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Verification and Validation of Encapsulation Flow Models in GOMA, Version 1.1

Rekha R. Rao, Lisa A. Mondy, P. Randall Schunk, Phillip A. Sackinger, and Douglas B. Adolf

Prepared by
Sandia National Laboratories
Albuquerque, New Mexico 87185 and Livermore, California 94550

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Verification and Validation of Encapsulation Flow Models in GOMA, Version 1.1

Rekha R. Rao, Lisa A. Mondy and P. Randall Schunk
Multiphase Transport Processes

Phillip A. Sackinger
Thermal/Fluid Computational Engineering Sciences

Douglas B. Adolf
Organic Materials Aging and Reliability

Sandia National Laboratories
P.O. Box 5800
Albuquerque, New Mexico 87185-0834

Abstract

Encapsulation is a common process used in manufacturing most non-nuclear components including: firing sets, neutron generators, trajectory sensing signal generators (TSSGs), arming, fusing and firing devices (AF&Fs), radars, programmers, connectors, and batteries. Encapsulation is used to contain high voltage, to mitigate stress and vibration and to protect against moisture. The purpose of the ASCI Encapsulation project is to develop a simulation capability that will allow us to aid in the encapsulation design process, especially for neutron generators.

The introduction of an encapsulant poses many problems because of the need to balance ease of processing and properties necessary to achieve the design benefits such as tailored encapsulant properties, optimized cure schedule and reduced failure rates. Encapsulants can fail through fracture or delamination as a result of cure shrinkage, thermally induced residual stresses, voids or incomplete component embedding and particle gradients. Manufacturing design requirements include 1) maintaining uniform composition of particles in order to maintain the desired thermal

coefficient of expansion (CTE) and density, 2) mitigating void formation during mold fill, 3) mitigating cure and thermally induced stresses during cure and cool down, and 4) eliminating delamination and fracture due to cure shrinkage/thermal strains. The first two require modeling of the fluid phase, and it is proposed to use the finite element code GOMA to accomplish this. The latter two require modeling of the solid state; however, ideally the effects of particle distribution would be included in the calculations, and thus initial conditions would be set from GOMA predictions. These models, once they are verified and validated, will be transitioned into the SIERRA framework and the ARIA code. This will facilitate exchange of data with the solid mechanics calculations in SIERRA/ADAGIO.

Changes in the encapsulation process design of the 4380 neutron generator, which is in production, must be minimal, in order to avoid delays in meeting production schedules. However, concern over the processibility of the encapsulant materials and the indications that voids were occurring have resulted in rather extensive changes to the process to date, and further changes based on sound scientific principles would not be arbitrarily ruled out. The primary driver for improved computational modeling capabilities is for the design of the upcoming 4531 neutron generator. In this generator, a completely new encapsulant material is being proposed, primarily in order to replace a carcinogenic curing agent with a more benign material. Because a new material is required, computational modeling could 1) help design the material itself, 2) aid in the design and optimization of the encapsulation process to be used with this new material, 3) determine the consequences of material and process changes and minimize any adverse effects, and 4) provide confidence in the material as it ages.

A "Phenomena Identification Ranking Table" (PIRT) that lists the physics models needed to understand the fluid phase phenomena in the encapsulation process has been developed. These models can be put into five major categories: 1) single-phase fluid flow 2) interface tracking/free surface flows 3) multiphase flows 4) energy transport 5) polymerization. The categories are then discussed in terms of the comprehensive physics models for encapsulation that are included within them. Categories 2 (free-surface flows including bubble dynamics) and 3 (multiphase flow including particle migration, sedimentation and degassing), are particularly poorly understood, thus work in model development is focused on these areas.

A verification plan for GOMA encapsulation models has been created. This includes a description of the code and its broad range of applications, the software engineering practices used in developing and maintaining the code as well as the quality assurance work that has be done to ensure that the code works as specified. The encapsulation models currently in GOMA that must be verified are a level set algorithm for mold filling and bubble dynamics (degassing), a suspension model for particle migration and settling simulations, heat transfer, and an epoxy curing model. As other models are added to span the needs defined in the PIRT, more verification work will be done. An automated regression test suite has been developed so that the code authors can check their work as they develop the code and ensure that the new features they have added have not disabled any existing feature. The verification problems that have been run with GOMA are discussed, including comparisons with analytical solutions, semi-analytical solutions and benchmarking against other codes. Extensions to the exisiting verification test suite are also discussed to exercise some other features of the encapsulation models in GOMA.

A validation plan for the encapsulation flow models in GOMA has been developed. These include experiments that address each key phenomenon listed as “high” importance in the PIRT. In cases where the adequacy of the model is currently questioned, steps to be taken in model development are addressed. The validation plan is separated into a four-tiered suite. Tier I studies are designed to explore the separable effects. Tier II are coupled effects. Tier III studies integrate many coupled effects. And Tier IV is a final “certification experimental campaign” to assess the readiness of the code for stockpile computing. In addition, we give a summary of the near-term validation simulations and experiments that we have planned along with a time line for future validation work.

Acknowledgment

The authors would like to thank the many individual who reviewed the document including Cecily Romero, Wahid Hermina and Justine Johannes. We would also like to thank our Peer Review Panel, which included Amalia Lopez, Tom Baer, Gary Froehlich and Chuck Harjes, for their many insightful comments. In addition, we would like to express our appreciation to Tim Trucano for providing guidelines and answering questions regarding the development of a Verification and Validation Plan and to Jaime Moya, Marty Pilch and the Verification and Validation Project who have graciously supported this work. Discussions as to format and content with Mary Mcwherter-Payne and Justine Johannes have been invaluable.

1. Stockpile Drivers and DP Customer Requirements

1.1 Introduction

Encapsulation is a common process used in manufacturing most non-nuclear components including: firing sets, neutron generators, trajectory sensing signal generators (TSSGs), arming firing and fusing devices (AF&Fs), radars, programmers, connectors, and batteries. Encapsulation is used to contain high voltage, to mitigate stress and vibration and to protect against moisture. The purpose of the ASCI Encapsulation project is to develop a simulation capability that will allow us to aid in the encapsulation design process, especially for neutron generators.

Many encapsulants are a mixture of particles in epoxy resins. The particles are used to tailor encapsulant properties to meet performance requirements such as matching thermal expansion coefficients between the encapsulant and component and minimizing residual stresses resulting from encapsulant cure.

Encapsulation is a complex process involving the flow of material around the component in the fluid phase and the phase change of the encapsulant due to polymerization chemical reactions. When designing an encapsulation process for a neutron generator, or other high voltage devices, the component designers aim to achieve several qualities. First, they would to have an efficient delivery of the encapsulant into the mold, with complete embedding of the component and no voids, air pockets or knit lines. This implies that the encapsulant must have adequate processibility, e.g. the viscosity is low enough to allow the mixture to flow but still high enough to keep the particles in suspension. Also, since the epoxy constituent is polymerizing, the pot life of the encapsulant needs to be long enough to allow embedding of the component without significant curing.

Second, component designers would like to have homogeneous properties of the encapsulant so that there are not significant variations in material properties such as coefficient of thermal expansion and density, that are important to the performance of the neutron generator. This is complicated by the fact that the encapsulants are composite materials blending epoxy and particles, e.g. Epon/ALOX and Epon/GMB. This implies that the concentration of particles should be the same everywhere surrounding the component and also that we do not have macroscopic variations in concentrations from one component to the next. Also, since we are using two different encapsulants we want to control the mixing of the materials and also minimize splashing of one encapsulant into the domain of the other.

Third, the encapsulant process should not greatly increase the length of time it takes to produce a component. An efficient cure schedule is crucial, since the encapsulant oven cure is often the bottleneck in the manufacturing process. Also important in the cure is that the properties stay within specification in that again you want to maintain homogeneous properties and also avoid the growth of small bubbles into large voids.

Because of the complexity of the processes, predictive models for the mold filling, curing and cool down processes associated with encapsulation are required to ensure that the encapsulant meets performance requirements and that the process is efficient. Validated computational models are needed to aid in design of encapsulation processes to reduce manufacturing defects such as voids from incomplete mold filling and fractures resulting from residual stresses that can lead to failure. Models are needed to optimize the cure schedules used in order to speed production without degrading component performance. Furthermore, predictive models are needed to provide information on the effect of design changes proposed for other reasons (such as producing less toxic encapsulants by replacing the "Z" material). Finally, validated encapsulation models are also needed to determine the initial geometry and stress state for performance and aging simulations.

The proposed computational capabilities will move us into the new era where "Virtual Prototyping" replaces the lengthy and expensive build-test cycles currently in place. These models are difficult to develop, both to capture the correct physics and to efficiently solve the resulting equations. At each phase of the flow simulations, we must compare the results with experimental data to make sure that our models correctly represent the physics of the encapsulation process. The requirements that must be met are discussed in more detail in the following section.

1.2 Programmatic Requirements

1.2.1 Verification and Validation Plan Process Overview

Figure 1.1 summarizes the process used to develop the Verification and Validation Plan. We based our plan on the "Guidelines for Sandia ASCI Verification and Validation Plans - Content and Format: Version 2.0" [Pilch et al., 2001] and followed its guidance as to format and content. First we identified our stockpile driver for encapsulation, which in our case is neutron generator manufacturing (MC4380, MC4531). We translated this driver into a set of stockpile requirements for our computational modeling work. The stockpile drivers and requirements are given in Section 1 of this document. We want to 1) reduce defects 2) optimize the manufacturing process 3) utilize modeling and simulation to perform "virtual prototyping" and 4) provide initial conditions for solid mechanics and performance and aging calculations. Ties from the phenomenology to these four issues are given in the "phenomena identification ranking table" (PIRT) and discussed in Section 2. Section 3 discusses the software engineering practices used to produce the GOMA code and current and future verification activities including the process and metrics. Section 4 is devoted to the validation plan and links PIRT driven experiments to a four-tiered validation test suite. Some of the issues discussed are calibration versus validation, prioritization, process and metrics. Available documentation trees are also given for experimental activities. The software engineering, verification and validation activities all lead into our guidance for stockpile computing, which is discussed in Section 5. Here we give both process and technical guidance on how to carry out a high consequence calculation.

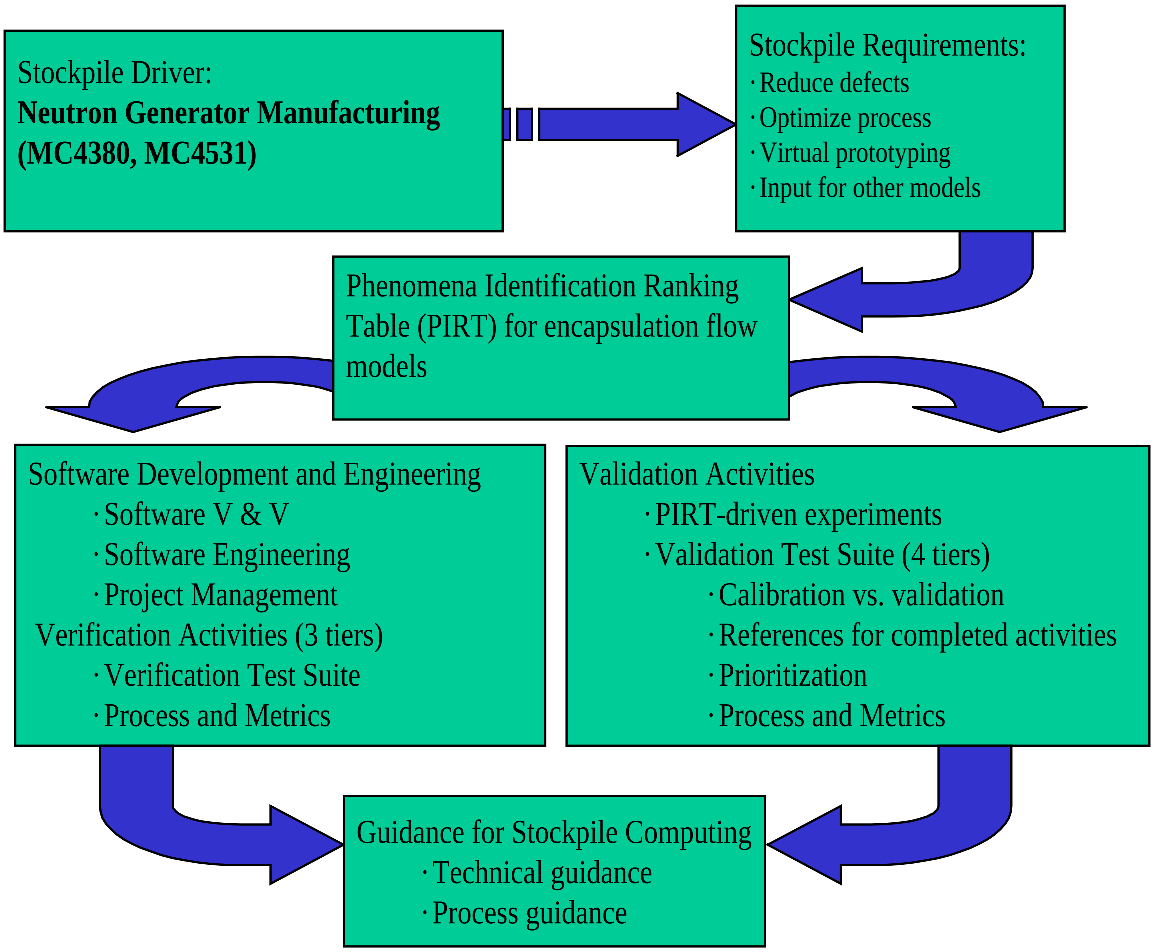

Figure 1.1: Verification and Validation Process Overview

1.2.2 Verification and Validation Plan Owners and Authors

Rekha Rao (9114) is the plan and process owner and has taken the lead in updating the plan and maintaining the documentation. She is the principal investigator (PI) on the ASCI Encapsulation and does code development and analysis in support of that project. The ASCI Encapsulation team is comprised of Doug Adolf (1811), Eric Lindgren (6131), Rekha Rao, Lisa Mondy (9114), Tom Baer (9114), David Lo (9123), Steve Burchett (9126) and Bob Chambers (9123). Lisa Mondy (9114) is the plan and process co-owner and has taken the lead in determining and documenting our experimental needs. She is the PI on the MAVEN Encapsulation Flow Models project and primarily and experimentalist and analyst. The MAVEN Team is comprised of Lisa Mondy, Doug Adolf, Bob Lagasse (1811), Tim O'Hern (9112) and Howard Arris (14172). Doug Adolf is our reality check from the Neutron Generator Production Team (Barbara Wells (14405), Howard Arris (14172), Todd Haverlock (2561), Doyle Morgan (2561), Matt Donelly (14172), Manny Trujillo (14402), Mark Stavig, Jeff Keck, Steve Montgomery, Doug Adolf, Steve Burchett, Rekha Rao, Lisa Mondy). Doug Adolf is an experimentalist and theoretician from the material science center, but has been working on encapsulation production issues for more than ten years. Randy Schunk (9114) and Phil Sackinger (9141) are primary code developers for GOMA and responsible for much of the existing software quality assurance. Auxiliary support for the plan and reference material were provided by three different teams: ASCI Encapsulation, MAVEN Encapsulation and the GOMA Code Team (Phil Sackinger, Randy Schunk, Tom Baer, Rekha Rao, David Noble (9113), Duane Labreche (9114), Harry Moffat (9114), Matt Hopkins (9117), Sam Subia (9141)).

