformation may be possible to facilitate modeling of fixed cylindrical vessels with rotating internals (e.g. mixing jets, impellers). The transformation is from the cylindrical coordinate system in the fixed tank reference frame to the rotating frame of the internal apparatus. This would require that the internals be located on, and rotate about, the vessel centerline. In TEMPEST, the moving vessel walls and floor could be implemented with the moving boundary logic.

In this memo I have derived the additional terms that this transformation introduces into the momentum equations. These terms could be included in TEMPEST and would be invoked as part of a rotating reference frame option. Perry Meyer checked my derivation and his corrections are included.

A fixed cylindrical vessel with coaxially located internals rotating at a constant rate, ω , can be represented with fixed internals and with the vessel rotating about the centerline with the same rate but in the opposite direction,

Lab Frame

Impeller Frame

provided that the following variable transformations are made,

$$\theta = \theta' - \omega t \quad (1)$$

$$u_\theta = u'_\theta - \omega r \quad (2)$$

(lengths and velocities in the other coordinate directions are equivalent).

Derivatives in θ are also affected.

$$\frac{\partial}{\partial \theta} = \frac{\partial}{\partial \theta'} \left(\frac{\partial \theta'}{\partial \theta} \right) \quad (3)$$

By (1),

$$\frac{\partial \theta'}{\partial \theta} = 1 + \omega \frac{\partial t}{\partial \theta} = 1 + \frac{\omega r}{u_\theta} = 1 + \frac{\omega r}{u_{\theta'} - \omega r} = \frac{u_{\theta'}}{u_{\theta'} - \omega r} \quad (4)$$

Therefore

$$\frac{\partial}{\partial \theta} = \frac{u_{\theta'}}{u_{\theta'} - \omega r} \frac{\partial}{\partial \theta'} \quad (5)$$

Consider the inviscid momentum equations in cylindrical coordinates,

$$\frac{Du_r}{Dt} - \frac{u_\theta^2}{r} = -\frac{1}{\rho} \frac{\partial p}{\partial r} \quad (6)$$

$$\frac{Du_\theta}{Dt} + \frac{u_r u_\theta}{r} = -\frac{1}{\rho r} \frac{\partial p}{\partial \theta} \quad (7)$$

$$\frac{Du_z}{Dt} = -\frac{1}{\rho} \frac{\partial p}{\partial z} \quad (8)$$

where D/Dt is the substantial derivative

$$\frac{D}{Dt} = \frac{\partial}{\partial t} + u_r \frac{\partial}{\partial r} + \frac{u_\theta}{r} \frac{\partial}{\partial \theta} + u_z \frac{\partial}{\partial z} \quad (9)$$

Transforming D/Dt by substitution of (2) and (5) into (9) leads to an equivalent expression in the primed coordinates

$$\frac{D'}{Dt} = \frac{\partial}{\partial t} + u'_r \frac{\partial}{\partial r'} + \left(\frac{u'_\theta - r\omega}{r'} \right) \left(\frac{u'_\theta}{u'_\theta - r\omega} \right) \frac{\partial}{\partial \theta'} + u'_z \frac{\partial}{\partial z'} = \frac{D}{Dt} \quad (10)$$

Substitution into the momentum equations yields

r-momentum

$$\frac{Du'_r}{Dt} - \frac{1}{r} (u'^2_\theta + r^2 \omega^2 - 2u'_\theta r \omega) = -\frac{1}{\rho} \frac{\partial p}{\partial r} \quad (11)$$

$$\frac{Du'_r}{Dt} - \frac{u'^2_\theta}{r} - r\omega^2 + 2u'_\theta \omega = -\frac{1}{\rho} \frac{\partial p}{\partial r} \quad (12)$$

θ -momentum

$$\frac{D}{Dt} (u'_\theta - r\omega) + \frac{u'_r}{r} (u'_\theta - r\omega) = -\frac{1}{\rho r} \frac{\partial p}{\partial \theta'} \quad (13)$$

which, after expanding terms on the LHS and simplifying, becomes

$$\frac{Du'_\theta}{Dt} + \frac{u'_r u'_\theta}{r} - 2u'_r \omega = -\frac{1}{\rho r} \frac{\partial p}{\partial \theta'} \quad (14)$$

The z -momentum equation is unchanged under this transformation.

