IMPROVEMENT AND VERIFICATION OF
FAST REACTOR SAFETY ANALYSIS TECHNIQUES

Progress Report

James F. Jackson
Department of Chemical Engineering
Brigham Young University
Provo, Utah

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ABSTRACT

A number of improvements and refinements have been made to the VENUS-II analysis of the KIWI-TNT experiment. The final calculations for this study are now being performed. Areas of difference that appeared during the initial VENUS-II/PAD intercomparison study have been investigated and largely resolved. In particular, the treatment of the energy-of-vaporization was examined and found not to have a significant effect on the calculated temperatures. The next round of comparison calculations are currently underway. A study aimed at comparing and evaluating different methods of characterizing work-energy or damage-potential of core-disruptive accidents has been initiated.

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INTRODUCTION AND SCOPE

The progress described in this report is broken into four subtask areas. Three of these areas (VENUS-II Experimental Comparisons, Accident Characterization, and Code Acquisition) correspond directly to subtasks identified in the 189a. The fourth area is a combination of two subtasks (VENUS-II/PAD study and Disassembly Analysis Comparison Studies).

VENUS-II/PAD INTERCOMPARISON STUDY

There were two main areas of difference noted in the initial round of VENUS-II/PAD intercomparison calculations.^{1,2} First, it was noted that the VENUS-II peak temperature increases were somewhat larger than those predicted by the PAD code. Second, the VENUS-II work potentials were considerably larger than the material kinetic energies calculated by the PAD code. Both of these areas of difference have now been investigated and it appears they can be resolved in the next round of calculations.

It was initially thought^{1,2} that the disagreement in the peak temperatures might be related to the different treatment of the latent heat-of-vaporization in the two codes. In particular, the VENUS-II code does not explicitly account for the energy of vaporization. This is because the corresponding states calculations that served as a basis for the equation-of-state indicated that the effect of vaporization was insignificant within the range where the code is applicable. The equation-of-state in the PAD code, on the other hand, treats the energy of vaporization via the Clausius-Clapeyron equation. Since the VENUS-II

temperatures were considerably higher, it was decided to determine whether this could be due to neglecting the heat-of-vaporization.

Estimates of the energy of vaporization can be obtained from the Clapeyron equation. This is a rigorous thermo-dynamic relationship and can be written in form³

$$\frac{dP}{dT} = \frac{h_v}{T \left(\frac{1}{\rho_v} - \frac{1}{\rho_l} \right)} \quad (1)$$

where:

P = equilibrium vapor pressure

T = absolute temperature

h_v = latent heat of vaporization

ρ_v = vapor density

ρ_l = liquid density

The vapor latent energy density, $\rho_v h_v$, can be obtained directly from equation (1), and takes the following form

$$\rho_v h_v = \left(1 - \frac{\rho_v}{\rho_l} \right) T \frac{dP}{dT} \quad (2)$$

The energy required to produce sufficient vapor to fill a volume, V_r , is then given by

$$E_v = \rho_v h_v V_r \quad (3)$$

In situations where the vapor pressure is relatively low, it can be assumed that $\rho_v \ll \rho_l$. In this case, equation (2) reduces to

$$\rho_v h_v \approx T \frac{dP}{dT} \quad (4)$$

and $\rho_v h_v$ can be obtained directly from the vapor pressure expression.

This approach has been used previously⁴ to estimate vaporization energy

and is the basis for the approach used in the POOL code⁵ (which was one of the codes included in the intercomparison calculations).

It should be noted that equation (4) is not valid for conditions approaching the critical point. As the critical point is approached, ρ_v approaches ρ_ℓ and h_v approaches zero. This behavior would be correctly predicted by equation (2), but not by equation (4). Use of equation (4) in this regime would tend to over-estimate the energy going into vaporization.

If in addition to assuming $\rho_v \ll \rho_\ell$ one assumes that the vapor-phase can be treated as an ideal gas, then equation (4) can be readily transformed into the Clausius-Clapeyron equation.

$$\frac{dP}{P} = \frac{h_v}{R T^2} dT \quad (5)$$

Finally, if it is further assumed that h_v is independent of temperature, equation (5) can be integrated to give

$$P = (\text{const}) e^{\frac{h_v}{RT}} \quad (6)$$

This is the form of the vapor pressure expression used in the PAD code. This expression should provide reasonable results at conditions well below the critical point, but would tend to underpredict the temperature increase as the temperature approaches the critical point.

Qualitatively then, the situation can be summarized as follows. The VENUS-II approach tends to overestimate the temperature increase associated with a given fission-energy deposition by ignoring the energy required to produce fuel vapor. This approach was taken because the corresponding states calculations on which the VENUS-II equation-of-state

is based indicated that the vaporization energy was insignificant over the range of conditions typically encountered in disassembly calculations. The PAD code, on the other hand, explicitly accounts for the energy of vaporization, but does so with an approach that tends to overestimate the effect (and therefore underestimate the temperature increase) at conditions approaching the critical point. It should also be noted that the vaporization energy effect is most significant at conditions near the critical point where the vapor density starts to rapidly increase.

In order to assess the accuracy of the VENUS-II treatment, a number of calculations were performed to determine the magnitude of the vaporization energy for various disassembly conditions. This was done by starting with equation (2). The vapor pressure expression in VENUS-II has the form

$$P = \exp(a \ln T + \frac{b}{T} + c), \quad (7)$$

so that equation (2) becomes

$$\rho_V h_V = P(a - \frac{b}{T}) (1 - \frac{\rho_V}{\rho_L}) \quad (8)$$

The vapor density, ρ_V , was estimated from the law of rectilinear diameters which states⁶

$$\frac{\rho_L + \rho_V}{2} = \rho_C + D (T_C - T)$$

where:

ρ_C = critical density

T_C = critical temperature

D = a constant determined from known low temperature conditions

A typical computational mesh-cell was considered that had equal volumes of liquid fuel and fuel vapor. The temperature increases that

would result from various increases in internal energy were calculated with and without the consideration of the energy of vaporization. The error that resulted from ignoring the heat of vaporization is plotted in figure 1 as a function of the final temperature. Thus, this figure shows how much the VENUS-II code overestimates the calculated temperatures as a result of neglecting the heat of vaporization.