1.3 Customer Drivers and Requirements

1.3.1 Customer Base

Encapsulation is a common process used in manufacturing most non-nuclear components including: firing sets, neutron generators, trajectory sensing signal generators (TSSGs), AF&Fs, radars, programmers, connectors, and batteries. Each of these components have short and long term weapons systems drivers for development of predictive simulation tools. This Verification and Validation plan is mainly focused on the neutron generator encapsulants. As such, our primary customer is the Sandia neutron generator production team.

1.3.2 Critical Applications

Two general classes of encapsulants are used for DP components: 1) particle-filled epoxy resins consisting of high (40-60%) volume fraction alumina particles or glass micro-balloons, and 2) polyurethane foams. This work will focus primarily on particle-filled epoxy resins, since these so called "hard encapsulants" are more critical to the performance of the components that they embed. Encapsulation is used to contain high voltage, mitigate stress and vibration and to protect against moisture. The particles in the epoxy resins are used to tailor encapsulant properties to meet performance requirements such as matching thermal expansion coefficients between the encapsulant and component and minimizing residual stresses resulting from encapsulant cure. These requirements of the encapsulant are truly critical to the integrity of the neutron generator function.

The introduction of an encapsulant poses many problems because of the need to balance ease of processing and properties necessary to achieve the design benefits described above. Allied Signal/Federal Manufacturing &Technology reports that encapsulation defects are the second leading cause of quality inspection findings for the Firing Set Production Area. Encapsulants can fail through fracture or delamination as a result of cure shrinkage, thermally induced residual stresses, voids or incomplete component embedding and particle gradients. Manufacturing design requirements include 1) maintaining uniform composition of particles in order to maintain the desired thermal coefficient of expansion (CTE), 2) mitigating void formation during mold fill, 3) mitigating cure and thermally induced stresses during cure and cool down, and 4) eliminating delamination and fracture due to cure shrinkage/thermal strains. The first two require modeling of the fluid phase, and it is proposed to use the finite element code GOMA to accomplish this. The latter two require modeling of the solid state; however, ideally the effects of particle distribution would be included in the calculations, and thus initial conditions would be set from GOMA predictions. As the encapsulation models are transitioned into the SIERRA framework, code to code interactions will be facilitated for fluid, solid and performance calculations.

Besides the need for modeling to help design the process to reduce defects, the process also needs to be optimized to produce quality products efficiently. The encapsulation process is often the “bottleneck” in production schedules. Optimization can only be achieved with accurate models, as will be discussed more in *Impact*.

There are several specific categories of predictions that are needed. First, the modeling would be used to design appropriate encapsulant materials. This would entail both designing “from the ground up” a new encapsulant to meet a specific performance requirement while maintaining processibility or modifying existing materials to improve performance or processibility. In conjunction with this, modeling is needed to predict the minimum in viscosity for optimal processibility. For example, the epoxy goes through a maximum temperature because of the exothermic reaction taking place. This maximum in temperature is usually near the minimum viscosity (although with polymerization taking place this is not necessarily true). When to pour and how long to degas is related to the dependence of the viscosity on temperature, degree of cure, etc. If process changes are needed to improve the degassing or pouring steps, or because of the behavior of a new material, modeling would provide input into the feasibility of redesigned manufacturing processes.

In the pouring step, predictions are needed of the extent of mold filling completion. In other words, the designer needs to be able to predict if unfilled regions due to flow hydrodynamics and knit line dynamics exist. Similarly, one needs to predict the location of microscopic bubble nucleation sites that will grow into voids upon degassing. These types of predictions will help optimize process design and design of the encapsulant distribution system.

Most neutron generator designs specify the use of two encapsulants. Mixing of the two is feared to degrade the performance of both, as they are designed specifically to have very different properties. Models are needed to predict mixing at the interface between the two encapsulants (currently glass microballoons (GMB)/Epon and alumina (Alox)/Epon) in different processing scenarios as part of the process design.

A very important part of the process design is the cure schedule. Predictions in the fluid phase specifically are needed to optimize cure schedule with regards to bubble degassing and particle flotation. These calculations are needed in conjunction with solid phase calculations to minimize residual stresses. The results of the fluid phase calculations ideally would be used as initial conditions for solid mechanics simulations; particle concentration, temperature and extent of cure.

1.3.3 Schedule

Changes in the encapsulation process design of the current neutron generator being produced (the 4380) must be minimal, in order to avoid delays in meeting production schedules. However, concern over the processibility of the encapsulant materials and the indications that voids were occurring have resulted in rather extensive changes to the process to date, and further changes based on sound scientific principles would not be arbitrarily ruled out. The primary driver for improved computational modeling capabilities, however, is for the design of the upcoming 4531 neutron generator. In this generator, a completely new encapsulant material is being proposed, primarily in order to replace a carcinogenic curing agent with a more benign material. Because a new material is required, computational modeling could 1) help design the material itself, 2) aid in the design and optimization of the encapsulation process to be used with this new material, and 3) determine the consequences of material and process changes and minimize any adverse effects. The 4531 is currently scheduled to start production in 2009. Obviously, the material and process design must be finalized before that date to allow time for the production of the necessary materials and tooling. Because of the technical challenges involved in computationally modeling the complex encapsulation process, work must continue at least at the current pace in order to be able to positively impact this design.

1.3.4 Impact of Software

Designing a good encapsulation process is essentially an optimization problem where competing physical effects must be traded off: for instance, a cure schedule designed to reduce thermal stresses may cause large gradients in the particle concentration, so these two effects must be balanced with the cost function taking into account both of these phenomena.

Traditionally, encapsulation processes have been “seat-of-the-pants” designs with as much guesswork as science involved. Because of the complexities of the multiple phenomena involved, this has been the necessary procedure to date. When a material or process worked, any changes to the procedure would be highly discouraged. This is the logical consequence of the chaotic physical processes involved, in which small changes to initial conditions result in large variations later. It is not clear whether or not we are working near a “cliff” in the operability window, in which changing one parameter can lead to a nonperforming neutron generator. Encapsulation is the last stage of the component build, so errors in encapsulation are very expensive since all the subcomponents are lost as well.

However, without adequate knowledge of the physics and the ability to model such nonlinear systems, no optimization can take place. Up to this point the cost function has been estimated by hand; for example, as the approximate difference between the standard oven cure schedule for the neutron generator and a new proposed cure schedule. The goal of the ASCI Encapsulation work is to automate the optimization process using multiple realizations of the full three-dimensional model from mold filling to cure.

Although the ability to optimize existing processes is the more immediate problem, perhaps the most impact will be gained with the ability to design, from the ground up, a new process that is required because of some other design change (for example, miniaturization of a component, or, as in the case of the 4531, concern over safety and health issues.) In this case, because no fundamental understanding of the processes has been developed and no modeling has been possible, extensive testing at every step of the design is required currently.

For production neutron generators a number of tests are routinely performed. These include X-ray (to determine voids), X-ray microscopy (to check voids and particle gradients), single element tests and full generator tests. It is very difficult to get the production engineers to provide neutron generators for testing, since this decreases their yield and they each cost upwards of $60k. Validated predictive modeling could replace these tests with much more cost efficient simulations.

1.3.5 Technical Risks

In trying to develop models that can accurately predict the flow and particle migration in filled epoxy suspensions, many complexities arise. First, the epoxies themselves are curing, thereby transitioning from the fluid state to the solid state. This requires knowledge of the kinetics of reaction that must be found via experiments. These kinetics must then be incorporated into a model for the entire suspension, which is then added to GOMA and validated with more experimental data.

The second complexity is the behavior of the particles in the epoxy. The particles have a significant effect, changing the fluid behavior from fluid-like in some regions to solid-like in others. Though we have a relatively good grasp of what the behavior might be for monomodal suspensions, ones which have particles all the same size, for the real suspensions in our encapsulant materials, we must try to simulate the effects of systems of particles that have a broad range of sizes, shapes and densities. These polydispersities are difficult to represent in a model suitable for implementation in a finite element code. Even to get data to allow us to produce such a model requires numerous experiments in the lab, as well as numerical experiments with our particle level boundary element code.

The third complexity arises because the current suspension model is poorly conditioned numerically and difficult to integrate. For example, particle settling terms make the equations hyperbolic, necessitating the use of the specialty methods, and often leading to numerical instabilities that grow in time.

The fourth complexity involves the difficulty in modeling mold filling operations even for simple fluids. The process requires tracking of a fluid interface whose location is unknown a priori. Therefore, these free and moving boundary problems require knowledge of the pertinent physics and special numerical methods to do so. Furthermore, the mold filling operations used in the manufacture of neutron generators require that one liquid encapsulant be poured on top of another, yet the lower encapsulant may not touch the components in the upper section. This adds the fifth complexity in that one must minimize splashing and mixing of two suspensions: processes that are poorly understood at present.

Finally, the sixth complexity is the need to predict degassing operations -- essentially three-phase flow and, again, beyond current modeling capabilities. Yet this three-phase flow may determine whether or not residual voids are left in the final product, and voids are thought to be the most likely source of dielectric breakdown and neutron generator failure caused by the encapsulant. These six submodels will be discussed again in the section “Identifying Key Phenomena”.

1.3.6 Accuracy Required

Absolute accuracy is not required in order to have positive effects in the design and optimization of neutron generator encapsulation. Trends in results can be used to compare the benefits of one material or cure schedule over another, without the absolute time scales or material properties being known. However, because the physics include chaotic systems, these results would have to be used with caution to avoid misguided interpretation of trends in the computational results.

However, if the details of the encapsulation process design for any new neutron generator (or other weapon component) becomes highly dependent on computational modeling due to a shortage of development time or funding, the consequences of erroneous results could be very serious. For example, the resulting process could be too difficult to perform (e.g. the encapsulant does not flow properly into the mold and around the components). To correct problems empirically would necessarily require a delay in production schedule to redesign, retool, retrain personnel and retry. Furthermore, if the process appears to work, but the particles become segregated or undetectable voids form, the neutron generator would likely fail to perform.

1.3.7 Computer Platforms

The goal of the ASCI Encapsulation work is to automate the optimization process using multiple realizations of the full three-dimensional model from mold filling to cure. The detailed three-dimensional models themselves will necessitate the use of Tflop computing with large amounts of data storage; for true optimization, the next generation of computers will be required.

1.3.8 Immediate Users

Using the software may require experts in the physical phenomena being described and in the numerical methods necessary to reach an accurate converged solution. We foresee that the Engineering Sciences Center will continue to supply this expertise. However, GOMA has almost 60 users at the Lab and in industry who range in expertise from undergraduate students to metallurgist, so it is possible to train staff who are not familiar with numerical analysis and fluid dynamics to obtain useful information from the code. Template problems with easy to use front ends can be setup for use by encapsulation designers and manufacturing technicians. We foresee these templates as the next stage in the development of the code.

2. Phenomena Identification Ranking Table (PIRT)

2.1 Process for PIRT Development

At the onset of the Encapsulation Project, we spent time determining the most relevant phenomena needed for modeling the encapsulation process by a process of brainstorming with the MAVEN Encapsulation Flow Models Team, the ASCI Encapsulation Team and the Neutron Generator Encapsulation Production Team. From these brainstorming sessions, we developed a broad list of important of the physics that needed to be included in our modeling effort. From the general list, Lisa Mondy and Rekha Rao developed more detailed information specific subcategories that could be used to guide the fluid phase modeling.

Once the phenomena had been determined, the necessity of the models with regards to four major categories was evaluated: reduction of defects, process optimization, virtual prototyping and initial conditions for stress/performance/aging calculations. Expert judgement was used in the evaluation process. The main physical issues associated with each of these categories is given in bullet form below.

Reduce Defects

- Maintaining uniform composition of particles (coefficient of thermal expansion, density, dielectric properties, etc.)
- Mitigating void formation during mold fill
- Mitigating cure and thermally induced stresses
- Eliminating delamination/fracture

Optimize process

- Minimize cure schedule
- Maximize processibility

Virtual prototyping

- Tailor encapsulant properties
- Reduce build/test cycles

Initial conditions for stress/performance/aging calculations

- Particle concentration
- Extent of reaction
- Thermal history

Finally the adequacy of the model was determined based on previous validation efforts.

