PROMPT BURST ENERGETICS (PBE) EXPERIMENT ANALYSES USING THE SIMMER-II COMPUTER CODE

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ABSTRACT

Two of the Prompt Burst Energetics (PBE) in-pile experiments conducted at Sandia Laboratories PBE-5S and PBE-SG2, have been investigated with SIMMER-II. These two tests utilize fresh uranium oxide and fresh uranium carbide pins, respectively, in stagnant sodium. The purpose of the analysis is to investigate the applicability of SIMMER-II to this type of experiment. Qualitative agreement with measured data is seen for PBE-5S. PBE-SG2 results agree somewhat less well but demonstrate SIMMER-II's potential for describing fuel-coolant-interactions with further model development.

INTRODUCTION

The Prompt Burst Energetics (PBE) experiments[1,2] are a series of in-pile tests conducted at Sandia Laboratories in the Annular Core Pulse Reactor (ACPR) and more recently in the Annular Core Research Reactor (ACRR). These experiments are designed to evaluate the pressure behavior of fuel and coolant as working fluids during a hypothetical prompt burst disassembly in an LMFBR. Herein we present preliminary analyses of PBE-5S, an oxide fuel experiment, and PBE-SG2, a carbide fuel experiment. These analyses have been performed with the SIMMER-II[3] accident-analysis computer code developed at Los Alamos Scientific Laboratories.

The purpose of the Sandia/LASL SIMMER PBE analysis program is threefold: (1) to investigate the usability of SIMMER in analyzing these complex experiments, (2) to provide insight into the separate pressure-generation and pressure-quenching mechanisms in these experiments, and finally (3) to provide information for model development and verification for the ongoing SIMMER evaluation effort. These preliminary calculations are, of necessity, mainly for demonstration purposes although some information concerning separate mechanisms in the experiments can be garnered. Impact on SIMMER model verification requires additional more extensive calculations.

The initial series of PBE experiments use a single fuel pin in a fluted channel. Pressure transducers are mounted at the top and bottom of the channel. Also, at the top of the channel there is a movable piston connected to a linear motion transducer. For both experiments listed above, the channel is filled with sodium. A complete description of the initial series of PBE experiments can be found in References 1 and 2 and in a paper by Reil and Young at this meeting.[4]

In the experiments the pressure data recording locations are substantially removed from the pressure source. Therefore, to determine the effects of channel geometry it is necessary to perform detailed hydrodynamic calculations.[5] Also, measured pressures are not necessarily the result of fuel vapor pressure alone and, therefore, the effect of fuel-to-coolant heat transfer must be included in the analysis. The SIMMER-II computer code, which was used to perform these analyses, is a two-dimensional, multi-phase Eulerian code that includes material motion, shock propagation and heat transfer models among other effects. Reference 3 contains a detailed description of the SIMMER-II computer code.

PBE-5S ANALYSIS

The initial SIMMER analysis was performed on the PBE-5S uranium oxide pin experiment which is not atypical of the sodium-in oxide series as a whole. In this experiment the pin was failed using a single maximum pulse in the ACPR which resulted in an axial peak energy deposition of about 2350 J/g in the 14% enriched fuel pin. The experimental configuration was modeled in SIMMER as shown in Figure 1. The model consists of a single fuel pin in a coolant channel below a movable piston. Failure is assumed to be a full circumferential break 10 mm high with an area of approximately 1.3×10^{-4} m^2. The calculation was started at the point of pin failure with initial conditions obtained using the EXPAND pin failure code.[6] These initial conditions are summarized in Table I. Coefficients of the analytical equation-of-state for UO_2 in SIMMER were based on Reil's upper energy curve[7] and the Benson data.[8] Two radial and three axial temperature zones were described within the fuel pin with a peak temperature of 4648 K and a corresponding vapor pressure of 20.0 MPa. The initial temperature of the coolant and structure material was set at 770 K with a pressure of 0.28 MPa. Nuclear heating from the tail of the pulse was included.

Analysis of the PBE-5S was started at pin failure and extends 2.0 ms into the transient. The experimental diagnostics included pressure histories taken at both the top and bottom of the pin and the piston displacement. A direct comparison of the predicted and measured pressure trace characteristics is shown in Figure 2 and summarized in Table II. Discrepancies occur in the magnitude of the initial pressure peak, in the frequency of the pulses and in the decay of the pressure train. The calculation has not been run far enough into the problem to determine the conversion efficiency of thermal into kinetic energy. The calculated pressure was found to be predominately due to fuel vapor pressure. Although the calculations do not indicate any significant sodium vapor pressure, its presence cannot yet be precluded. Further experiments will be required to provide confirmatory evidence.