In summary, the balance of forces in the impeller reference frame are described by equations (8), (12) and (14), which are repeated here for convenience.

$$\frac{Du'_r}{Dt} - \frac{u'^2_\theta}{r} - r\omega^2 + 2u'_\theta \omega = -\frac{1}{\rho} \frac{\partial p}{\partial r} \quad (15)$$

$$\frac{Du'_\theta}{Dt} + \frac{u'_r u'_\theta}{r} - 2u'_r \omega = -\frac{1}{\rho r} \frac{\partial p}{\partial \theta'} \quad (16)$$

$$\frac{Du_z}{Dt} = -\frac{1}{\rho} \frac{\partial p}{\partial z} \quad (17)$$

The transformation results in two new terms in the r -momentum equation: $r\omega^2$ is the centripital force and $2u'_\theta \omega$ is the Coriolis force. Only the Coriolis force term is added to the θ -momentum equation. Batchelor¹ gives a good description of the influence of these terms on a rotating flow field. As a check on limiting cases, note that all three correction terms go to zero with vessel rotation rate, ω . Also, for the case of rigid body rotation ($u'_\theta = r\omega$) the LHS of (15) and (16) is zero (i.e. no net pressure gradients). These three terms are what need to be added to TEMPEST, and would be selectively turned on when modeling the flow in a fixed vessel using a rotating reference frame.

1. Batchelor, *An Introduction to Fluid Mechanics*, Cambridge University Press, 1967, p. 555.

Attachment 2

Pressure Gradient Term ($1/\rho \times \partial p / \partial r$)

I = 2

pgrad

II Print II 21 Feb 1994 II post.plt II Fine Grid T = 2.46 TEMPEST ver. N83.5d

Total Centrifugal Force Term (u_θ^2/r)

$l = 2$

clld

40
36
32
28
24
20
16
12
8
4
0

Centrifugal Force Term
Due to Rotating Vessel ($r\omega^2$)

$l = 2$

crbm

Coriolis Force Term ($2u_0\omega$)

$l = 2$

corl

70
63
56
49
42
35
28
21
14
7
0

$$2u_{\theta}\omega - u_{\theta}^2/r - r\omega^2$$

| = 2

sum

$$u_{\theta}/r \partial u_r / \partial \theta$$

$l = 2$

adv2

Print II 21 Feb 1994 II post.plt II Fine Grid T = 2.4s TEMPEST ver. N33.5d

$u_z \partial u / \partial z$

$l = 2$

adv3

II Print II 21 Feb 1994 II post.plt II Fine Grid, T = 2.4s, TEMPEST ver. N33.5d

$u, \partial u / \partial r$

$I = 2$

adv1

Attachment 3

Plot at time = 0.001 seconds

qaid: REI test problem
Cylindrical Stirred Reactor - Fine Grid

Computational Grid

r-x plane at K = 25

J = 1 to 38

I = 1 to 29

tempest/n33.5 d 02aug92 13jun93 2/12/94 13:15:56

Plot at time = 0.001 seconds

qaid: REI test problem

Cylindrical Stirred Reactor - Fine Grid

tempest/n33.5 d 02aug92 13jun93 2/12/94 13:16:56

r-z plane at l = 2

J = 1 to 38

K = 1 to 50

Computational Grid

Plot at time = 0.001 seconds

qaid: REI test problem
Cylindrical Stirred Reactor - Fine Grid

Initial Condition
Rigid Body Motion ($V_\theta = \omega r$)
from blade tip to wall
 $\vec{V} = 0$ within blade region

tempest/ n33.5 d 02aug92 13jun93 2/12/94 13:15:56

r-x plane at K = 25

J = 1 to 38

I = 1 to 29

Vmax = 2.166
→

Plot at time = 0.001 seconds

qaid: REI test problem
Cylindrical Stirred Reactor - Fine Grid

Boundary Conditions
at Floor:

← Rigid body motion ($V_\theta = \omega r$)

at Top Surface:
free slip

tempest/ n33.5 d 02aug92 13jun93 2/12/94 13:15:56

r-x plane at $K = 1$

$J = 1$ to 38

$I = 1$ to 29 .