2.2 Identifying Key Phenomena

Table 1 provides a first approximation to a bottom-up review of the phenomenological models for the encapsulation flow models. The importance of the main physical phenomena to the four main goals of the modeling are listed. The adequacy of the current models are then estimated. When the model exists and is deemed acceptable for predictive modeling it is marked with an “A” for “adequate.” In many cases (marked with a question mark) parameter studies are required to determine quantitatively the current model adequacy. In some cases, the model is nonexistent or only partially exists (marked with an “I” for “inadequate”)

Phenomena	Importance to:				Ade quac y
	Reduce defects	Optimize processes	Virtual Prototyping	Defining initial state for performance/ aging models	
Fluid Flow/ Momentum Transport					
A. Fluid Flow of single-phase liquid	Medium	Low	Medium	Low	A
B. Gas/fluid interface tracking	High	High	High	High	I
B.-1 Mold Filling	High	High	High	High	I
B-1a Single fluid phase	High	High	High	High	A
B-1b Multiple fluid phases	High	High	High	High	I
B-2 Multiple Interfaces/ Bubble dynamics in single liquid phase	High	High	High	High	I
B-2a Isolated bubble nucleation	High	High	High	High	I
B-2b Single bubble growth & transport through single fluid phase	Medium	Medium	Medium	Medium	A
C. Multiphase flow	High	High	High	High	I
C-1 Particle Dynamics	High	High	High	High	I
C-1a. Particle hydrodynamic interactions/migration	High	High	High	High	I

Phenomena	Importance to:				Adequacy
	Reduce defects	Optimize processes	Virtual Prototyping	Defining initial state for performance/ aging models	
C-1b Particle nonhydrodynamic interactions	Low (GMB) to Medium (Alox)	Low (GMB) to Medium (Alox)	Low (GMB) to Medium (Alox)	Low (GMB) to High (Alox)	I
C-1c Particle sedimentation	High	High	High	High	I
C-1d Solid/fluid interface physics/chemistry	Low to Medium	Low to Medium	Medium	Medium	I
C-2. Bubble/particle interactions (3-phase flow)	High	High	High	High	I
C -3. 2-Fluid mixing	Medium	Medium	Medium	High	I
C-3a. Mixing of 2 single-phase fluids	Low	Medium	Medium	Medium	I
C-3b. Mixing of 2 suspensions	Medium	Medium	Medium	High	I
C-3c. Mixing of 2 suspensions with air entrapment	Medium	Medium	Medium	High	I
Energy Balance					
D. Energy transport	Medium	High	Medium	Medium	A
E. Energy production / chemical reactions	Medium	High	Medium	Medium	I
Coupled Energy/Momentum	Medium	High	Medium	Medium	I
F. Epoxy/curative rheology	High	High	High	High	I

Phenomena	Importance to:				Ade quac y
	Reduce defects	Optimize processes	Virtual Prototyping	Defining initial state for performance/ aging models	
G. Extent of reaction (uniformity of cure)	High	High	High	High	I

2.3 Explanation of PIRT

2.3.1 Fluid Flow

A. Fluid flow of a single phase liquid

The equations of momentum conservation and continuity are well known for single phase fluids. The adequacy of the model for generalized Newtonian fluids is well documented in the literature, and validation in simple flow geometries is not thought necessary at this time.

B. Gas/fluid interface tracking

Any time more than one phase is involved, the models are less likely to be adequate for a complex application. This is a high priority issue since incomplete embedding of components (mold filling) and bubble nucleation and growth (bubble dynamics) can lead to fracture during thermal cycling and performance failure.

B-1. Mold filling

Tracking of a single interface during mold filling is in general a far more tractable problem than tracking multiple interfaces. Although the PIRT lists this phenomenon overall as “inadequate”, this black or white rendition of needs in the PIRT does not allow the shades of gray that actually exist.

B-1a. Single fluid phase

Tracking of a single gas/liquid interface is probably achieved well with GOMA, as documented in other applications such as found in coating flows. Nevertheless, the mold filling simulation tool available in GOMA needs to be made more robust for gas phase representation. Three dimensional simulations of the neutron generator geometry will be required, which in turn requires expensive parallel computations. Validation exercises will be useful.

B-1b. Multiple fluid phases

Tracking the interface between two liquids with comparable viscosities will require some model development. The model for relatively slow, uniform filling will probably be adequate with a minimum of development time. However, not so straightforward is the development of a model to describe the mixing of one fluid layer into another, as occurs in neutron generator encapsulation when one encapsulant is injected on top of another already in place. This phenomena is listed separately as C-3.

B-2. Multiple interfaces/bubble dynamics in a single liquid phase

Although much literature exists for the dynamics of single bubbles in a liquid, detailed models require extensive computations. Some model development will be required to modify the existing boundary element model (BEM) to simulate deforming gas bubbles. The approximations necessary to do this will need to be compared with more exact models. Multiple, interacting bubbles are listed separately as C-2.

B-2a. Isolated bubble nucleation

This is still a very active research area. Depending on the application, models can range from adequate to nonexistent. Experiments are needed to determine the type of nucleation (homogeneous vs. film) and the type of gas involved (entrapped air vs. encapsulant vaporization) dominating the encapsulation degassing process. The probability of bubble nucleation with processing conditions and temporal and spatial location must be determined.

B-2b. Single bubble growth & transport through a single liquid phase

In general, this topic is better understood than nucleation. However, as mentioned above, the complexity of the physics will cause some model development to be necessary in order to render the problem tractable, *e.g.* interfacial mass transfer, compressibility, etc.

2.3.2 Multiphase Flow

C. Multiphase flow

Multiphase fluid flow is another high priority area because inhomogeneities in particle concentration due to migration and settling can lead to poor shock wave propagation, dielectric breakdown and CTE mismatch. All of these issues can lead to failure.

C-1. Particle dynamics

Although in principle the equations of motion can be written for any system, the multiple interfaces involved in particle or bubble flows render the combined simulation impractical. Recently developed BEM models are capable of solving the creeping flow equations for on the order of 1000 particles. Even here, some approximations are required when the particles are very close to each other. At the particle concentrations used in encapsulants, extremely close contact is inevitable. Nonhydrodynamic effects can also become important at very close contact even for relatively large particles (>10 microns) that are usual in encapsulants. Some encapsulants commonly used at

Sandia, most notably those with the standard alumina powder, do have particles whose rheology is dominated by the "fines" or the smaller particles of the size distribution. In these encapsulants, nonhydrodynamic effects are extremely important.

In all systems, there are so many particles that BEM techniques cannot be used to describe the actual process application. These simulations instead can be used on a representative volume of suspension in order to better understand the overall effect of multiple particle interactions. In order to model applications such as encapsulation, continuum approximations are needed. These approximations would attempt to describe the relevant physics in terms that are easier to solve numerically in a Navier-Stokes solver such as GOMA.

Because both interacting particles and bubbles are present in most encapsulants, and because modeling of all aspects of the encapsulation process requires constitutive formulations for the materials involved, validating these equations has in the past, and is expected to be in the future, one of the primary validation tasks needed.

C-1a. Particle hydrodynamic interactions/migration

The first two-phase constitutive equation to be tested in the encapsulation model is based on coupling conservation of mass and momentum for the fluid with an additional advection-diffusion equation which describes the evolution of the particle concentration field [Leighton and Acrivos 1987, Phillips et al. 1992]. The concentration equation is coupled to the momentum equation through a concentration-dependent viscosity. This constitutive model was validated earlier for suspensions of relatively large (>100 microns), uniformly sized, neutrally buoyant spheres in viscous Newtonian liquids, in which the particles interact primarily through hydrodynamic forces [Subia et al. 1998]. For more complex suspensions the equation set must be modified to allow for effects of differences in particle size, shape, and density, as well as any additional particle interaction forces (e.g. colloidal, electrostatic).

The constituent equation used to model encapsulant flow with the computational code GOMA requires at least three empirically derived coefficients to describe the rheology of a suspension. Quiescent settling experiments can be used to determine the hindered settling function, which is one of the three coefficients and a function of particle concentration.

Ideally, we would determine the shear-induced migration terms (the other two empirical coefficients) from a flow experiment with neutrally buoyant particles. However, for the very heavy Alox and the very light GMB, fluids with matching densities do not exist. We can only measure the total particle migration in one geometry (under multiple conditions), assume the form of the hindered settling function, fit the remaining two coefficients to the data, and then perform validation experiments in another flow field. Both GMB and Alox suspensions were tested in a wide-gap Couette (counter-rotating concentric cylinders) device and sheared at one of two constant rates (the center shaft turning at either 52 or 26 rpm and the outer cylinder held constant). Although in a quiescent suspension, settling of the Alox (or the floating of the GMB) is almost immediately evident, the shear-induced migration competes with buoyancy effects, so that the formation of a clear zone at the top (or bottom) only occurs at lower rotation rates.

With these data, combined with data for well characterized, monodisperse, “ideal” suspensions collected in more fundamental programs [Abbott et al. 1991, Tetlow et al. 1998], it is expected that we will be able to extract the necessary model coefficients. However, the “ideal” suspensions were of much larger particles relative to the flow gap, and may not be representative of the small-sized powders used in encapsulants. Furthermore, the earlier data show disturbing trends in that the effect of particle size on the diffusion coefficients does not scale as the particle size squared (assumed in the model) and is not independent of the concentration of particles. This may be an indication that the particles used were too large. Ideally, more data would be collected with representative sizes in neutrally buoyant suspending fluids and with settling particles such as the more uniform AA-5 and AA-18 alumina powders. The effects of polydispersity of the standard alumina would then also become more evident. Other results may be required at different rotation rates, as well.

Another constitutive equation that has recently shown good results is the suspension balance model [Nott and Brady, 1994]. Although similar to the diffusive flux model, here two momentum equations are solved, one for the particle phase and one for the suspension phase as a whole. In some versions, and additional equation analogous to an energy equation is also solved. The “energy” equation attempts to account for the finite effects of the ratio of particle size to characteristic flow diameter. These are fluctuations in the local velocity with respect to the average velocity, something that has been seen in suspensions [Segre et al., 2001]. However, the equation also adds four adjustable parameters determined through experimental data, and therefore, requires additional data. Some data, for example the value of the fluctuations of particle velocity at or near walls, is difficult at best to obtain, although BEM simulations may aid in developing reasonable approximations.

Both the suspension balance model and the diffusive flux equation require additional terms in curvilinear flows. Because mold filling involves flow around embedded objects and complex geometries, it is likely that the models as published to date will be inadequate for this application. The most promising method to account for multidirectional flow effects is to determine the full stress tensor for the principle directions of flow and then use a transformation matrix to write the flow at each nodal point in terms of the principle directions [Morris and Boulay, 1999, Fang et al., 2001]. (It is thought that the normal stresses evolving due to particle interactions become very important in nonviscometric flows.) Although in some flow fields this can only be accomplished approximately, preliminary comparisons with data show promise. More model development is needed and more data is needed for multidimensional flows.

C-1b. Particle nonhydrodynamic interactions

Developing boundary element techniques can handle complex geometries and concentrated systems; however, as two surfaces approach, the model breaks down due to lack of knowledge at the molecular scale. In addition, while classical molecular mechanics techniques can probe greater size dimensions with the latest computers and algorithms, reproducing continuum level phenomena is not regularly possible. In order to bridge the region between hydrodynamically dominated systems (typically particles > 10 microns) and phenomena controlled at the molecular level, one could apply Density Functional Theory and molecular dynamics to modify state-of-the-art boundary element methods to resolve appropriate boundary conditions and, in particular, the singularity occurring when two surfaces become close. Surface interactions need to be determined for different continuous phases, where ionic and Coulombic attractions can dominate and lead to agglomeration of particles. This is a research topic that has to date been unexplored, since this has been deemed a low priority area.

C-1c. Particle sedimentation

When particles settle en masse, fluid flows back through the particles slowing the settling rate. The amount of velocity retardation that occurs is highly dependent on the concentration of particles and also on the particle shape and size distribution. Settling of uniform spheres is well documented in the literature and an expression, albeit empirical, is available to describe the sedimentation velocity as a function of concentration. The effects of polydispersity (in both size and density) is less well known, but is likely to be important in encapsulation. The settling rate, in part, determines the cure schedule and is, therefore, very important to model accurately. Validation studies on actual encapsulation systems are required.

C-1d. Solid/fluid interface physics/chemistry

All multiphase phenomena discussed here can be affected by the surface chemistry of the particles interacting with the epoxy suspending fluid. Preliminary studies of particles with various surface coatings have shown a marked effect on the suspension rheology. In an ideal world, all validation studies would be repeated with various surface coatings. The new 459 encapsulant has shown marked non-Newtonian rheology that occurs through interactions between particle surfaces and the curing agent. This gives the appearance of particles in a shear-thinning suspending fluid.

C-2. Bubble/particle interactions

Further complications to particle sedimentation occur during degassing. Here, interaction with rising bubbles may greatly slow the sedimentation of heavy particles (desirable) or greatly increase the separation of light particles such as glass microballoons (undesirable). However, there is empirical evidence that the separation of mixtures of light (bubbles) and heavy (alumina) particles can actually be enhanced when the two species form preferential lanes in which to flow, leading to a much more rapid particle sedimentation [Altobelli and Mondy, 2001]. Phenomenological discovery studies and later validation experimental studies are clearly needed.

C-3. 2-Fluid mixing

This is presently a hole in the process of validating encapsulation processes. Until recent changes to the neutron generator mold filling process (in large part caused by recent MAVEN sponsored flow visualization studies), this was of little concern because one fluid was poured (with a gently gravity feed) on top of the other. However, the current process calls for one fluid to be injected (under pressure) across the top surface of another. Furthermore, because of performance concerns, it is desired that none of the lower encapsulant splash onto components to be surrounded by the upper encapsulant.

C-3a. Mixing of 2 single-phase fluids

Although difficult, the mixing of two Newtonian fluids is in theory possible to model. Nevertheless, the complexity of the phenomena would require validation to gain added confidence in the model.

