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June 13, 1994

Dr. A. Behbahani
U. S. Nuclear Regulatory Commission
Office of Nuclear Regulatory Research
Accident Evaluation Branch
Division of System Research
Mail Stop TWF-K8
Washington, D. C. 20555-0001

Subject: **Ex-vessel calculations for the CE System 80+ using GT3F computer code. Contract No. NRC 92-04-045, Task Order 4.**

Dear Dr. Behbahani,

Attached please find a review of the results of GT3F calculations for CE System 80+ performed at Georgia Institute of Technology (memorandum from H. Esmaili to M. Khatib-Rahbar dated June 13, 1994) and the report entitled "Analysis of Ex-Vessel Steam Explosions for the Combustion Engineering System 80+ Using the *GT3F™* Computer Code." If you have any further questions, please do not hesitate to contact me.

Sincerely,

M. Khatib-Rahbar

cc: H. Esmaili, ERI
ERI/NRC-045 file

MEMORANDUM
ENERGY RESEARCH, INC.

TO: M. Khatib-Rahbar

FROM: H. Esmaili H.E.

SUBJECT: CE System 80+ Ex-vessel Calculations Using GT3F Computer Code

DATE: June 13, 1994

I have reviewed the results of the CE system 80+ ex-vessel FCI calculations performed at Georgia Institute of Technology using GT3F computer code by Drs. Abdel-Khalik and Ghiassian. These results were transmitted to ERI in the form of a report entitled "An Analysis of Ex-Vessel Steam Explosions for the Combustion Engineering System 80+ Using the *GT3F™* Computer Code (June 1994)." They were requested to perform three simulations using the initial and boundary conditions established in ERI/NRC 94-201 which are listed below:

(1) Scenario-A base case assuming a single instrument tube penetration failure (0.03 m diameter) in the central region of the lower head.

(2) Scenario-A base case assuming a single instrument tube penetration failure (0.03 m diameter) on the side of the lower head near the corbel supports (see Figure 6, page 31 of ERI/NRC 94-201, showing the lower head penetrations). These side penetrations are approximately 0.1-0.2 m away from the corbel supports.

(3) Scenario-A with 8 instrument tube penetration failures in the central region of the lower head (sensitivity case S-4 in ERI/NRC 94-201).

In addition, the code was used to simulate KROTOS-21 test to obtain insights into the fragmentation model parameters and achieve best agreement with the experimental data. These parameters were subsequently used in the CE System 80+ calculations. A discussion of the particle breakup (premixing phase) and fine fragmentation (propagation phase) models was also provided.

There are a number of comments and concerns regarding these calculations that I will try to expound further in the following sections.

I. General Comment

In all the plant calculations using GT3F, the water pool temperature was set at 393 K (saturated pool). The saturated water pool condition leads to higher local vapor void fractions as the melt enters the pool and exchanges energy with the coolant. A higher local vapor void fraction somewhat mitigates the maximum pressures that can be reached in the explosion zone. In the

three scenarios mentioned above, the water pool temperature was assumed to be 353 in ERI/NRC 94-201 (the water pool was subcooled by 40 K). Therefore, it is not possible to directly compare the GT3F results with TEXAS and IFCI calculations. However, a sensitivity case using TEXAS with a saturated water pool was performed in ERI/NRC 94-201. In that calculation, there was a 40% reduction in the maximum explosion pressure (and a corresponding 30% reduction in the local pressure impulse) when the water pool temperature was raised to 393 K.

II. Central Instrument Tube Failure

II.1 The axial length of the computational domain was 5.4 m, thus the top of the computational domain appears to be a free surface. There is no discussion on the imposed boundary conditions during the premixing and propagation calculations.