The peak fule temperature in case A1 of the initial comparison calculations was 5620°K (see Ref 1). It is seen from figure 1 that the error in this calculation is less than 0.3% or about 16°K. Thus, the 860°K difference between the VENUS-II and PAD calculations was not a result of ignoring the vaporization energy in VENUS-II.

It is interesting to note that the maximum error in the VENUS-II temperature calculations is only a few percent and peaks at about the critical temperature (8000°K). The fractional error decreases above the critical temperature because further liquid-vapor phase transition cannot occur. Since expansions much larger than those considered in these sample calculations are usually not encountered in VENUS-II calculations, it appears the assumption that the energy of vaporization can be ignored in VENUS-II is well justified. In most calculations of interest, the final temperatures are rarely above about 6000°K, so that the maximum error would only be about 1%.

It turned out that the differences in the calculated peak temperatures were largely due to having an incorrect peak-to-average power in the distribution set up for the spherical geometry PAD calculations. This will be corrected in future calculations.

Figure 1. Error in VENUS-II calculated temperatures that results from neglecting the heat-of-vaporization.

The second area of difference was the comparison of the PAD kinetic energies to the VENUS-II work potential results. As noted previously¹, these results are not directly comparable because the PAD calculations were terminated at an elevated pressure which the VENUS-II calculations considered an expansion down to 1 atm. Two options have recently been added to the VENUS-II code to provide full P-V-Work expansions. One of the options was described briefly in the previous progress report². The second option was recently developed at ANL⁷ and is based on the Clausius-Clapeyron relationship. Use of these expansions will allow a comparison of the work-potentials and kinetic energies at comparable pressures.

Other minor modifications to the intercomparison cases have been agreed upon and the final cases are being run.

VENUS-II EXPERIMENTAL COMPARISONS

The initial analysis of the KIWI-TNT excursion described in the previous progress report has been carefully evaluated. On the basis of this, a number of improvements and corrections have been implemented into the calculation.

Many of the improvements were related to different aspects of the equation-of-state. For example, a new vapor pressure expression was developed that provides a more accurate fit to Mantell's data⁸ in the temperature range above 4500°K. This new expression has the form

$$P_v = 0.388 \times 10^{17} \exp [1.04 \times 10^5/T]$$

where:

P_v = vapor pressure in dynes/cm²

T = temperature in °K

The single-phase pressure formulation was also corrected to provide phase-transition points that were in better agreement with available bulk expansion data. The earlier formulation had led to single-phase pressures at somewhat lower temperatures. This caused a premature disassembly of the core and a subsequent decrease in the fission energy release.

A new method of calculating the temperature changes from an explicit temperature-dependent specific-heat for graphite was also implemented. Previously, the heat capacity was implicit in an internal-energy temperature relationship derived from corresponding states calculations. The approach was modified to provide better agreement with measured values of the heat capacity.

Finally, a study of the high temperature behavior of graphite indicated that accounting for the energy of sublimation could be significant when calculating large displacements. It was desired to carry out the calculations to rather large expansions to allow comparison of the calculated core and reflector boundary motion with experimental measurements.⁹ As a result, considerable effort went into developing a technique for accurately accounting for this effect. This involved developing explicit expressions for temperature dependent solid and vapor-phase densities.

Other areas of improvement included implementing better reactivity worth distributions and initial delayed neutron concentrations.

VENUS-II calculations including all of the above improvements are being carried out. Results to date predict a total energy release that is somewhat larger than the initial calculations presented earlier.²

The power burst is turned over mainly because of the negative temperature coefficient with a vapor pressure driven disassembly providing ultimate shutdown of the system. A final version of the calculation will be completed and documented during the next quarter.

An initial VENUS-II calculation of the SNAPTRAN-2 excursion was also completed. A preliminary evaluation indicated an improved equation-of-state for ZrH_2 was needed. A new equation-of-state has been developed along the lines of the graphite equation-of-state being used in the KIWI-TNT calculations. Improvements in the reactivity worth distributions also appeared necessary, and such improvements are currently being pursued.

ACCIDENT CHARACTERIZATION

A study to intercompare and evaluate various characterizations of work-energy has been initiated. The initial stage of the study is being based on calculations previously performed on the FTR. These calculations are being used because the REXCO damage evaluation calculations have already been performed. The REXCO calculations are an essential part of the intercomparison and are the most difficult to perform of the various work-energy approaches being considered.

Plans are also being made to extend the study to larger sized systems. Some of the VENUS-II/PAD intercomparison calculations discussed earlier will be useful in this regard, since they are being performed on a demo-sized reactor. The final stage of the study will consider a 1000 Mw system.

CODE ACQUISITION

A special code⁷ to calculate the P-V-Work expansion following a VENUS-II calculation has been obtained from ANL and implemented into our version of VENUS-II. This calculation is being used in both the VENUS-II/PAD comparison calculation and the accident characterization study. It is also being compared with a similar type calculation derived from corresponding states calculations.²

The ANL parametric model¹⁰ has been made operational for use in the accident characterization study.

Final check-out of the telephone link to the CDC-7600 computer at Berkeley is underway.

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