C-3b. Mixing of 2 suspensions

The mixing of two suspensions, as actually occurs in the neutron generator encapsulation process is extremely difficult to model. The first requirement is that well validated constitutive equations exist; therefore, this topic must be deferred to later in the program. However, limited experimental data exist that shows enhanced mixing occurs with suspensions. In other words, modeling with idealized Newtonian fluids may not give results even close to the actual behavior of suspensions.

C-3c. Mixing of 2 suspensions with air entrapment

If the above is difficult, the modeling of the actual mixing of two suspensions in other than a vacuum may be intractable for many years yet. Again, here not only must the rheological behavior of two suspensions be well known and the osmotic forces between particles, but the interaction of bubbles must also be well described.

2.3.3 Energy transport

D. Energy transport

The equations of energy conservation are well known for single phase fluids. The adequacy of the model for generalized Newtonian fluids is well documented in the literature, and validation in simple flow geometries is not thought necessary at this time. However, the properties of multiphase fluids are not known, although approximations based on local volume fraction are the likely form. Validation studies to confirm the assumed properties will be necessary. Viscous heating is also likely to be affected by the fact that two or more phases are present.

2.3.4 Energy production/chemical reactions

E. Energy production/chemical reactions

The reaction kinetics of the epoxy polymerization must be determined experimentally, as well as any effects of the presence of particles and bubbles. This is intimately coupled to the properties of the encapsulant and the concentration of particles as described in the following section. The effects of bubbles during degassing (which happens early in the cure process) are presently unknown and may need to be added to the experimental procedures described in the following section.

2.3.5 Epoxy/Curative Rheology and Extent of Reaction

F. Epoxy/Curative Rheology and G. Extent of reaction

Determination of a particular encapsulant's rheology requires rheometric measurements of encapsulant rheology over time and at several constant temperatures. This liquid characterization is non-trivial due to the numerous dependencies we need to investigate. For example, processing typically occurs from temperatures of 65 to 95^{o}C over which the viscosity can change by a factor of 7. The curing reaction is exothermic, so even higher temperatures can be reached without careful processing. More dramatic, however, is the dependence on state of cure, since at the gel point, the viscosity becomes essentially infinite. A SAND report [Adolf, Stommen, and Johnson, 1997a] documents the extensive testing done on a currently used encapsulant material, Epon 828 (or Epon 826) cured with either diethanolamine (DEA) or Shell Curing Agent "Z", both alone and filled with a rubber toughening agent CTBN. This report describes formalisms that capture these dependencies. This model has been implemented into GOMA.

Similar testing done on the 459 encapsulant has also been published [Adolf, 1999, Mondy et al., 1999]. Dramatic changes are seen in the viscosity during processing due to polymerization and thermal effects. Because Sandia only uses filled epoxies, the dependence of viscosity upon filler fraction is also required. Therefore, bulk rheology measurements are also needed on encapsulant materials filled with particles, such as GMB, Alox, or β-eucryptite (β-eu) at various solid loadings, including the exceptionally high loadings that may be seen in regions affected by gravitational settling of the particles. The dependence on filler fraction is also dramatic. The addition of 45 volume per cent alumina can increase the viscosity by a factor of 70 and even induce non-Newtonian behavior. Because neither type of particle stays well mixed in suspension, the dependence across a range of volume fractions must be determined. The rheological models developed in the SAND report mentioned above are dependent on a number of thermophysical properties. Parameters for the model outlined in the SAND report are listed in that document for the 459 encapsulant, both particle filled and unfilled. The filler affects more than the individual values of these parameters, because the properties are actually dependent on the filler fraction, local variations in properties can exist if local variations in the filler fraction exist. This is the subject of an earlier subsection.

3. Verification Plan

3.1 Software Verification Requirements

Software verification requirements are easily derivable from two sources: the PIRT for encapsulation (see previous Section) and the 5-Year Plan [Rao et al., 2000]. The PIRT clearly defines the types of mathematical models that need to be verified and the 5-Year Plan gives the schedule for when these models must be verified. Not all models described in the PIRT currently exist in GOMA, *i.e.* we cannot currently perform degassing simulations using the code. The focus of this verification plan will be on verifying the models that are currently extant in GOMA, models which we rely upon to perform weapon component simulations. These include the fluid mechanics/interface tracking (PIRT elements A, B-1, B-2b), suspension migration and settling (PIRT elements C-1a, C2c, C3a, G), energy transport (PIRT elements D, E) and the epoxy curing/curative rheology (PIRT element F, G). The suspension and curing models all take advantage of the mass transport algorithms in GOMA. In particular, one of the key deliverables for FY 2000 was to simulate epoxy cure and settling in a MC4531 geometry, thus for last year we focused on verifying the epoxy curing and settling models. As new models are added to GOMA from the PIRT, the verification plan will also be modified accordingly. PIRT elements that currently do not exist as models in GOMA or only exist in a rudimentary form include bubble nucleation (B-2a), particle nonhydrodynamic interactions (C-1b), solid/fluid interfacial chemistry/physics (C-1d), bubble/particle interactions (C-2) and two suspension mixing (C-3b, C-3c).

3.2 Software Development Process Description (SQA&SE)

3.2.1 Software Development Process

3.2.1.1 Requirements Management

The requirements for the software are laid out in the encapsulation PIRT detailed in section 2. These requirements will be managed using the Encapsulation V&V Plan in conjunction with the 5-Year Plan.

3.2.1.2 Project Planning

In FY98, considerable effort went into constructing a 5-Year Plan for ASCI Encapsulation that was linked to weapons system development such as neutron generators, TSSG and firesets, all of which are encapsulation components. This 5-Year Plan is being used to guide the development of GOMA for encapsulation simulations. Every year since its compilation, we have updated the 5-year Plan with respect to deliverables, delivery dates and focus of effort. We meet with our customers on a bimonthly basis. These meeting often inspire changes in the direction of the research/analysis efforts. Changes to the 5-Year Plan, which is a living document, are made through the baseline change forms. The links between the 5-Year Plan and the V&V plan are given in the previous section on Verification Requirements.

3.2.1.3 Project Tracking and Oversight

Project tracking is carried out in a hierarchical system. The ASCI Encapsulation program manager tracks the progress of the project through communication with the staff working on the project. The tasks and milestones from the 5-Year Plan are communicated to the ASCI Program Management through the implementation plan that are written for the ASCI Manufacturing Program Manager. Progress regarding the task and milestones are tracked through quarterly reports.

3.2.1.4 Sub-contract Management

Experimental validation is provided by the MAVEN project on Encapsulation. The ASCI manufacturing project provided input to the MAVEN Experimental Plan ensuring that the necessary experiments for validation are carried out. Communication between the ASCI Encapsulation Project and the MAVEN Encapsulation Project take place through MAVEN and ASCI meetings, since several of the MAVEN investigators are also on the ASCI project. Additional support from MAVEN to ASCI is provided between direct communication by the PIs.

The ASCI GOMA Project is responsible for providing parallelized infrastructure and the ASCI Red Port of all the capabilities needed to model the encapsulation process. The Encapsulation PI provided input to the GOMA project on parallel capability needs and time-line for the capability which is synchronized with the 5-Year Plan. Communication with the ASCI GOMA project occurs through GOMA meetings and by direct communication between the PIs.

Improved preconditioners and iterative solvers are needed to solve the complex, stiff problems common in encapsulation applications within a manageable amount of time. These preconditioners and solvers are provided by the LDRD entitled “Hybrid Sparse-Dense Incomplete Factorization Preconditioners” [Heroux, 1999] in which a new class of preconditioners based on equation types as well as matrix structure is being implemented into AZTEC [Hutchinson, 1995]. Input as to needs for encapsulation are provided by the ASCI Encapsulation PI who is also a member of the LDRD team. ASCI Algorithms funding is also helping with the development of an advance level set technique that can be used for multiphase flow modeling such as mold filling. Several of the staff members involved with that project also work on ASCI Encapsulation.

Additional services include pre- and post-processing as discussed in following sections. The ASCI Encapsulation project also relies on SIERRA to provide us with the next-generation of encapsulation modeling tools (e.g. ARIA, PRESTO/ADAGIO, and CALORE).

3.2.1.5 Software Quality Assurance (SQA)

Software quality assurance practices have been used to a certain extent during the development of GOMA (see section on software engineering). Further QA is needed; it would be valuable to hire a contractor who could devote full time effort to the QA and verification of the code. Currently a contractor has been hired at a half-time effort to rewrite the input parser using lex and yak protocols. The new input parser will be more robust and easier to modify or to add features. The most significant portion of the input parser rewrite is that a echo file is being produced that regurgitates all the setting and material parameters that the code will use. This provides an easy file format for doing input file audits/inspections and verifying that the correct input properties are being used. Further information on the SQA of GOMA can be found in the GOMA Tri-Lab Survey [Peercy et al., 2000] and the GOMA developer's manual [Schunk et al., 2000].

3.2.1.6 Configuration Management

Details of configuration management for GOMA are given in the next subsection and in the GOMA developer's manual [Schunk et al., 2000].

3.2.2 Software Engineering of GOMA

In this section, we give a brief description of GOMA and its capabilities. Details of the code can be found in the GOMA Manual and other selected publications including code tutorials [cf. Schunk et al. 1997, Schunk and Labreche, 1998, Schunk et al, 1999, Schunk et al, 2000] and the developer's manual [Schunk et al., 2000]. We follow the description of GOMA by a discussion of the software engineering and quality assurance practices used in the development of the code. A more detailed and complete discussion of software engineering for GOMA can be found in the GOMA Tri-Lab Survey [Peercy et al., 2000] and the GOMA developer's manual [Schunk et al., 2000].

3.2.2.1 Description of GOMA

"*GOMA*", which means *rubber, gum,* or *elastic* in Spanish, is a two- or three-dimensional finite element program currently being advanced and specialized for the analysis of manufacturing flows and related processes that involve one or more transport fields, i.e., any combination of heat, mass, momentum (solid and fluid) and species transport fields. Specifically, the processes for which *GOMA* is suited are those which contain free or moving boundaries between dissimilar materials or phases or complex rheology in fixed domains.

The class of problems treated by *GOMA* is those described by any one or a combination of the incompressible form of the momentum conservation equation for generalized Newtonian fluids, the momentum conservation and differential stress constitutive equations for viscoelastic fluids, saturated and unsaturated flow through porous media, the energy conservation equation, the equations of quasi-static equilibrium of an elastic solid, and any number of additional or auxiliary species convection-diffusion-reaction equations. Details of several advanced examples from capillary hydrodynamics, melting and solidification, particle migration, and polymer processing may be found elsewhere [Sackinger et al. 1995, Cairncross et al. 1995, Chen et al. 1995, Schunk et al. 1997, Baer et al, 2000, Cairncross et al, 2000, Rao et al, 2001a, Rao et al, 2001b].

For encapsulation problems, two types of general models are currently being used in GOMA. The generalized Newtonian momentum transport equations are coupled with species equations to simulate the transport of particles and the curing of the epoxy through an extent of reaction equation. This capability allows us to study particle migration through viscous resuspension [Leighton and Acrivos, 1987] as well as settling or flotation due to the difference in density between the particles and the suspending fluid. We can also simulate this with the added complexity of a polymerizing suspending fluid. At some point, the particle migration models will be coupled with our mold filling capability. Currently, we use a level set equation to track the location of the free surface as a function of time. The level set algorithm has not yet been augmented to take into account suspension flows and is now limited to Newtonian fluids. The level set method is also being used to study single bubble dynamics to provide insight into degassing.

3.2.2.2 Numerical Methods

GOMA is based primarily upon the Galerkin finite element method, with some extension for hyperbolic systems such as Petrov-Galerkin, pressure stabilization [Droux and Hughes, 1994] and discontinuous Galerkin [Johnson, 1990]. For detailed discussions of our numerical method, please see the GOMA manual [Schunk et al., 1997] and the GOMA developer's manual [Schunk et al., 2000].

3.2.2.3 Portability, Libraries and Accessibility

GOMA has been developed primarily on a SUN system running the Solaris operating system (most recently SunOS 5.8), using the standard SUN compiler suite. However, we routinely use the openly accessible GNU compiler suite to aid in our support of all other UNIX systems, including parallel shared memory and distributed memory platforms running MPI. Other supported UNIX operating systems include HP-UX, AIX, IRIX, Linux, UNICOS, and a POSIX-compliant platform called Interix (available on Windows NT). The code has also been ported to specialty UNIX operating systems such as those available on the ASCI Red Machine and Sandia's CPlant. Many of the machine dependencies in the program have been isolated using C preprocessor directives. See the GOMA developer's manual for details of the libraries and dependencies [Schunk et al., 2000].

Generally, pre- and post-processing is performed outside of *GOMA*, although some post-processing of results is available within the program. This separation of the functionality permits the use of alternative solid-modeling and mesh-generation software and visualization packages of choice, insofar as they may be interfaced with the EXODUS II finite element data model.

Pre-processing options include mesh generation via FASTQ [Blacker, 1988], CUBIT [CUBIT Development Team, 1999], or PATRAN [PDA Engineering, 1990]. These mesh generators currently support and will output a finite element database in the EXODUS II format, the latter through a specially constructed add on to PATRAN that allows for an EXODUS Preference.

Post-processing options include BLOT [Gilkey and Glick, 1989] and AVS. The latter visualization package, particularly AVS/Express, may be conveniently accessed using MUSTAFA [Glass, 1995].

3.2.2.4 GOMA Source Control

Source code control for GOMA is performed using the Concurrent Versions System (CVS), a publicly-available program distributed under the GNU General Public License. Full source code distributions and some documentation may be found at the web site for Cyclic Software (`http://www.cyclic.com/cvs/info.html`) or any one of many mirror sites (e.g., *www.loria.fr/~molli/cvs-index.html*.) CVS is a system for managing sequential incremental changes to a collection of files under its control. A particular strength of CVS is its ability to manage concurrent changes by more than one developer. CVS may be built in a highly-capable server configuration on most UNIX platforms and client versions as well as simplified non-client/server versions may be built for UNIX as well as for operating systems such as Windows NT/95, OS/2 and VMS. The CPU and memory requirements of CVS are generally modest.

