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date: June 20, 1983

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subject: Status of Core Melt Programs - March-April, 1983

I. Core Melt-Coolant Interactions (CMCI)

1. Intermediate Scale Experiments

The first four EXO-FITS-CM tests have been conducted with the conditions and results summarized in Table 1. The objective of these tests was to investigate the coarse mixing process (using relatively deep water with low subcooling to obtain longer observation time with less likelihood of triggering an explosion). However, all tests to date have produced an explosion triggered at the surface. Through an oversight in test 1 no record was made of the debris remaining in the intact water vessel, but in tests 2 to 4, quenched melt (in the respective amounts 3.8, 4.3 and 3.5 kg) was recovered from the bottom of the vessel remaining. From the high speed photographic records, the surface interaction occurred when the leading edge of the melt had penetrated a few inches into the water. The submerged melt was then driven to the bottom of the vessel with no explosion occurring, while the majority of the melt (still above the water surface) was scattered to distances up to 100 ft. from the interaction site.

The unexpected persistence of surface triggered phenomena in these circumstances has allowed the gathering of coarse mixing data on only portions of the delivered melt. Furthermore, these data, representing a type of forced coarse mixing following the surface interaction, appear somewhat different from those obtained in earlier tests where an explosion was triggered after the melt contacted the base of the water vessel. Future tests in this series will be aimed at understanding this surface triggering phenomenon.

Table 1. EXO-FITS-CM RESULTS

Melt: Iron-alumina. All tests produced surface-triggered explosions after melt had penetrated coolant a few inches.

Test, Date	Melt Mass, kg		Water vessel cross-section x depth, ft^3	Approx. subcooling, °C	Drop height, ft.	Residual melt in vessel, kg
	loaded	delivered				
1 3/22/83	20	18.7	1 x 1 x 4	9	1.0	0
2 4/1/83	20	18.3	1 x 1 x 4	4	1.0	3.8
3 4/19/83	20	18.5	2 x 2 x 4	3	1.5	4.3
4 4/27/83	20	18.9	2 x 2 x 2	3	3.7	3.5

2. Modelling and Analysis of CMCI

2.1 A Comparison of the Computer Codes SIMMER-II and CSQII (J. M. McGlaun)

2.1.1 Introduction

Modelling of steam explosion phenomena is an important aspect of the CMCI program. Steam explosion experiments have been modelled at SNLA with the two-dimensional, multi-material wavecode CSQII [1,2]. Another computer program that could be used to simulate steam explosion phenomena is the two-dimensional, multi-material, LMFBR, fluid-dynamics code SIMMER-II [3]. CSQII was selected for these calculations because it was considered to be a reliable and appropriate code, because of our familiarity with it and because of the very low cost that would be required to evaluate it for CMCI applications. Getting a large code like SIMMER-II running, becoming familiar with the physical models and learning how to efficiently run the code is very expensive and time-consuming. Nevertheless, we recently attempted to assess and compare the physical models and numerical algorithms in the two codes for applications to simulate steam explosion phenomena. The assessment of CSQII is based on the reference manual [1], and our extensive experience in running the code. The assessment of SIMMER-II is based on the reference manual [3], discussions with other staff and our previous code running experience.

2.1.2 Physical Models and Numerical Methods

Both CSQII and SIMMER-II are two-dimensional multi-material codes that calculate the thermo-mechanical behavior of materials. Both of the codes conserve mass, momentum and energy. CSQII uses finite difference approximations to the conservation equations that are second-order accurate for uniform spatial and temporal grids. SIMMER-II uses equations similar to the Kachina equations, [4]. Both codes allow material to be solid, liquid or vapor. CSQII allows up to ten materials in a calculation. SIMMER-II was designed for LMFBR analysis and is restricted to five specified materials: fuel, steel, sodium, control material and fission gas. Both codes assume all the materials in a cell are at the same pressure.

The two codes use different physical models to calculate the temperature of the material in a computational cell. CSQII assumes all the materials in a cell have the same temperature. The temperature of the mixture is selected to conserve energy. This physical model prevents hot and cold material from coexisting in the same computational cell and precludes modelling nonequilibrium effects. This can lead to a non-physical numerical energy transfer from a hot

material to a cold material. SIMMER-II assumes all gases in a cell have the same temperature but each solid and liquid may have its own temperature. This allows hot and cold materials to coexist in the same cell and allows modelling nonequilibrium effects.