In the SIMMER analysis the magnitude of the initial pressure peaks are underpredicted by about 30%. However, this error is within the uncertainty in the energy deposition and in the fuel equation-of-state. The slope of the fuel vapor pressure curve is so steep that a 7% increase in the peak temperature doubles the initial pressure in the pin. The misprediction of the frequency of the pressure pulses is most probably due to geometric modeling approximations for the pressure vessel. In sensitivity studies on model changes, it was observed that the inclusion of the sodium fill tubes located at the top and bottom of the vessel significantly decreases the frequency of the pressure train by increasing the effective sodium path length.

Causes for the slow pressure decay in the calculation are more difficult to isolate. The rate of decay is controlled by the pressure source at the break location, the quenching mechanisms in the channel, and for the top

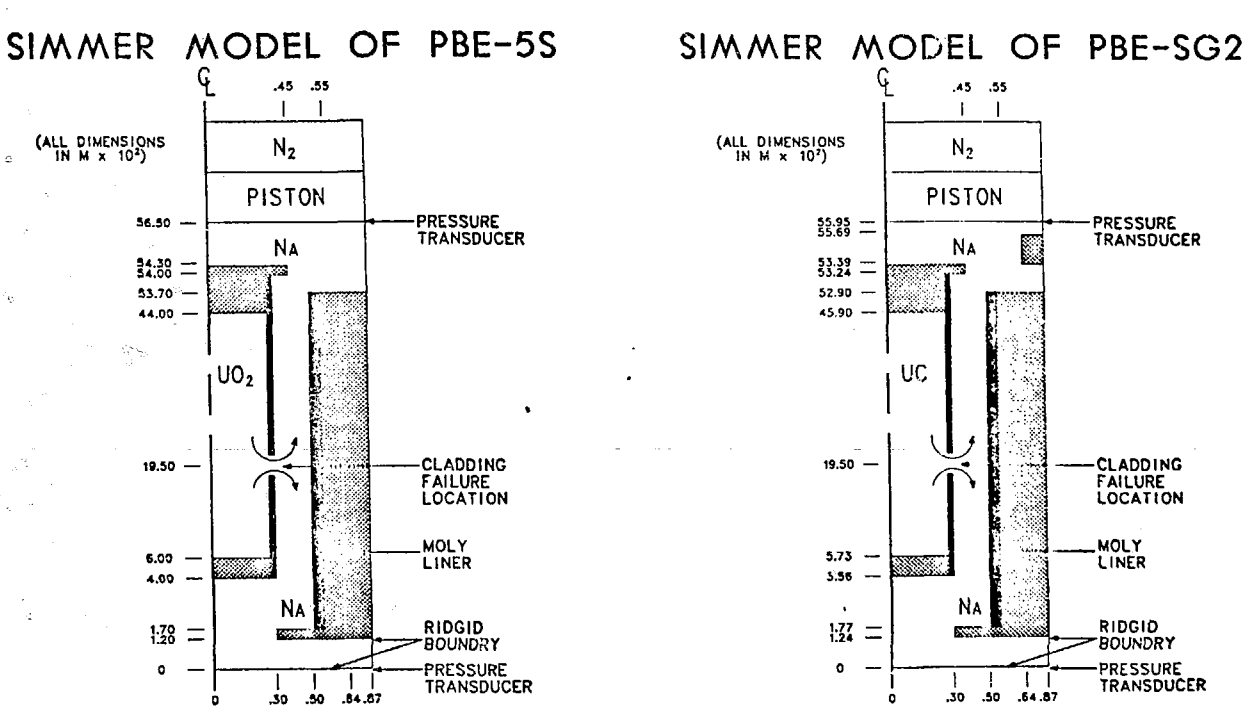


Figure 1. SIMMER MODELS

Table 1. SIMMER INITIAL CONDITIONS

	PBE-5S	Case 1	PBE-SG2 Case 2	Case 3
Fuel Type	UO_2	UC	UC	UC
Fuel Mass (Kg)	6.4×10^{-2}	8.0×10^{-2}	8.0×10^{-2}	8.0×10^{-4}
Fuel Temp (K)	Peak 4648	Uniform 6942	Peak 6942	Peak 6098
Fuel Vapor Pressure (MPa)	20.0	20.0	20.0	4.5
Sodium Temp. (K)	770	770	770	770
Area of Cladding Break (m^2)	1.8×10^{-4}	1.8×10^{-4}	1.8×10^{-4}	1.8×10^{-4}
Cladding Temp. (K)	770	770	1500	880
Top Boundary	Free Piston	Rigid	Free Piston	Free Piston
Bottom Boundary	Rigid	Rigid	Rigid	Rigid