Access to the CVS repository of GOMA is password controlled and limited to the developers of GOMA. CVS allows the seven primary developers, and the nine part-time developers, to work concurrently. CVS is used to automatically merge changes made by different developers maintaining a unified version of the code, including all improvements, in the source code repository. CVS also allows versions of the code to be checked out by date, if an older version of the code is desired for comparison and to help find any changes that may have inadvertently introduced bugs.

3.2.2.5 Programming Standards and Style

GOMA is written in the C programming language [specifically Kernighan and Ritchie, 1988, C with ANSI extensions]. As of 2001, all declarations and definitions of the routines have been reworked to use strict ANSI standard function prototypes to enhance data type checking. Furthermore, the function prototypes declarations are confined to one instance in an include file that provides the identical prototype declaration to all files that require it. Guidelines for development in GOMA have evolved on an ad hoc basis and are only recently being formalized. Among the recommendations are the following tenets:

- Desist from proliferating global variables unless they are absolutely necessary.
- Provide ANSI prototype function declarations in a single place.
- For actual function definitions, try to put the name of the function in the first column.
- Use all caps for C preprocessor definitions including any macros. Other variables should be lower case and/or mixed case.
- Use distinctive names for those global variables, like “After_Thought” instead of “i”, which is likely to conflict with the name of an automatic variable.
- Use descriptive comments like what the function does, what it needs, what it affects, limitations, who is the author, who has modified it and any other significant notes.
- Be concise with I/O! Maximum information in the least space! Is this print statement really necessary?
- Do not clog your routine with unused variables or functions.
- Initialize all variables before use.
- Close up case statements with break; and include a default case.

- Error check. Make descriptive error messages that include a reasonable prescription for the fix. Suggest to the user not only what his likely problem is, but make it easy to figure out what the solution is to the problem.
- Generalize: after about 27 if() blocks with each variable named, it might suggest the use of a function!
- Write speedy code where lucidity is not sacrificed.
- Use boolean variables for clarity.
- Indent properly. Emacs will do this automatically for you.
- Try not to run over the 80 column limit if possible. Never go over the 132 column limit.
- Never throw a global variable into the argument list of a function.
- Make sure to free all memory that has been dynamically allocated.
- Insofar as possible, keep your development code current with the repository. Do frequent updates with others changes and check in your own changes after verifying them with the regression test suite.

In addition to these guidelines, it is strongly suggested to make use of diagnostic tools. For example, (i) use Purify, ccmalloc, or ElectricFence to look for memory leaks, overwriting of array bounds and uninitialized memory accesses; (ii) run different problems in the regression test suite, not just one that exercises the new feature you just added; (iii) run the compiler with warning messages activated (e.g., gcc -Wall) to indicate sections of code that may cause portability problems later; (iv) run lint; and (v) run the numerical Jacobian checker to make sure you have implemented your analytical Jacobian contributions correctly (it is all too easy to make an error).

By following these guidelines, the GOMA developers will be able to implement useful features in a way that is more robust, less likely to break other features, and in a way that is less likely to break itself when put under more severe testing later. The C programming language has been criticized in the past as a “write-only” language, a reputation it gained as obfuscated code is easy to write. The GOMA developers are motivated to adhere to coding guidelines because they recognize that a small investment of effort during coding can lead to big time savings in future debugging and future feature addition to a code that is lucid and robust. More information about programming style and standards can be found in the GOMA Developer’s Manual [Schunk et al, 2000].

3.2.2.6 Bug Tracking and Bug Resolution

In this aspect of production computing, the GOMA code and the GOMA development team have extensive experience “in the fire”. Primary support coordinators (Duane Labreche and Randy Schunk, 9114) handle most of the support calls (with a demand that they come by email unless they are “show stoppers” as is described in the attachments below). They either answer the question or fix the bug, or dispatch the problem to one of the 15 developers, as appropriate. There are still areas for improvement. Serious bugs are addressed immediately and aid is given to analysts who are having trouble running a particular problem. Analyst show stoppers often take the form of errors in the input file. Thus the input file echo will save everyone time and irritation.

A more formalized bug tracking system also exists. All bugs are entered into an issue tracking system developed by Matt Hopkins with support from Michael Martinez [Hopkins and Martinez, 2000]. The issue tracking system is based on a MySQL database (freeware) that is preprocessed using PHP and compiled to an Apache Web server (http://www.engsci.sandia.gov/goma/issue-track/index.php). New issues/bugs can be added, modified or closed by anyone who is in the net-pub GOMA group. As discussed above, show stopping bugs are fixed as soon as possible by the development team. The issue tracking database is more useful for longer term issues such as desired new features, clean up, bugs with current work-arounds and as a place to document undocumented features that cause the code to run in a way that the user is not prepared for. Fields held in the current data base include severity, contact person, work estimate, description of issue, originator and whether the issue is open or closed.

3.2.2.7 Software Inspections

Currently, formal software inspections are not carried out for the GOMA code. For the most part, guidelines are only enforced by peer pressure, are not dictated as absolutes and rely upon the goodwill of each developer. For the most part, this has been successful. In the future, we hope to use compiler warnings and an automated configuration and build process to catch the most blatant examples of bad coding practice. However, additional reviews would be helpful in enforcing more subtle guidelines. A code may be strictly correct C, produce no compiler warnings and yet be incomprehensible, confusing and/or difficult to modify, whether to fix a bug or to add a feature. Code reviews, if funded and staffed, would be an avenue to the promotion of robust, modifiable code.

Some informal review already occurs by virtue of the team model that has been used for some of the GOMA development. In the team model, one developer will write a function and another developer will test and modify the function. Code written by one developer is often rewritten by another to make it more robust and efficient or to extend its functionality to suit another purpose not originally foreseen. In addition, if we plan to make major changes to the architecture of GOMA, we will send emails or have a meeting to ensure that all the developers agree with the changes.

3.2.2.8 Regression Testing & Coverage Analysis

A regression test suite currently exists containing about 80 fairly complicated problems that exercise a broad range of code features. Currently, guidelines demand that developers test that these problems be run before changes are committed to the central repository. For the external user base, however, rigorous testing of all problems occurs on multiple platforms before a major release to these users. Even though the process is automated to run every night, bug fixes can still require a substantial investment of time on the part of the support personnel.

Additionally, the regression test suites covers a range of desired checks. At the most basic level, the tests verify that current code snapshots from the repository will build cleanly without producing compiler warnings. Secondly, the current code executable runs each of the sample test problems without terminating abnormally (e.g., Bus error or Segmentation fault). Thirdly, a quantitative comparison between the results of the simulation and the results of a reference baseline simulation should show no differences, unless the developer believes the newer results to be more reliable, in which case a new standard reference is to be established. Finally, the preceding checks are performed on a variety of hardware and software platforms and using any range of different compilation and linking options that may be pertinent. This however is not currently automated.

In the future, we plan to extend our regression test suite to an even broader class of problems. Indeed, some of the formal verification problems used to demonstrate code correctness will be used as part of the routine regression tests that current releases must pass. In addition, we will use a coverage testing tool, such as Pure_Coverage, to ensure that we test as many parts of the code as possible with the test suite. Given the complexity of the logic in parts of GOMA, the latter task is particularly important.

3.2.2.9 Regression Test Suite

A Goma verification test suite containing 80 problems that can be run automatically each evening using scripts has been developed. The test suite can also be used by developers before checking in to the CVS Repository to insure that the new features added did not jeopardize the workings of the code. A description of the regression test suite, its sample problems and usage can be found elsewhere [Moffat and Labreche, 2001].

3.2.2.10 Metrics for Software Development Process

The metrics for determining the adequacy of the code are straightforward. Since we have more that 60 users throughout the lab and in industry, we deem the satisfaction and continuing use of GOMA by the user-base to be an ultimate metric. In addition, GOMA must reproducibly provide verifiable answers to application problems. Thus, our second metric is that the code performs reliably and predictably on standard verification problems as well as comparisons with experimental validation studies.

Unfortunately, no formal metrics exist that provide a detailed picture of the effectiveness of GOMA software development. Intuitively, GOMA software developers are aware of the practical benefits of following established guidelines and best practices, but not all of these best practices have been incorporated into the GOMA development process as yet. Consequently, some aggravation with the time to fix bugs, time to develop new features, time to prepare a verifiable release

CD for external customers could be alleviated if more funding and personnel were devoted to putting in place more of the known best practices.

3.2.3 Issues and Challenges for Software Engineering

GOMA is a code that began life as the product of an LDRD, as a vehicle for research. It was not designed from the beginning as a production code. In fact, much of the development has been driven by specific applications that demand a particular feature be developed in the shortest possible time. However, the rapid developing of a particular feature in a research code for use on a particular application will not generally align with the best software engineering practices. It is only the conscience of the developer, later augmented with the plaintive cries of the user base, that has mandated generality and robustness in the GOMA code. Without money specifically targeted for software engineering efforts that the application projects do not want to fund, the GOMA code has been relegated to accumulating more features as a priority to testing and verification of existing features.

Surprisingly, considering the history of the GOMA development model, the code has done quite well in the production setting. However, there are many improvements that are needed to maintain the quality of the software as the user base continues to grow. A list of the needed software engineering improvements is given below:

- More complete coverage of all problem types in the regression test suite. GOMA currently has 114 equations, 150 boundary conditions and 654 distinct input deck parameters. It is a daunting task to create a test suite that can exercise all of these features, particularly when combinatorial effects are considered that are responsible for a significant fraction of the bugs that are found.
- More debugging tools built into the code such as i) input deck regeneration, ii) helpful symbolic annotations of all residuals and matrix contributions and iii) improved diagnostics, such as internal trace backs.
- Update/completion of the developer’s manual [Schunk et al., 2000]. Currently there are many developers who, while knowledgeable, are not intimate with the details of the entire code. A completed developer’s manual, updated with the latest GOMA changes, could be invaluable to new and experienced users alike.
- Code speed-up. A feature-laden code designed for correctness and extensibility is not necessarily fast. “*First make it right, then make it fast.*” With the verification tests, the first of these admonitions is satisfied. It is time to address the needs of the second.
- Rewrite of many sections with software engineering practices in mind to make the code more robust and maintainable, including new data structures that are designed to reflect the actual usage patterns that have been deployed over the first five years.
- More comments in the code so others can easily track the intent of the original code developer. Comments represent documentation at the most immediate level and learning to write good comments usually only comes with experience or training.

3.3 Software Verification Testing Plan

3.3.1 Equations and Numerical Method

References giving a description of the equations and numerical method used to simulate encapsulation processes are given below. The primary models currently available are a level set solver for mold filling and single bubble dynamics (degassing), a suspension model for particle settling and migration simulations, and an epoxy curing model.

3.3.1.1 Level Set Algorithm

A common technique for modeling processes with fluid-fluid interfaces in complex, intricate geometries is the level set method. Details of this algorithm can be found elsewhere [Schunk et al., 2000; Noble et al., 2001].

3.3.1.2 Suspension Model

Flowing suspensions of particles in viscous liquids are found to exhibit particle migration in creeping flow and in the absence of significant nonhydrodynamic effects [Leighton and Acrivos, 1987]. Here we are focusing on suspensions of noncolloidal particles, where the particle size is greater than 10 μm. Scaling arguments have been used to identify the three major causes of particle migration, which are gradients in shear-rate, particle viscosity and relative viscosity. Phillips et al. [1992] used these scaling arguments to develop a continuum constitutive equation. The Phillips' model, also called the diffusive-flux model, uses a particle concentration dependent generalized Newtonian viscosity coupled with a diffusion equation to track the evolution of the particle concentration. This evolution equation takes into account shear-induced migration and particle-particle interactions.

Zhang and Acrivos [1994] extended the Phillips' model to account for effects caused by density differences between the particles and solvent. We base much of our work on theirs with some significant modifications. The viscosity depends on the particle concentration. The suspension's behavior is quite nonlinear, ranging from highly viscous solid-like behavior at the limit of maximum packing (ϕ_m) to much lower viscosity in the pure fluid (μ_o) region. Here we use a Krieger model [1972], since it is found to agree well with experimental data. In the Krieger model, *n* is a parameter that is used to best fit the viscosity data.

Details of our equations, numerical method and implementation can be found in a variety of sources such as internal Sandia memoranda and peered reviewed journals [See for instance; Rao et al., 1997; Tetlow et al., 1998: Subia et al., 1998: Sun, 1998; Romero, 1999; Rao et al., 2001a: Rao et al., 2001b, Fang et al., 2001].

3.3.1.3 Epoxy Curing and Viscosity Model

Liquid epoxy exhibits thermophysical properties that require highly nonlinear models. Its apparent viscosity as seen in the experiments, for example, is a strong function of time, the extent of cure, the concentration of filler, and temperature [Adolf et al., 1997a]. In order to understand how the liquid properties impact the final structural integrity of cured, solid epoxy, many characterization experiments were carried out to accurately model the curing kinetics as well as temperature dependency [Adolf et al., 1996, Adolf et al., 1997]. Details of the equations and numerical method of the reaction kinetics and the viscosity-temperature relations for 828/Z, 828/DEA, 826/459 (459 in short) liquid epoxy systems can be found elsewhere [Sun, 1999; Rao et al., 2001c]. Two types of fillers commonly considered are GMB and ALOX. For the curing epoxy a momentum, continuity, energy, suspension migration and extent of reaction equation must be solved making it computationally intensive.

3.3.2 Additional Software/Other Technologies

Additional software is frequently used in conjunction with GOMA. In order to initiate a GOMA simulation a finite element mesh must be provided in the EXODUS II file format. Mesh generation tools used to accomplish this step include FASTQ, GEN3D, GJOIN, CUBIT and PATRAN. Some of the mesh generation tools make use of CAD files that describe the overall geometry of the region that is to be simulated; other applications (e.g., ProEngineer) may be used for the generation of the basic problem geometry.