II.2 The fuel volume fractions in the computational domain at various times during the premixing calculation are shown in Figure 2.3. The melt is observed to reach the bottom of the coolant pool between 1 to 1.25 seconds (TEXAS and IFCI predictions have shown that the melt would only penetrate to the bottom of the corbel support in 1 second). This implies that the average melt velocity should be approximately 5 m/s in the water pool, thus indicating that the melt particles hardly slow down as they travel in the water pool. In addition, there is practically no radial dispersion of the melt jet, i.e., the melt remains primarily in the inner radial node.

II.3 The distributions of the vapor void fraction in the axial direction in the computational domain exhibit cell like structures of high local vapor void fractions. The cause of this behavior is not explained.

II.4 It is stated on page 2 of the report that "*Triggering was assumed to take place on the axis of symmetry of the jet, 4.1 m above the bottom of the liquid pool which corresponds to the mid plane elevation of the submerged portion of the corbel supports.*" From Figure 2.1 in the report, the mid plane elevation of the corbel support region is at 4.5 m. It is further stated that "*Triggering was simulated in the code by assuming that, at the triggering time, 10% of the molten fuel in node (1,21) underwent complete fragmentation in one time step (2 μs).*" It is not clear how these values were selected. For example, if the initial fragmentation was 20%, would the resulting explosion pressures be affected?

II.5 The report states on page 4 that "*The pressure impulses predicted by the TEXAS code are significantly higher, however, and are in the 12 to 42 kPa-s range.*" The TEXAS predicted pressure impulses for the saturated pool (which is the case in the GT3F calculations) ranged from 3 to 31 kPa-s corresponding to the explosion zone and should not be compared to impulse loads on the corbel support wall. Unfortunately, the pressure impulses in the explosion zone were not reported for the GT3F calculations. These values should be reported.

II.6 The propagation phase of the interaction was simulated using two radial node sizes of 3 cm and 6 cm. The report states on page 4 that "... *the predicted peak pressures are considerably higher for the smaller radial node size.*" and it further states that "... *reducing the radial node size ... had a slight effect on the predicted pressure impulse distributions.*" The peak pressures in the explosion zone from Figures 2.10 and 2.11 show that by increasing the radial node size from 3 cm to 6 cm, the peak pressure is decreased from about 16.5 bars (node 1,17) to about 14.5 bars (node 1,19) suggesting a 12% decrease. I do not consider this a significant change. The pressure impulses on the corbel support show the reverse trend, i.e., increasing the radial node size tends to increase the pressure impulse (albeit it is only a slight variation). In addition, even the radial node size of 3 cm does not resolve the boundary of the melt jet (the radius of the melt jet is 1.5 cm). This may have an impact on the particle breakup (see also comment VI.2).

II.7 The maximum pressure at the corbel support (Node 50,17) is approximately 13 bars compared to the maximum pressure of 16.5 bars in the explosion zone at node 1,17 (see Figure 2.10) which indicates that the mitigating effect of radial pressure decay is minimal. The pressure history at node (50,17) indicates that by the end of the simulation (15 ms), the pressure at the corbel support has not significantly decreased. Therefore, it appears that the GT3F predictions of the maximum impulse on the corbel support would be even higher than indicated, had the simulation been continued for a longer time period.

III. Outer Instrument Tube Failure

III.1 As far as premixing is concerned, the same comments (II.1, II.2, and II.3) also apply here.

III.2 The maximum pressure in the explosion zone is approximately 72 bars (Figure 3.9) which is substantially higher than the previous case with a central instrument tube failure even though the mass of melt in the coolant pool is similar for both cases. For this case however, the diameter of the computational domain (30 cm) was significantly smaller (compared to 300 cm for the central instrument tube failure). This was done primarily to perform two-dimensional calculations in polar cylindrical coordinates. The effect of confinement is a possible source of this discrepancy. In reality, however, such confinement does not exist and one would expect similar pressures in the explosion zone for both cases if the melt fragmentation rates are the same. For an outer instrument tube penetration, a simulation with a larger computational domain should be reported to correct this non-physical behavior. The simulation can be performed by increasing the radial extent of the computational domain and placing a flow obstruction to simulate the presence of the corbel support.