The codes use different physical models to handle material interpenetration. CSQII uses a sophisticated interface tracking algorithm to preserve interfaces and inhibit material diffusion as materials move through the mesh. This allows materials to move through the mesh without interpenetrating and mixing. SIMMER-II has no interface tracking scheme so materials will interpenetrate and diffuse when they move through the mesh. This diffusion is strongly dependent on the mesh size.

The assumed geometry of the materials in a cell differs between the two codes. SIMMER-II assumes the liquid is in the form of droplets suspended in a continuous vapor phase. The droplet size determines the surface area which strongly influences the heat transfer between the liquid and gas. CSQII does not assign a particle size to the materials in a cell. It assumes the surface tension energy of the particles is small with respect to the total internal energy. All the materials are at the same temperature so there is no heat conduction calculated between materials in a computational cell.

The equations of state used by the two codes are different. CSQII uses the ANEOS [5] package that calculates a thermodynamically consistent equation of state. Solid, liquid, vapor and mixed phases are simulated by ANEOS. Mixed-phase states are treated as an equilibrium mixture of liquid and vapor. Tabular equations of state may be used by CSQII. A special equation of state for water has been developed for CSQII that reproduces the steam table values. SIMMER-II uses analytic or tabular (SESAME) equations of state. The analytic equations of state are simple and may not be adequate for some materials. Mixed phases are treated as two materials, one liquid and one vapor. This allows nonequilibrium treatment of mixed phase materials. Liquids and solids are assumed incompressible.

Both codes model heat conduction but between different objects. CSQII can calculate both heat conduction and radiation heat transfer between computational cells. This feature has not yet been used on any of the steam explosion calculations. SIMMER-II calculates heat conduction between materials inside a computational cell. Heat conduction is modelled by temperature difference type models. The gas-liquid and gas-solid heat-transfer coefficients are functions of the average thermal conductivity of the vapor mixture, Reynolds number, vapor mixture Prandtl number and

bubble or hydraulic diameter. The liquid-liquid heat-transfer rate is the product of the collision frequency and the energy exchange per collision. SIMMER-II does not calculate heat conduction between computational cells. The only energy transfer between cells occurs due to mechanical work (PdV) and convection of energy with material.

The models used to determine the velocity of the materials are different between the two codes. CSQII assumes the velocity of a material is the velocity of the cell boundary. All materials move with the same velocity, i.e., there is no slip between materials. Rigid interfaces may be defined that coincide with the mesh. SIMMER-II assumes that all liquids move at the same velocity and that all vapors move at the same velocity but these two velocities may be different. Solid material is stationary. Drag forces between materials moving at different velocities are calculated and included in the momentum balance. The liquid-vapor drag correlation results from a combination of Stokes flow over a sphere for low Reynolds numbers and a form drag correlation for spheres for high Reynolds numbers.

Donor cell methods are used for convecting momentum and energy with the mass moved between cells. CSQII uses a second-order accurate convection scheme with a monotonicity restriction that inhibits oscillations, [6]. SIMMER-II uses a first order accurate convection scheme that assumes the material properties are uniform across a computational cell. The user may input parameters that control interpolated values (higher order accurate values) but these schemes can generate oscillations because no monotonicity restriction is used.

CSQII has a rezone capability but SIMMER-II does not. This allows CSQII to run the early portion of the calculation with a fine mesh, then rezone to a coarse mesh to speed the calculation of the late time behavior. If a fine mesh was used in SIMMER-II to inhibit the material diffusion, then the fine mesh would have to be used throughout the calculation.

2.1.3 Conclusions

It is not clear that SIMMER-II would give a better answer than CSQII or vice versa. Each code has its strengths and weaknesses and one might give a better result for a part of the problem than the other. CSQII has a non-physical numerical energy transfer arising from the assumption that all the materials in a computational cell have the same temperature. SIMMER-II has a non-physical numerical material transfer (diffusion) because of the assumption that all materials in a cell are well mixed (no interface tracking). Some of the intra-cell exchange function physics

in SIMMER-II may be ineffective because the temperatures may not be accurately calculated by the simple equations of state.