Many analyses with GOMA make extensive use of the APREPRO preprocessing language that facilitates the use of named variables as well as many useful arithmetic, logical and string operations. GOMA will initiate a system call to run APREPRO to preprocess the input file as well as the material files.

Parallel GOMA simulations require the BRK tool and the underlying CHACO graph partitioning engine in order to properly decompose problems for use on distributed memory message passing computers. Conversely, results from a parallel GOMA simulation must be recomposed into a single monolithic file suitable for visualization or other post processing using the FIX tool.

Sequential GOMA simulations are sometimes controlled in the context of optimization wrappers such as DAKOTA that can also be used to aid in parameter estimation. Auxiliary software such as ARPACK can be used with GOMA to perform generalized eigenvalue calculations for the analysis of stability and frequency response. Finally, post processing of GOMA results typically involves visualization software such as BLOT, MUSTAFA, or XMGR.

3.3.3 Verification Test Suite Process Development

The process for developing the verification test suite is as follows. The first step was to develop a list of models that must be verified. This information is derivable directly from the PIRT. We broke the modeling down into the following categories: fluid mechanics, coupled fluid mechanics with mass or energy transport, suspension test problems, level set test problems and curing epoxy test problems.

Once the list was finalized, the GOMA team had a brainstorming team and filled in the problems that had been run or that should be run to verify each class of physics models. The authors then documented this work in the form of a verification test suite and added appropriate references for work that was completed, when available.

3.3.4 Verification Test Suite

A description of the verification test suite for the models used in encapsulation flow is given below. We also discuss briefly test problems that exercise other models in GOMA. The majority of our verification efforts have been in Tier I, or comparison with analytical solutions, and Tier II, code to code comparisons. Less has been done in the Tier III area, or tests against semi-analytical solutions. As part of the verification process, we plan to hire a contractor to assemble all the verification problems that have been run and should be run with GOMA into a comprehensive SAND report.

3.3.4.1 Tier I

Below we have listed the analytical solutions that have been or will be used to test GOMA modules pertinent to encapsulation, which include basic generalized Newtonian fluid mechanics, suspension model, interface tracking and the epoxy curing model. If the problem is completed, no further information is given unless a memo exists documenting the process. If the problem has not yet been completed, the year it will be completed is indicated. Unless otherwise indicated, we have achieved good agreement between GOMA and the analytical solutions, e.g. less than 5% error. The choice of the 5% error criteria based on computer roundoff error, truncation error, engineering judgement and common sense.

<u>Fluid Mechanics Tests</u>
These problems test the basic momentum and continuity equations along with the finite element implementation. Exercises submodels used in PIRT elements A, B, C but does not provide complete coverage.

- Axisymmetric Newtonian pipe flow.
- Rotated axisymmetric Newtonian pipe flow, at 30^o, 45^o and 60^o. This tests cross terms in the equations.
- 3-D Newtonian pipe flow.
- 2-D Newtonian channel flow.
- Startup Poiseuille flow. (This tests our transient implementation of the equations.)
- Newtonian parallel plate viscometer. This tests the swirling flow capability. [Lindgren, 2000a]

- Newtonian cone and plate viscometer. This tests the swirling flow capability in a slightly more complex geometry. [Lindgren, 2000b]
- Newtonian flow into a line sink. This tests cross terms in the equations. [Baer, 2000].

Fluid Mechanics with Mass/Energy Transport Tests

These problems test the fluid mechanics along with the mass transport or energy transport equations and their numerical implementation. Mass and energy transport can often be posed as identical equations. Since we use the concentration equations for our suspension model it is critical that they be well tested. So tests that exercise the concentration and energy equations in a different context are still relevant. Exercises submodels used in PIRT elements A, B, C, D, F and G, but does not provide complete coverage.

- Graetz problem: pipe flow with temperature or concentration gradients due to wall boundary conditions.
- Flow over a heated sphere, *i.e.* Oseen's solution at zero Reynold's number. This problem also tests the post-processing of heat/mass fluxes in GOMA.
- Stefan tube. (This also tests the Stefan-Maxwell equations for concentrated, non-Fickian diffusion.)
- Vapor-liquid equilibrium and Raoult's law.
- Axisymmetric diffusion of mass from a point or a plane compared to theory of images solution. (**FY02**)
- Axisymmetric diffusion of energy from a point or a plane compared to theory of images solution. (**FY02**)
- 3D diffusion of mass from a point or a plane compared to theory of images solution. (**FY03**)
- 3D diffusion of energy from a point or a plane compared to theory of images solution. (**FY03**)
- Stefan problem of phase change in a slab. This also tests our free surface/moving mesh algorithm. (**FY04**)

Suspension Test Problems

These tests exercise the suspension model, including the augmented Phillip's model using the concentration equation, the momentum equation and the continuity equation along with their transient finite element implementation. Exercises submodels used in PIRT elements C-1 but does not provide complete coverage.

- Flow of a suspension in a Couette viscometer. An analytical solution exists for the Phillip's model [Subia, 1997].
- Suspension settling with two fronts coming together [Baer, 1999].
- Flow of a suspension in a pipe (axisymmetric). An analytical solution exists for the Phillip's model [Baer, 1998].

Level Set Test Problems

These problems test the volume of fluid algorithm for simulating mold filling as well as the basic equations of fluid mechanics. Exercises submodels used in PIRT elements A and B but does not provide complete coverage.

- 1-D mold filling problem. Comparison of plug flow front movement with analytical solution.
- Capillary imbibition in 2D [Noble et al., 2001].
- Comparison of mold filling results with Hele-Shaw solution. (**FY02**)

<u>Epoxy Curing Model</u>
These problems test the extent of reaction equation, which couples to the viscosity function, as well as the basic equations of fluid mechanics. Exercises submodels used in PIRT elements D, E and G but does not provide complete coverage.

- Isothermal homogeneous reaction (**FY01**).

3.3.4.2 Tier II

Below we have listed the semi-analytical solutions (or comparison to ODEs) that have been or will be used to test GOMA modules pertinent to encapsulation, which include basic generalized Newtonian fluid mechanics, suspension model, level set capability and the epoxy curing model. We will indicate if the problem has not yet been completed and when we plan to complete it. Unless otherwise indicated, we have achieved good agreement between GOMA and the semi-analytical solutions.

<u>Fluid Mechanics Tests</u>
These problems test the basic momentum and continuity equations along with the finite element implementation. Exercises submodels used in PIRT elements A, B, C but does not provide complete coverage.

- Pipe flow of a Giesekus fluid. (This also tests the viscoelastic flow capability.)
- Pipe flow of a Phan-Thien Tanner fluid. (This also tests the viscoelastic flow capability.)
- Pipe flow of a Carreau fluid. (This also tests the generalized Newtonian capability.)
- Coating flow problem. (This also tests the free surface/moving mesh algorithm.) **(FY03)**
- Tensioned web coating flow. (This also tests the free surface/moving mesh algorithm as well as the solid-fluid interaction sections of the code.) **(FY03)**

<u>Suspension Test Problems</u>
These tests exercise the suspension model, including the augmented Phillip's model using the concentration equation, the momentum equation and the continuity equation along with their transient finite element implementation. Exercises submodels used in PIRT elements B-2 but does not provide complete coverage.

- Flow of a suspension in a Couette viscometer. Comparison with 1-D finite difference solution.

- Pipe flow of suspension using inflow condition from another simulation [Baer, 1998].

3.3.4.3 Tier III

Below we have listed the code to code comparisons that have been or will be used to test GOMA modules pertinent to encapsulation, which include basic generalized Newtonian fluid mechanics, suspension model, level set capability and the epoxy curing model. We will indicate if the problem has not yet been completed. Unless otherwise indicated, we have achieved good agreement between GOMA and the code it was benchmarked against.

<u>Fluid Mechanics Tests</u>
These problems test the basic momentum and continuity equations along with the finite element implementation. Exercises submodels used in PIRT elements A, B, C but does not provide complete coverage.

- Planar extrudate swell of a Maxwell fluid: Comparison to POLYFOW [Rao, 1996].
- Axisymmetric extrudate swell of a Newtonian fluid: Comparison to FIDAP [Rao, 1995].
- Planar four to one contraction flow of a Newtonian fluid: Comparison to MPSALSA.
- Axisymmetric four to one contraction of a Newtonian fluid: Comparison to FIDAP [Torczynski, 2000]
- Flow past a sphere with a Phan-Thien-Tanner fluid: Comparison to POLYFLOW [Hartt, 2001]
- Flow past two spheres with a Phan-Thien-Tanner fluid: Comparison to POLYFLOW [Hartt, 2001]
- Flow over a backward-facing step: Comparison to published benchmark results of Gresho et al. [1993] (**FY03**)

<u>Fluid Mechanics with Mass/Energy Transport Tests</u>
These problems test the fluid mechanics along with the mass transport or energy transport equations along with their numerical implementation. Mass and energy transport can often be posed as identical equations.

- Metal melting in axisymmetric coordinate system using an enthalpy method. Comparison of GOMA with FIDAP [Schunk, 1996].
- 1-D oven drying with mass transfer at surface: Comparison to Kodak drying code. (This problem does not test fluid mechanics, but does exercise the energy equation, mass transport with diffusion, Flory-Huggins, and the transient algorithm [Sun and Bell, 1999].)
- Natural convection in a square region at increasing Rayleigh number: Comparison with MP-SALSA [Evans, 2000].

<u>Suspension Test Problems</u>
These tests exercise the suspension model, including the augmented Phillip’s model using the concentration equation, the momentum equation and the continuity equation along with their tran-

sient finite element implementation. Exercises submodels used in PIRT elements B-2 but does not provide complete coverage.

- Flow of a suspension in a Couette viscometer: Comparison to NACHOS [Subia, 1998].
- Flow of a suspension in an eccentric cylinder: Comparison to NACHOS. (**FY02**)

Level Set Test Problems

These problems test the volume of fluid algorithm for simulating mold filling as well as the basic equations of fluid mechanics. Exercises submodels used in PIRT elements A and B but does not provide complete coverage.

- Axisymmetric mold filling: Comparison to FIDAP. (**FY02**)
- Bubble rise: Comparison between level set model and moving mesh model [Noble et al., 2001].
- Mold filling in 3D pipe: Comparison to FIDAP. (**FY03**)
- Mold filling in more complex 3D geometry: Comparison to FIDAP. (**FY03**)

Epoxy Curing Model

These problems test the extent of reaction equation, which couples to the viscosity function, as well as the basic equations of fluid mechanics. Exercises submodels used in PIRT elements D, E and G but does not provide complete coverage.

- Non-isothermal epoxy curing without particle settling in a stainless steel mold around a kovar tube: Comparison with COYOTE [Rao et al., 2001c].
- Non-isothermal epoxy curing without particle settling in a stainless steel mold: Comparison with COYOTE (**FY01**).

4. Validation Plan

4.1 Validation Process and Metrics

To date we have successfully validated the code against a number of experiments. We have tested the code predictions of single phase flow in a large number of scenarios and with several fluid constitutive equations [Pedersen, 1997; Secor, 1998; Sun and Bell, 1999]. Recently we have also begun to model mold filling with and bubble rise in a Newtonian fluid using a new “level-set” formulation [Noble et al., 2001]. Validation experiments to test these two flows have also been initiated.

The suspension constitutive equation has been tested to see if the predictions of particle migration are accurate in well controlled experiments on ideal systems [Subia et al., 1998] and on the actual encapsulants [Sun, 1999, Romero, 1999]. Here, we assess 1) qualitative agreement as to the direction of the particle motion, 2) quantitative measurements of the resulting concentration gradients, and 3) quantitative measurements of the rate of migration. In most applications for neutron generators, the first is the most important. In order to determine if there is a problem during processing, we must primarily know where the particles are likely to end up. If the second and third are within engineering accuracy, say within 30%, trends can be established for different processing scenarios or different encapsulant formulations. With recent improvements to the constitutive equations [Fang et al., 2001] we correctly predict the direction and steady-state concentration of a wide range of suspended particle sizes undergoing a variety of flows. With regard to gravity induced flows, we have managed to also match satisfactorily the rate of particle movement [Rao et al., 2001a]. The above tests were done using a Newtonian suspending fluid, which is a good model for Epon 828 and 826 and for the standard “Z-cured” encapsulants before vitrification. With a non-Newtonian suspending fluid, we have only matched the direction of particle motion [Rao et al., 2001b] to date. However, this was not tested with our most recent improvements to the constitutive equation. The new 459 encapsulants are markedly non-Newtonian.

The exothermic polymerization reaction affects the temperature of the material, and the viscosity of the encapsulant with time, extent of reaction, and temperature. The changing viscosity in turn determines the final particle concentration gradients. We have compared GOMA predictions of temperature to experimental measurements and obtained reasonable results (within 10%) [Rao et al., 2001c]. We also are comparing predictions of the final particle concentrations with post-cure microscopy data. The tests completed to date show correct predictions of trends (for example, the alumina particles do not settle appreciably in 459 but the GMB do) and to an engineering approximation (within the desired 30%) correct quantitative predictions of extent and rate of migration.

Open issues in suspension modeling include the above mentioned non-Newtonian effects and improving the predictions of rate of migration. We also are developing better means to model mold filling operations and are actively involved in benchmarking the code against experiments in simple fluids and ideal suspensions. The biggest challenge we face is to develop appropriate models for degassing. The former two efforts are our highest priorities for future work. Because of the difficulties associated with the development of degassing models and limited resources, the latter is lower in priority.

Uncertainty quantification has been a somewhat neglected effort thus far, since much of our uncertainty arises from model uncertainty as opposed to parameter uncertainty. Model uncertainty arises from several of our physics models, with the Phillips model being the largest source of error. Once the model uncertainty has been eliminated, we will work on parameter uncertainty issues.

4.2 Organization of Validation Plan

The following sections outline the model and experiments, either completed or planned, that address each phenomenon listed in the PIRT discussed in Section 2. In cases where the adequacy of the model is currently questioned, steps to be taken in model development are addressed. The validation plan is separated into a four-tiered suite. Tier I studies are designed to explore the separable effects. Tier II are coupled effects. Tier III studies integrate many coupled effects. And Tier IV is a final "certification experimental campaign" to assess the readiness of the code for stockpile computing.