IV. Multiple Instrument Tube Failures

IV.1 The results of the propagation calculations for this case is suspect since the explosion pressures are significantly lower than the other two cases even though the mass of fuel is increased by a factor of eight. This has been reflected in the report.

IV.2 The report states on page 8 that "*Such low concentrations of molten fuel are evidently unrealistic, and do not provide the necessary conditions for a steam explosion ...*". Clearly, given the selected radial nodalization for this simulation, the low fuel concentration was expected. I am confused as to why it was decided to proceed with this calculation using the coarse nodalization when the authors knew that an energetic explosion would not occur. The results of the propagation calculation, therefore, are nonsensical as mentioned previously (see comment IV.1).

V. Recommendations for Future Work

V.1 It is recommended in the report to perform the propagation calculations for the central and outer instrument tube failure cases by assuming that the triggering occurs at the bottom of pool upon fuel impact. The rationale for these additional calculations are not clear. From the results of the premixing calculations, it is evident that fuel impact with the bottom of the pool occurs between 1 to 1.25 seconds (see also comment II.2). Therefore, as far as premixing results are concerned, the distributions of the coolant and fuel are not expected to be significantly different. If the point is to examine the effect of triggering, no clear evidence has been offered as to how this variation would change the results. Also, considering the fact that the size of the computational domain in the outer instrument tube failure may not be adequate (see comment III.2), I do not think that additional calculations would shed any new light on the results.

V.2 The report suggests that the simulation with failure of multiple instrument tube penetrations be repeated with a finer radial mesh since the results of this simulation is questionable. However, the authors also maintain that a two-dimensional calculation even with a finer radial nodalization may not be adequate and they recommend a three-dimensional calculations. I do not recommend three-dimensional calculations at this point since these simulations are very time consuming. In addition, performing a three-dimensional calculation with a small slice of the actual system domain (1/4 of the cross-sectional area) may not be reasonable given the nonuniform distribution of the lower head instrument tube penetrations and lack of adequate experimental validation of the parametric fine fragmentation model in the GT3F computer code (see also comment VII.2).

VI. Particle Breakup and Fine Fragmentation Models in GT3F Computer Code

VI.1 Equation (21) should be written as,

$$V_{r,c} = \left| \frac{\alpha' \rho_1 \overline{U}_1 + (1-\alpha')\rho_2 \overline{U}_2}{\rho_c} - \overline{U}_3 \right| \qquad (21)$$

and in equation (19), *rho*$_c$ should be replaced by ρ_c.

VI.2 It is not clear from the discussion on pages 68 and 69 of the report how the particle breakup model is actually implemented in the code, i.e., how is the interfacial surface area between the melt and coolant calculated given the particle breakup model (Equation 19).

VI.3 On page 69, the report states that "*The latter limit is imposed based on the model validation with experimental data ...*". The limit refers to the lower bound particle diameter of 1 cm during the premixing calculation. Do the authors refer to the KROTOS-21 test as the experimental data or are there any other justification for the specification of this lower limit? It also appears that specification of a lower limit brings into question the validity of the breakup model (Equation 19) in the GT3F computer code.

VI.4 For the fine fragmentation model during the propagation phase of the interaction, the fragmentation criteria is based on a critical Weber number and the rate of fragmentation is given by Equation (18). If the melt particles start to quench and solidify, is there a provision in the code to cease fragmentation? The constant of proportionality in Equation (18) has been specified as 1/6. Is this an adjustable parameter or is the critical Weber number criteria the only model parameter? For example, the GT3F fragmentation model is similar to the model employed in the ESPROSE computer code[1]. However, in the ESPROSE formulation, an enhancement factor is introduced to the fragmentation rate to account for possible thermal effects on fragmentation rate.

VII. Simulation of KROTOS-21 Steam Explosion Experiment

VII.1 There is no discussion of the radial nodalization.