$V_{\max} = 2.166$
→

Plot at time = 2.400 seconds

qaid: REI test problem
Cylindrical Stirred Reactor - Fine Grid

Mid-plane of Blade
($z^* = 0.0$)

tempest/n33.5 d 02aug92 13jun93 2/16/94 9:36:45

r-x plane at K = 25

J = 1 to 38

I = 1 to 29

A-20

Vmax = 2.089

Plot at time = 2.400 seconds

qaid: REI test problem
Cylindrical Stirred Reactor - Fine Grid

tempest/n33.5 d 02aug92 13jun93 2/16/94 9:36:45

r-z plane at l = 2

J = 1 to 38

K = 1 to 50

$\theta = 0^\circ$

Plot at time = 2.400 seconds

qaid: REI test problem
Cylindrical Stirred Reactor - Fine Grid

r-z plane at l = 7

J = 1 to 38

K = 1 to 50

Vmax = 0.482
→

$$\theta = 12^\circ$$

Plot at time = 2.400 seconds

qaid: REI test problem
Cylindrical Stirred Reactor - Fine Grid

tempest/n33.5 d 02aug92 13jun93 2/16/94 9:36:45

r-z plane at l = 12

J = 1 to 38

K = 1 to 50

Vmax = 0.481

$\alpha = 24^\circ$

Plot at time = 2.400 seconds

qaid: REI test problem

Cylindrical Stirred Reactor - Fine Grid

$\phi = 35^\circ$

r-z plane at $l = 17$

J = 1 to 38

K = 1 to 50

$V_{max} = 0.475$

Plot at time = 2.400 seconds

qaid: REI test problem

Cylindrical Stirred Reactor - Fine Grid

tempest/n33.5 d 02aug92 13jun93 2/16/94 9:36:45

$\theta = 46^\circ$

r-z plane at l = 22

J = 1 to 38

K = 1 to 50

Vmax = 0.497
→

Appendix B

Letter from REI Outlining Follow-On Work

REACTION
ENGINEERING
INTERNATIONAL

August 11, 1994

Dr. James A. Fort
Battelle
Pacific Northwest laboratories
Battelle Boulevard
Richland, Washington 99352

Dear Jim:

Since we last met with Battelle about the CPI initiative we have had a number of important events occur. I have enclosed a brief report on what we at REI see as the major issues that have arisen since our joint draft proposal to Dow. The report shows how we propose to resolve each of these issues. We would like you to review them, distribute them to those at Battelle who are, or who might be, involved in this program, and give us some feedback from the PNL perspective.

I have listed what we propose as the next steps to be taken in this initiative. If you agree, we should identify a meeting time and place as soon as possible. We can then identify the agenda for the meeting and make assignments to each participant.

Let me know what you think,

Philip J. Smith

Computational Reacting Flow Tools (cfd-based) for the Chemical Process Industry: **Some Issues and Proposed Resolutions (August, 1994)**

Scope of Proposed Work:

Discussions with the chemical process industry have raised questions regarding the scope of work as proposed in our previous meetings. Some parties have indicated that the preliminary task statements were too ambitious. Others have suggested that the scope should include only reacting flow systems. In this regard Dow has identified three target areas important to them for computational tool development: mixing tanks, multi-phase (polymer) flows, and reactive flows.