The numerical energy transfer in CSQII will make it difficult to analyze the late-time part of the problem after the pressures have equilibrated but should not seriously influence the early time pressure driven phenomena. The numerical material transfer in SIMMER-II may drive the calculation away from the correct answer as the materials move through the computational mesh. The simple equations of state may negate the multi-temperature feature of SIMMER-II because the heat conduction is based on the temperature differences and the temperatures may not be accurately calculated by the simple equation of state.

CSQII can do an adequate job of calculating the early time behavior, e.g. pressure wave propagation and motion of material. CSQII may not be the best tool for analyzing the late time pressure and temperature because it is strongly influenced by the energy flow between the liquid and vapor. SIMMER-II has the features to handle the late time energy flow between materials if the equations of state are adequate and there is no hydrogen burn. The numerical material transfer may make an accurate, early portion of the calculation. With SIMMER-II, one does not have the option of running the early part of the problem with a finely zoned mesh to inhibit material transfer and then rezoning to a coarser mesh to speed the calculation when the materials are well mixed.

We tentatively conclude the following: At very low cost (approximately 0.5 man-year), we have demonstrated that CSQII can do an adequate job of evaluating CMCI experiments. Although it is possible that SIMMER-II could be modified to do similar calculations, we are certain that the cost would be much higher. We do not currently feel that this additional cost is justified to meet the program's needs.

2.2 Monte Carlo Analysis of Steam Explosions

(D. V. Swenson, A. J. Wickett, M. Berman)

The first draft of a report on the new Monte Carlo analysis of steam explosions has been prepared. At this point, despite substantial research, the principal conclusion is that the combined uncertainty of the containment failure probability from an invessel steam explosion is still large. The new results show that the most important parameter (affecting both lower plenum failure and containment failure) is the pour diameter of melt from the core barrel into the lower plenum: this directly affects the mass of molten core that can participate in the steam explosion.

Additional details will be given in the appropriate semiannual report.

2.3 Analysis and Modelling of CMCI
(M. L. Corradini)

During the last two months we have begun work in a number of areas:

(1) We are participating with N. A. Evans in assisting A. Benjamin in short term calculations for rebaselining previous predictions for the RSSMAP and IREP, in regard to the steam spike phenomena and core melt-coolant mixing during ex-vessel interactions;

(2) We are developing a model for the minimum film boiling point considering sphere size and velocity; this effort seems to be able to explain data on film collapse on solid spheres of different sizes and may explain triggering of the single droplet tests of Nelson. We also intend to apply it to the variable triggering processes observed in the FITS experiments, considering noncondensible gases;

(3) We have a conceptual model for fuel melt fragmentation in the single droplet experiments of Nelson. The model is a follow-on of the initial efforts of vapor film collapse and Taylor instability growth. It is actually a synthesis of many past ideas on fuel fragmentation gathered together in a mechanistic framework. Film collapse calculations are now underway;

(4) Finally, we are developing a model for the expansion phase of the interaction. These expansion dynamics are important for the mechanical energy derived from a steam explosions (as identified by the Steam Explosion Review Committee), and also for steam spike considerations and core melt dispersal in ex-vessel situations where an explosion may or may not occur.

References

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II. Molten Core/Concrete Interactions
(R. K. Cole, Jr., D. P Kelly, M. A. Ellis)

1. New CORCON Models

The new crust-formation/freezing model was installed as described in our last letter, to produce Version 1.02.00. We are continuing to gain experience with it, and searching for possible problem areas. A calculation for the sample problem included in the CORCON-MOD1 manual, including this model, was carried out through 10 hours of interaction time. The results showed solidification of 10 cm on the bottom of the metal layer, and 20 cm on its side, and of a few millimeters on the surface of the oxide at the end of this time. The principal effect of the crust model, compared to a calculation using Version 1.02.00 with the model disabled, is a change in the shape of the eroded cavity. The total concrete erosions predicted by the two calculations were the same within a fraction of a percent, demonstrating the degree to which the problem is dominated by conservation of energy. The shape change was caused by a decrease in ablation by the metal as its interfaces with concrete solidified, and a compensating increase in ablation by the oxide. (The temperature of the oxide increased in response to the increased thermal resistance in the downward direction.)