The following subsections contain tables of the validation tests completed or planned for the future. Where possible, references to documentation are provided for completed tests. For each planned test, a unique identifier is provided, including the PIRT chart number, the tier of the test, and a number (so more than one test in the category can be planned). Prioritization is also included in these tables. The priority was determined through consideration of the importance of the phenomena (PIRT Table 1) to the customer as well as a combination of the difficulty of developing a model for the phenomena and the available funding. If the amount of effort required was beyond the anticipated funding level, we rated that task with lower priority relative to other more attainable goals. If, on the other hand, the model has been determined to be adequate and validated adequately already, we also rated the priority as very low.

In addition to the validation tests listed, we have performed sensitivity analysis to determine the effects of various parameters that must be measured experimentally. For example, we have varied thermal conductivities, heat transfer coefficients, hindered settling functions, diffusivities/particle size for the Phillips model, viscosity, and density. Much of this work is very recent and has not been documented to date. We have tried to state in the table and text where additional calibration data are needed.

4.3 Tier I

TABLE 2 Validation Test Plan Linked to PIRT

Phenomena	Tests Planned or Completed (reference)	Priority 1=high 5=low
	Tier I	
Fluid Flow/ Momentum Transport		
A. Fluid Flow of single-phase liquid	Completed for Newtonian and Carreau models (Secor 1998, Pedersen 1997, Sun & Bell 1999).	5
B. Gas/fluid interface tracking		
B.-1 Mold Filling		
B-1a Single fluid phase	B1a-I-1.Newtonian 3-D model compared to data (some available in Romero 2001). B1a-I-2. Non-Newtonian.	1
B-1b Multiple fluid phases	See Tier II	
B-2 Multiple Interfaces/ Bubble dynamics in single liquid phase		
B-2a Isolated bubble nucleation	No tests planned due to model uncertainty and low priority.	5
B-2b Single bubble growth & transport through single fluid phase	B2b-I-1. Compare level-set formulation to flow visualization of bubble transport through single Newtonian fluid. B2b-I-2. Non-Newtonian.	3
C. Multiphase flow		
C-1 Particle Dynamics		

Phenomena	Tests Planned or Completed (reference) Tier I	Priority 1=high 5=low
C-1a. Particle hydrodynamic interactions/migration	C1a-I-1. Effects of particle concentration on viscosity [complete except for 459: Adolf et al. 1997, Mondy et al. 1998, Adolf et al. 2000]. C1a-I-2. Ideal uniform neutrally buoyant particles -calibration of coefficients and validation. Some additional data required. Multiple flow fields [Abbott et al. 1991, Subia et al. 1998, Tetlow et al. 1998, Fang et al. 2001].	1
C-1b Particle nonhydrodynamic interactions	No tests planned -- phenomena not thought important for present encapsulants.	5
C-1c Particle sedimentation	C1c-I-1. Sedimentation in otherwise quiescent fluid. Monodisperse and polydisperse particle sizes [Romero 1999, Rao et al 2001].	1
C-1d Solid/fluid interface physics/chemistry	see Tier II	
C-2. Bubble/particle interactions (3-phase flow)		
C-2a. 3 phase flow (sedimentation)	see Tier II	
C-2b. 3 phase flow (general)	No tests planned -- phenomena not dominant in encapsulation process.	5
C -3. 2-Fluid mixing		
C-3a. Mixing of 2 single-phase fluids	C3a-I-1.Newtonian model compared to data [some available in Romero 2001].	4
C-3b. Mixing of 2 suspensions	see Tier II	4

Phenomena	Tests Planned or Completed (reference) Tier I	Priority 1=high 5=low
C-3c. Mixing of 2 suspensions with air entrapment	No tests planned -- beyond the scope of this study.	5
D. Energy Balance		
D-1. Energy transport	Model adequate in well understood material, but suspension calibration data needed.	5
D-2. Energy production / chemical reactions	See Tier II.	3
E. Coupled Energy/ Momentum		
E-1. Epoxy/curative rheology	See Tier III.	1
E-2. Extent of reaction (uniformity of cure)	No tests planned -- beyond the scope of this study.	5

There are a few separable effects that need to be studied in order to build robust models. The flow of single phase fluids (A) exhibiting several types of constitutive equations have been modeled extensively with GOMA in the past. Further experiments and modeling are not considered necessary for simple flows. Phenomenon B-1a is another example; however, in this case little data exists for direct code comparison. Mold filling simulations with GOMA of a single viscous Newtonian fluid at constant temperature in model neutron generator geometries should be compared to flow visualization data (instrumented flow visualization experiments of the encapsulation process to determine location of fill front.)

Another separable effect is B-2b, the rise of a single bubble through a single phase. Little additional data are thought to be required here, because examples exist in the literature; however, data collection is straightforward and may be desirable to obtain experimental conditions relevant to encapsulation processes. Particle tracking algorithms existing in GOMA need to be tested against suitable data to see if they are adequate to track a bubble during degassing. The new level-set formulation also can be tested against flow visualization data of the deformation of a bubble rising in a single phase fluid.

Another suite of studies that fit into this category involves the mixing of two fluids in a simple geometry as one flows over the other (C-3a). Suitable flow visualization studies may exist in the literature. However, experiments where the viscosities, flow rates, and geometries are close to that of the application are desirable. Recent data taken by Romero begin to address this problem.

The sub-grid physics model based on the boundary element method (BEM) will also require validation. The BEM code results are used to obtain information that is impractical or impossible to obtain with experiments. However, the code needs to be validated against experiment where possible. These codes have been extensively verified and validated against analytical solutions and experiments for up to a few interacting solid particles [Dingman et al. 1992, Mondy and Ingber 1993]. In order to modify this code to study bubbles (B-2 and C-2), we will need to compare the results to single bubble data. Bubble nucleation is not as well understood; nevertheless, is it not expected that additional single bubble nucleation experimental studies will be necessary, since we are generally interested in the nucleation of many bubbles during the degassing process.

Particle nonhydrodynamic (C-1b) effects in dilute systems can be isolated as well, numerically with a modified BEM coupled with FDT, and experimentally with an atomic force microscope. Aspects of interface chemistry (C-1d) can also be studied by varying the properties of the fluid and particles (especially the addition of surface coatings on the particles). Further validation experiments would be necessary, similar to those listed in Dingman et al. [1992], but with small particles and video microfocus. This is a research topic that has been neglected to date in the ASCI program. Although some encapsulant particles are small enough for nonhydrodynamic forces to be significant, most encapsulants used to date are made up of larger particles. Miniaturization of components will lead to smaller particles being used. However, balancing the required resources with the projected funding has led us to rate this effort as lowest priority for the present.

Other aspects of multiphase flow (C) can be categorized as separable effects, although the model would be built directly into the continuum description of suspensions. Experimental studies of particle migration of neutrally buoyant particles of uniform size should be completed first (C-1a). Then the same studies should be repeated to determine the effects of size and shape, and finally the effects of polydisperse sizes. These studies of migration need to be done in several unidirectional flow fields and simple 1-D curvilinear fields. Some of the experimental work has been completed; however, the simulations need to be repeated for modified constitutive equations, especially if the suspension balance model is adopted. Some experiments will need to be augmented by studies with parameters in the range of those expected during encapsulation. Particle sedimentation in otherwise quiescent suspensions (C-1c) also needs to be repeated (both simulations and experiments) for polydisperse particles, especially those actually used in encapsulants. Much of this work, too, has been completed.

The experiments on particle migration and sedimentation to date combine calibration studies with validation studies. For example, diffusion/sedimentation coefficients in the diffusive-flux constitutive equation are determined empirically through a set of experiments with one type of particle. The assumed dependence of the migration rate to the particle size is then validated with a separate set of experiments using a different particle size. Other validation studies include measuring and predicting particle migration in various flow fields. References include calibration of the coefficients with uniform spheres neutrally buoyant in a Newtonian liquid flowing in a wide gap Couette apparatus [Abbott et al., 1991, Tetlow et al., 1998], validation of the model for roughened spheres [Tetlow et al., 1998] and rods [Mondy 1994], and validation in various flow fields [Subia, 1999, Sun, 1998]. The Sun work showed that the original diffusive-flux constitutive equation was unsatisfactory in curvilinear flow fields. An improved constitutive equation [Fang et al. 2001] was subsequently developed. Validation computations need to be completed for this new formulation. The remaining Tier I experimental need is for measurements of particle concentrations in a complex three-dimensional flow.

In solving the energy equations (D), properties of the suspension will be needed. Heat capacities and thermal conductivities need to be approximated as functions of particle volume fraction and temperature (and properties of the epoxy and particles). Calibration data must be taken or assumed from literature values and additional data to validate these approximations will probably be needed. Much of this work has been completed [Burchett et al. 1997, Adolf 2001].

4.4 Tier II

Phenomena	Tests Planned or Completed (reference) Tier II	Priority 1=high 5=low
Fluid Flow/ Momentum Transport		
A. Fluid Flow of single-phase liquid	See Tier I.	
B. Gas/fluid interface tracking		
B.-1 Mold Filling		
B-1a Single fluid phase	See Tier I.	
B-1b Multiple fluid phases	B1b-II-1. Mold filling visualization experiments with Newtonian single-phase liquids [some in Romero 2001]. B1b-II-2. Non-Newtonian single-phase -- see also Tier III.	2
B-2 Multiple Interfaces/ Bubble dynamics in single liquid phase		
B-2a Isolated bubble nucleation	See Tier I.	
B-2b Single bubble growth & transport through fluid phase	B2b-II-1. Compare level-set formulation to flow visualization of bubble transport through ideal suspension of neutrally buoyant particles. B2b-II-2. Transport through non-neutrally buoyant particles -- see also Tier I and Tier III (C1a-III-1).	3
C. Multiphase flow		
C-1 Particle Dynamics		

Phenomena	Tests Planned or Completed (reference) Tier II	Priority 1=high 5=low
C-1a. Particle hydrodynamic interactions/migration	C1a-II-1. Particle migration of more realistic systems, including gravity effects. C1a-II-2. Neutrally buoyant particle migration in non-Newtonian suspending fluid. see also Tier I and Tier III	1
C-1b Particle nonhydrodynamic interactions	See Tier I.	
C-1c Particle sedimentation	C1c-II-1. Sedimentation in curing systems (excluding 459) [Mondy et al., 1998; Sun 1999; Lagasse & Thompson 2001].	1
C-1d Solid/fluid interface physics/chemistry	C1d-II-1. Completed experiments show that particle surface interactions are very important in 459 [Adolf, 2000; Mondy et al., 2000]. Further data required to determine rheology. See also Tier 3 (C1a-III-1).	1
C-2. Bubble/particle interactions (3-phase flow)		
C-2a. 3 phase flow (sedimentation)	C2a-II-1. Sedimentation of two separate particle phases.	3
C-2b. 3 phase flow (general)	See Tier I.	
C -3. 2-Fluid mixing		
C-3a. Mixing of 2 single-phase fluids	See Tier I.	
C-3b. Mixing of 2 suspensions	C3b-II-1.Model compared to data on single phase liquid mixing with suspension [some available in Romero, 2001].	4

Phenomena	Tests Planned or Completed (reference) Tier II	Priority 1=high 5=low
C-3c. Mixing of 2 suspensions with air entrapment	See Tier I.	
D. Energy Balance		
D-1. Energy transport	See Tier I.	
D-2. Energy production / chemical reactions	D2-II-1. Compare model to temperature/stress data.	2
E. Coupled Energy/ Momentum		
E-1. Epoxy/curative rheology	See Tier III.	
E-2. Extent of reaction (uniformity of cure)	See Tier I.	

Coupled effects include particle movement of idealized neutrally buoyant suspensions in more complex multi-dimensional flows, where stresses in the suspension are difficult to resolve. For example, branching pipe simulations of suspension flow need to be compared with NMR data.

Coupled effects also include situations when both buoyancy and shear rate gradients drive migration. A series of experiments need to be completed and GOMA results compared with each constitutive equation (this will also provide an opportunity to optimize the coefficients describing the particle migration and hindered settling).

Additional experiments are also needed for single bubble transport in a suspension where particles will hamper transport.

Curing of the epoxy (D and E) affects the temperature and viscosity of the suspending epoxy. This process is inherently a coupled process, and rheological studies are required as described in the PIRT section.

Mixing two simple fluids can also be categorized as coupled effects (involving solving equations of motion of each phase and following interfaces). Mold filling studies involving two fluids are also related to this work.

4.5 Tier III

TABLE 4 Validation Test Plan Linked to PIRT

Phenomena	Tests Planned or Completed (reference)	Priority 1=high 5=low
	Tier III	
Fluid Flow/ Momentum Transport		
A. Fluid Flow of single-phase liquid	See Tier I.	
B. Gas/fluid interface tracking		
B.-1 Mold Filling		
B-1a Single fluid phase	See Tier I.	
B-1b Multiple fluid phases	See Tier II. B1b-III-1. Flow of a suspension and a pure fluid [some available Romero 2001]. B1b-III-2. Flow of two suspensions [some available Mondy et al., 1997; Mondy et al., 1998; Romero 2001].	
B-2 Multiple Interfaces/ Bubble dynamics in single liquid phase		
B-2a Isolated bubble nucleation	See Tier I.	
B-2b Single bubble growth & transport through fluid phase	See Tiers I and II.	
C. Multiphase flow		
C-1 Particle Dynamics		
C-1a. Particle hydrodynamic interactions/migration	C1a-III-1. Particle migration in non-Newtonian 459 encapsulant (rheology controlled by surface interactions). See also Tiers I and II.	3

Phenomena	Tests Planned or Completed (reference)	Priority 1=high 5=low
	Tier III	
C-1b Particle nonhydrodynamic interactions	See Tier I.	
C-1c Particle sedimentation	C1c-III-1. Sedimentation in curing 459 system (rheology controlled by surface interactions). See also Tiers I and II.	3
C-1d Solid/fluid interface physics/chemistry	See Tier II.	
C-2. Bubble/particle interactions (3-phase flow)		
C-2a. 3 phase flow (sedimentation)	C2a-III-1. Bubble flow in curing suspension.	4
C-2b. 3 phase flow (general)	See Tier I.	
C -3. 2-Fluid mixing		
C-3a. Mixing of 2 single-phase fluids	See Tier I.	
C-3b. Mixing of 2 suspensions	C3b-III-1. Model comparisons to curing suspensions (slices of interface after mold fill) (some data available: Mondy et al., 2000). See also Tier II	4
C-3c. Mixing of 2 suspensions with air entrapment	See Tier I.	
D. Energy Balance		
D-1. Energy transport	See Tier I.	