We propose that the scope of this work be narrowed to Computational Reacting Flow Tools for the Chemical Process Industry. The strength of the proposed team and the uniqueness of the CPI applications are in chemically reacting flow problems.

The developed tools will emphasize simulations of coupled physical and chemical processes including: homogeneous and heterogeneous reactions, multiple complex chemical kinetic mechanisms, laminar and turbulent flow fields, diffusive and convective mass transfer, and radiative, convective and conductive heat transfer. A second emphasis will be the ability to model complicated geometries relevant to the CPI and thereby proved the capabilities to simulate a wide range of reacting flow vessels, e.g. mixing tanks, crystallizers, process heaters, flow reactors, etc.

Computational Paradigm:

In using our own software tools for industrial reactive-flow applications we are continually confronted with the need for a new computational paradigm. This need is manifest in the following problems:

1. Every application requires a specific set of physical and chemical descriptions (models) that change from problem to problem. In the literature, we find many good fundamental models but are unable to expeditiously incorporate these models into our cfd-based tools.
2. With increasingly sophisticated applications there is continual pressure to reduce computational run times. Our experience has shown that different numerical methods have advantages for different reacting flow applications. Furthermore, numerical methods are continuously being improved. Unless we change the existing computational paradigm these improvements cannot be cost-effectively exploited.
3. Finally, a similar observation has been made with respect to vessel geometry. Each application requires different constraints on the type of defining mesh. Any new tool for the CPI needs to be flexible with respect to mesh structure, including the option to mix mesh types within the same simulation.

We are convinced that the above problems are not unique to our own software tools, but rather are common to all reacting flow simulation software used by industry.

The solution to these problems is to use a modern object-oriented computational paradigm. This object-oriented programming approach must be a flexible but proven technique for easy and rapid incorporation of evolving chemistry/physics models, new numerical methods, and multiple mesh architectures. This paradigm has been applied and proven in research cfd tools. However, the technology has not yet been transferred to commercial cfd codes.

We introduced this paradigm to Dow in previous meetings. Since that time we have had detailed discussions with the leading researchers who have developed object-oriented cfd codes. These researchers are willing to collaborate with us. Their involvement in this program would augment our team capabilities and increase the probability of success for delivering friendly, useful, and flexible tools.

Team Structure:

We propose the addition of the DOE/HPCC Grand Challenge Computational Center for Combustion as a member of the core team. This center is a network of leading researchers in the cfd community. The principle participants are:

Phil Colella, UC Berkeley/Lawrence Livermore National Laboratory
John Bell, Lawrence Livermore National Laboratory
Jeff Saltzman and group (C3), Los Alamos National Laboratory
Marsha Berger, NYU/Courant Institute

The HPCC center was established to create advanced cfd tools, with a particular focus on combustion applications. The center participants have a proven track record in developing object-oriented cfd tools.

Phil Colella, the project director of the DOE/HPCC Center, visited REI and listened to a presentation on the objectives of the CPI proposal. He subsequently discussed with his center participants the possibility of joining teams. They have told us that they would enthusiastically join the core CPI team.

Commercial Support:

Dow has expressed concern about the need for a commercial software vendor to provide user support for the delivered products. We remain amenable to this approach. However, as a result of our discussion with cfd developers, we remain concerned that any existing commercial vendor will have a vested interest in their own technology/user-base and thus may not be willing to support a new computational paradigm.

If a separate software-support company is needed, it will become apparent over the course of the development cycle. The CPI advisory board could then develop either a spin-off company, or empower an existing entity to provide that function.

Next Steps:

The first step should be a meeting with REI, Batelle, Dow and the HPCC team to prepare a strategic plan. In order to complete that plan we must have:

1. final agreement on the scope and objectives of the program;
2. agreement on core team participants and their roles;
3. identification of participating chemical companies.

After this meeting the core team should prepare the long discussed white paper on this initiative. The team must then identify the source and method of federal funding (e.g. DOE, NIST). Additionally, we must send team members out to recruit participation from other chemical companies.

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