Concurrent with this effort, we have begun development of the coolant-layer model. Other work has slowed progress, and the model is not yet operational, but no problems have been encountered.

2. Other Code Modifications

As part of the clean-up following the definition of Version 1.02.00, we have eliminated several unnecessary violations of ANSI coding standards. The resulting code, with two heavily commented exceptions, is accepted by most, if not all, current extensions of the 66 and 77 standards. (The extensions involved are generalized DATA statements and subscript forms compared to the 66 standard, and use of HOLLERITH data not included in the 77 standard.) Some additional checks on input were also implemented.

3. Interaction With the MELCOR Program

The MELCOR program involves development at Sandia Laboratories of a suite of codes to replace the current MARCH/MATADOR/CRAC sequence currently used for Severe Accident PRA work. As a part of this effort (and funded by it) we have written a summary description and evaluation of the models now used in the calculation of core/concrete interactions. Models included in codes other than CORCON, and other models that have never

been implemented in any code, were included in the evaluation. One significant conclusion of this work is that, in several areas, CORCON models involve significant "overkill" for PRA purposes (and possibly for other purposes, given the uncertainties in other models). Most prominent among these are the inclusion of many trace species in the compositions of the pool and of the gaseous products of the metal/gas reaction, and the extremely detailed spatial resolution of heat transfer at the pool/concrete interface. The possibility of simplification was not, of course, obvious at the time the detailed models were developed, and has only been learned through experience with these models. It would be advantageous to both programs (CORCON and MELCOR) to develop a "stripped" core/concrete interactions code, based primarily on CORCON. This could be used in MELCOR exactly as the INTER code (which was intended as a qualitative tool only) is in MARCH, while providing guidance as to which models in the full code could be simplified without significant loss.

4. Assessment

The question of a validation document for CORCON (MOD1) has been raised because of the use of CORCON in NUREG/CR 0956 ("Radionuclide Release under LWR Specific Accident Conditions," Volume I). Following discussions with Dr. Burson, we constructed an outline and a partial draft of such a report. (We appreciate fully the need for an independent assessment, but believe that the code developers themselves are in the best position to supply some of the information required for such an effort...nobody else could develop the detailed knowledge of the code's strengths and weaknesses in any reasonable amount of time.) One (minor) result of this exercise was the development of statistics on code size and internal documentation. The following table compares MOD1 (with C1 and C2 correction sets) with Version 1.02.00.

	MOD1	1.02.00
Lines of FORTRAN statements	5400	5700
Lines of non-blank comments	1200	1600
Lines of blank comments	900	1100
Total lines	7500	8400
Core required (octal) on Cyber 76	105000	64000

The volume of comments has grown faster than the volume of FORTRAN and, despite inclusion of the crust-formation/freezing model, Version 1.02.00 requires 25 percent less core than MOD1. We will continue to expand internal documentation and control code growth through the development of MOD2. Our assessment of CORCON-MOD1 during this reporting period has progressed to a point where three out of the four sections of

tests have been completed. The final two model sensitivity tests, transport properties and material properties, were completed. The metallic and oxidic mixture transport properties tested included viscosity, thermal conductivity, and surface tension. The first two transport properties, viscosity and thermal conductivity, were found to significantly affect heat transfer coefficients, and thus, the cooling rates of the melt. Layer surface tension was found to have much less of an effect on the primary results (e.g., concrete ablation and gas generation). The material properties tested included layer density and specific heat. Like viscosity and thermal conductivity, layer density is used in the calculation of heat transfer coefficients. Therefore, it was not surprising that changes in this material property impacted layer heat transfer and overall thermal behavior of the melt. Unlike the layer density, the layer specific heat does not enter into the calculation of the gas film heat transfer coefficients, but does in the calculation of the various pool layer heat transfer coefficients. Therefore, variations in specific heat (in the heat transfer coefficients only) had a less dramatic affect on the partition of decay heat, and thus, the ablation of concrete.