Phenomena	Tests Planned or Completed (reference)	Priority 1=high 5=low
	Tier III	
D-2. Energy production / chemical reactions	D2-III-1. Prediction and measurements of temperatures during cure of two suspensions in mold (limited data available: Arris 2000). See also Tier II.	3
E. Coupled Energy/ Momentum		
E-1. Epoxy/curative rheology	E1-III-1. Validation tests during arbitrary flows of filled 459 systems (see also C1d-II-1 and all Tier III tests listed under “C”).	4
E-2. Extent of reaction (uniformity of cure)	See Tier I.	

Actual applications involve mixing many coupled effects. An example is the pour of one suspension (after traveling through a series of pipes and flow splitters, all the while particles are migrating and sedimenting) on another allowing mixing at the interface. The first Tier III suite of model-to-data comparisons would examine the behavior of non-reacting, isothermal suspensions. Through flow visualization studies and instrumented fixtures, the development of concentration profiles, mixing layers, and velocity profiles would be determined. In the actual process, the temperature of the mix is changing with the polymerization reaction, as is the viscosity of the underlying epoxy. These coupled effects would be studied next. Finally, the complex rheology of the 459 encapsulant, where non-Newtonian effects are produced by particle surface interactions, would be included. These many coupled effects are difficult processes to model, yet central to mold filling operations for neutron generators. As such, most Tier III studies will not be performed in the near future.

Once the mold is filled, a period of quiescent settling and degassing occurs. The pressure is lowered and bubbles grow, travel up, and sometimes break at the surface of the fluid. This involves coupling many-body particle interactions with bubble-bubble and bubble-particle interactions. Bubble growth and removal by transport not only depend on material properties (e.g., fluid viscosity, surface tension, and phase purity), but also on conditions (e.g., local pressure, local effective density) that change during the process because of the bubble dynamics itself. The interaction between bubbles and particles is highly dependent on the length scales of the bubbles, particles, and flow channel, and on the distribution of particles and bubbles. Moreover, the flotation of bubbles can affect the distribution of particles. The process also involves competing time scales, as the optimal time needed to degas is often in conflict with the time scale of the ongoing polymerization reaction. Finally, the temperature also affects bubble size and transport. A complete study of the degassing process will necessarily be quite involved. As such, we have lowered the priority of this work.

After degassing, the encapsulant continues to cure and particles continue to sediment (or float). Post-cure x-ray data can determine the final particle distribution. The complex coupled effects of epoxy cure (with a cure schedule that contains steps at several different temperatures), rheology, and particle settling, should be studied in a simple geometry first. Post-cure x-ray data to determine particle concentration profiles can then be compared with GOMA predictions.

4.6 Tier IV

The final validation study would involve the complete process with all phenomena listed in Table 1 present. A well instrumented, well characterized study would need to be performed to compare GOMA predictions to models involving the four uses expected by the production facility. To reduce defects, we would focus on mold filling and degassing and do well instrumented tests, followed with x-ray studies of void locations to compare with predictions. To optimize the process, the model would be exercised to determine the best oven temperatures to minimize particle settling, maximize bubble flotation and minimize overall time in oven. Virtual prototyping could proceed with suggested changes to the encapsulant, such as modifying the standard alumina to use more uniform particles. The effects of the proposed changes in processibilty, defect formation, and cure times could then be explored. Finally, through extensive post-test analysis, the predictions of the final state of particles (and possible voids) could be tested against data, and then used to define the initial state for performance and aging models.

4.7 Summary of Suggested Near-Term Validation Studies

A brief outline of suggested validation simulations and experiments that could be accomplished in the next few years follows. This is by no means a complete description of the proposed work. However, this is intended to be a “living” document and, therefore, this section is envisioned to be updated with every version of this document to describe the validation exercises with the most urgency. Priority, with “1” being the highest, is listed in parentheses. Quarter and fiscal year of the proposed completion date is listed in brackets.

4.7.1 Mold Filling

B1a-I-1.Single Newtonian liquid, 3-D model, compared to data (1) [Q4 FY01]

B1a-I-2. Single Non-Newtonian, experiment and simulation (2) [Q3 FY02]

B1b-II-1. Model compared to mold filling visualization experiments with two Newtonian single-phase liquids (1) [Q4 FY01]
B1b-II-2. Two Non-Newtonian single-phase liquids, experiment and simulation (2) [Q4 FY02]

4.7.2 Multiple Interfaces/Bubble dynamics in single liquid phase

B2b-I-1. Compare level-set formulation to flow visualization of bubble transport through single Newtonian fluid. (2) [Q4 FY01]
B2b-I-2. Non-Newtonian (3) [Q1 FY02]

B2b-II-1. Compare level-set formulation to flow visualization of single bubble transport through ideal suspension of neutrally buoyant particles. (3) [Q3 FY02]
B2b-II-2. Transport through non-neutrally buoyant particles (3) [Q4 FY02]

4.7.3 Particle Dynamics

C1a-I-1. Effects of particle concentration on viscosity (except 459). Only if required for another encapsulant system.
C1a-I-2. Additional data on ideal uniform neutrally buoyant particles -calibration of coefficients and validation. (1) [Q4 FY01]
C1a-II-1.Particle migration of more realistic systems, including gravity effects. (1) [Q2 FY01]
C1a-II-2. Neutrally buoyant particle migration in non-Newtonian suspending fluid. (1) [Q2 FY01]
C1a-III-1. Particle migration in non-Newtonian 459 encapsulant (rheology controlled by surface interactions). (3) [Q4 FY02]

C1c-I-1. Sedimentation in otherwise quiescent fluid. Monodisperse and polydisperse particle sizes. Complete experiments in more complex geometries. Complete modeling at high concentrations and in more complex geometries. (1) [Q3 FY01]
C1c-II-1. Sedimentation in curing systems (excluding 459). (1) [Q3 FY01]

C1d-II-1. Completed experiments show that particle surface interactions are very important in 459 (Adolf SAND, Maven review 00). Gather data required to determine rheology/phenomena. (1) [Q4 FY01]
Model development completed. (2) [Q2 FY02]

4.7.4 Bubble/particle interactions (3-phase flow)

C2a-II-1. Sedimentation of two separate particle phases. (3) [Q3 FY02]

C2a-III-1. Bubble flow in curing suspension. (4) [Q4 FY03]

4.7.5 2-Fluid mixing

C3a-I-1. Newtonian model compared to data. (4) [Q4 FY03]

C3b-II-1. Model compared to data on single phase liquid mixing with suspension. (4) [Q4 FY03]
C3b-III-1. Model comparisons to curing suspensions (slices of interface after mold fill). (4) [Q4 FY03]

4.7.6 Energy Balance

D2-II-1. Compare model to temperature/stress data (2). [Q4 FY01]
D2-III-1. Prediction and measurements of temperatures during cure of two suspensions in mold. (3) [Q1 FY02]

4.7.7 Coupled Energy/Momentum

E1-III-1. Validation tests during arbitrary flows of filled systems, especially 459. (4) [Q4 FY03]

5. Protocols for Stockpile Computing

The aim of the encapsulation flow models in GOMA is to provide design guidance for the manufacturing of polymer embedded components such as neutron generators. For this reason, it is satisfactory for us to predict trends while not having achieved quantitative validation. In other words, if we can manage to produce simulation results that have 60% error, but always produce the correct trends we will have a validated tool to provide input to the encapsulation production team on cure schedule, processing conditions etc. If our validation proves to be within 10% error, we can successfully eliminate testing such a X-ray microscopy, X-rays and full generator performance. At this point in the life cycle of the code, we have required that expert analysts, who are also code developers, conduct the validation activities. This is because model uncertainty dominates our error analysis. The suspension model, for instance, is a constitutive equation that may or may not represent real particle migration in all the flow fields that are necessary to model the encapsulation process. For this reason, we have looked at a number of different constitutive equations as well as improvements to the one that is currently used. However, we can foresee a time in the near future where the code is "qualified" for use in stockpile computing. The following sections discuss the protocols and guidance suggested for use when we reach this stage.

5.1 Qualification of GOMA for Encapsulation Modeling

As we take GOMA through the paces outlined in this document in terms of verification and validation and documentation, along with the peer review process outlined elsewhere [Pilch et al., 2001], we will have developed a high level of confidence in the code and its performance with respect to encapsulation flow modeling. At this point in GOMA's development, the software will be robust and mature in all the significant algorithms for encapsulation and significant model uncertainty will have been eliminated. The code will run through the entire validation test suite and get the same answer, or a new defensible one, when new capabilities are checked into the CVS repository. This level of qualification implies that an expert analyst who can also fix bugs and implement new physics models is no longer necessary as the sole validation analyst. At this point, the code can be given to an analyst on the neutron generator production team who may not necessarily be an expert in meshing, numerical methods or visualization. However, the fact that the code has been "qualified" does not circumvent poor code usage that will give erroneous results. For this reason, an analyst accreditation process must be followed for users of GOMA with regards to stockpile computing applications. The process of accrediting an analysts is given in the following section.

5.2 Analyst Accreditation: Training and Expertise Required

GOMA has a wealth of training documentation and support. Tutorial memos with analogous problems directories (these include input files, material file, geometry, ExodusII output files and reduced output data) have been produced for a wide variety of applications [Schunk and

Labreche, 2001]. A mature user's manual with theory exists [Schunk et al., 1997] and a developers manual with details of the numerical methods and code architecture was recently completed [Schunk et al., 2000]. For most of our users at Sandia and industry, we begin with a GOMA training that goes through the basics of pre- and post-processing, code usage and tutorial example problems. On the second day of the training, the trainer helps new users set up problems of interest. One code delivery model has been pursued with the Specialty Metals Processing Consortium (SMPC) where specific tutorials and problems templates are provided to analysts who are metallurgists with little training in numerical methods. Scripts were developed specifically for the SMPC that allow only a few parameters to be changed such as overall shape of mesh but not topology, material parameters etc. This model has proved successful if a narrow range of applications is to be solved.

For our GOMA encapsulation flow models, we plan to follow a different model where the analyst is trained and accredited to have a high level of functionality. Prerequisites to undergo the accreditation process would be an engineering degree and some knowledge of numerical methods. We envision three levels of accreditation that would be run by the GOMA development team. Level 1 accreditation would imply that the user was familiar with the tutorial examples and can create a mesh, modify the input deck, run GOMA and analyze the results. Level II accreditation would involve a validation test suite that has already been simulated by an expert analyst who has archived the relevant data. The analyst in training would have to reproduce the experts analysts results from the ground up in a blind study, *e.g.* they would be required to create their own meshes, input/material files, run the problem and analyze the output. If a passing grade is received on Level II accreditation (85% or higher), the analyst candidate will be ready for Level III accreditation. Level III accreditation is the highest level achievable. It requires the candidate to run a validation simulation that has not been conducted before. This should be a complex, multiphysics problem and can be viewed as a thesis or research paper. The results would have to be presented and defended to a panel of experts from within Sandia, academia and industry. A passing grade must be achieved to reach Level III accreditation.

5.3 Guidance for Stockpile Computing

Thus far we have not worked out our entire methodology for performing stockpile computing. However, we have developed a few "rules of thumb" that should be generalizable. First and foremost, the analyst who performs these high level/high consequence computations must be either an expert analyst or an accredited analyst. For a simulation that will change a component in the stockpile, we will demand an extensive sensitivity analysis to determine which parameters affect the results the most. Once the analyst has determined the sensitive parameters, parameter uncertainty techniques will be used to bound the results of the calculation, e.g. size of clear zone, and determine a conservative value. It is envisioned that a Monte Carlo, Latin Hyper Cube approach that has been used so successful in waste management and probabilistic risk assessment at Sandia will be followed to reduce the size of the parameter space that must be searched [Iman and Shortencarier, 1983].

In addition to sensitivity studies to insure that the results are conservative and defensible, we will also conduct a double blind study in the center of the parameter space. Another accredited or expert analyst will be sequestered and required to reproduce selected results from the first analyst. If the results do not agree, an independent auditor from the code team would be called in to look for errors, oversights and other differences. Once independently reproducible results have been achieved, the next step in the process would be archiving the results. This would involve working closely with the team's quality assurance officer to insure that all the necessary materials have been saved, stored, labeled and documented in an appropriate fashion. A CD would be created containing the version of the code used for the analysis (source, library and executables needed for the build), input required to run the problem, ExodusII output and postprocessing results. A table of contents would exist elsewhere as a hard copy and as a living document on the web. Many of the protocols used for waste management will be useful here as well and there is much we can learn from other groups at Sandia [see for instance, Rao et al., 1992; Baer et al., 1994].

5.4 Conclusions

In this document, we have outlined the processes that we have undergone and are undergoing to provide qualified software for encapsulation flow models. We have established customer drivers for our analysis and code development efforts. We have investigated the relevant phenomenology of the process of interest and summarized this information in convenient tabular form termed a PIRT. We have also summarized the software quality assurance that has been performed on GOMA and referenced the appropriate documents. Both a verification and validation test plan has been developed along with a time line. In addition, we have provided guidance for accredited use of the encapsulation flow models in GOMA.

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