VII.2 Apart from the fact that multiple explosions were observed for the lower We number of 30, the first peak pressures (and also pressure wave arrival time) at locations K3 and K4 show better agreement with the experimental data compared to the simulation using We=100 (note also that last transducer was located in a region with a large local void

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[1] T. G. Theofanous et al., "Steam Explosions: Fundamentals and Energetic Behavior," NUREG/CR-5960, (1994).

fraction and may not be considered reliable[2]). It is not clear why the propagation calculations with We=30 demonstrate multiple explosions. It appears that more validation of the computer model is required by benchmarking it against different tests. For example, KROTOS-26 and KROTOS-28 tests produced very energetic explosions (peaks pressures in excess of 50 MPa were observed in KROTOS-28 test) and at this point there is no reason to believe that the Weber number specification of 100 would still be applicable under these conditions (even the constant of proportionality in Equation 18 may have to be modified). In light of these observations (e.g., see comment VI.4), do the authors believe that the fragmentation model and the model parameter (Weber number) in the GT3F code can be universally applied to other experiments and the plant calculations?

cc: A. Behbahani, NRC
F. Eltawila, NRC
S. Abdel-Khalik, GT
S. M. Ghiassian, GT

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[2] M. Burger et al., "Examination of Thermal Detonation Codes and Included Fragmentation Models by Means of Triggered Propagation Experiments in a Tin/Water Mixture." *Nuclear Engineering and Design*, **131**, 61-70 (1991).

S.I. ABDEL-KHALIK

Consultant
3579 Midvale Cove
Tucker, GA 30084

June 3, 1994

Dr. M. Khatib-Rahbar, President
Energy Research, Inc.
6290 Montrose Road
Rockville, MD 20852

Subject: Consulting Contract ERI-NRC-04-92-045, Ex-Vessel Steam Explosion Study for CE System 80+

Dear Dr. Khatib-Rahbar:

In accordance with the statement of work specified in your letter of April 12, 1994 under the above-referenced contract, we have performed the following fuel-water interaction calculations using the GT3F^{TM} computer program:

(1) Scenario-A base case assuming a single instrument tube penetration failure (0.03 m diameter) in the central region of the lower head

(2) Scenario-A base case assuming a single instrument tube penetration failure (0.03 m diameter) on the side of the lower head, 0.15 m away from the corbel support

(3) Scenario A with 8 instrument tube penetration failures in the central region of the lower head

The results of the calculations are described in the enclosed report, where the above cases (1), (2), and (3), are addressed in Sections 2, 3, and 4, respectively. Per your request, the details of the fragmentation models incorporated in GT3F^{TM} are also provided in Appendix A of the enclosed report. We also simulated, and performed parametric calculations for, the KROTOS Test # 21, whereby the GT3F^{TM} fragmentation model was adjusted to match the model-predicted and experimentally-measured pressure peaks. KROTOS Test 21 simulation and parametric calculations are described in Appendix B of the enclosed report.

Based on the calculated results, we recommend that the following additional analyses be performed.

(1) The propagation calculations reported here for single central and outer instrument tube penetration failures (cases (1) and (2) above) were based on the assumption that triggering occurred on the centerline of the melt jet one second after the initiation of premixing, at 4.1 m above the bottom of the water pool (midplane of the submerged corbel support). Similar calculations with triggering initiated at the bottom of the water pool upon melt impact should be performed.

(2) The two-dimensional (r,z) simulation of the multiple instrument tube penetration failure (case (3) above) in the polar cylindrical coordinates, as described in the enclosed report, is inadequate and results in unrealistically low pressure peaks. This case should be reanalyzed, using finer radial nodes. Additionally, a three-dimensional (r,θ,z) analysis is recommended.

We appreciate the opportunity to work with you on this interesting project. Please feel free to call either one of us if you have any questions.

Sincerely,

S.I. Abdel-Khalik
Consultant

S.M. Ghiaasiaan
Consultant