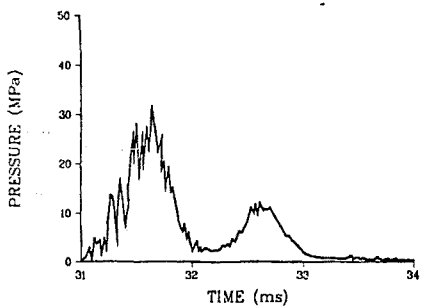
Table II. PBE-5S RESULTS

	Measured		Calculated	
	Top	Bottom	Top	Bottom
First Peak (MPa)	31.0	46.0	21.3	29.4
FWHM (ms)	0.35	0.28	0.45	0.25
Second Peak (MPa)	12.5	22.5	18.3	30.9
FWHM (ms)	0.40	0.32	0.53	0.40
First/Second Pressure Ratio	2.5	2.0	1.2	0.95
Period Between First and Second Peak	1.05	0.63	0.67	0.39
Bottom/Top Pressure Ratio of First Peaks	1.48		1.38	

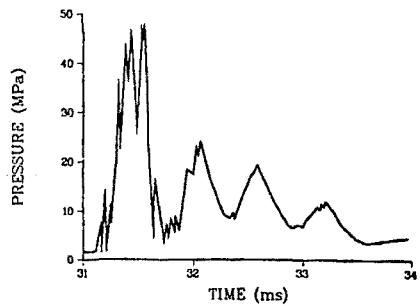
Table III. PBE-SG2 RESULTS

		SIMMER-II Calculations		
	Experiment	Case 1	Case 2	Case 3
Peak Pressure at Bottom (MPa)	190	160	82	67
Peak Pressure at Top (MPa)	170	175	70	57
Peak Pressure in Interaction Zone (MPa)	--	120	109	80
Pressure Ratio Top/Bottom	0.89	1.09	0.85	0.85
Mass of Fuel in Coolant Channel (Kg)	--	3.5×10^{-3}	3.0×10^{-3}	2.5×10^{-3}

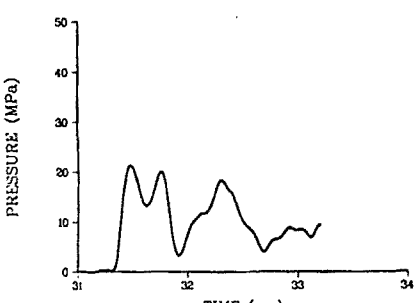
PBE-5S TOP PRESSURE TRACE



PBE-5S BOTTOM PRESSURE TRACE



CALCULATED TOP PRESSURE TRACE



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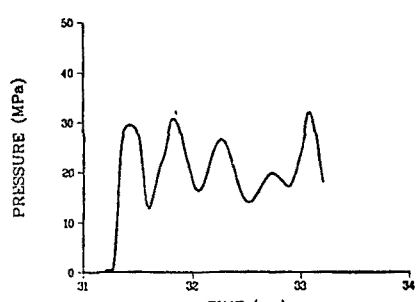


Figure 2. PBE-5S PRESSURE TRACES

transducer location, the motion of the piston. Poor modeling approximations in any of these areas could result in errors in the pressure decay. The rather coarse temperature grid used in the analysis may sustain the pressure source at too high a level. With a large peak temperature zone, little mixing and no inter-nodel conductive heat transfer (a SIMMER constraint), the temperature inside the pin decreases slowly and the fuel vapor keeps the channel pressure pumped up. Inside the channel phase changes were calculated using the single component vaporization/-condensation model in SIMMER. A component of the vapor field is allowed to condense only on structure or on its own liquid field component. Thus, fuel is not allowed to condense on liquid sodium. In the PBE experiments this quenching mechanism could be very important. Finally, the molten fuel-sodium heat transfer has a pronounced effect on the pressure generation. It is difficult to assess the accuracy of the heat transfer calculations in SIMMER. Additional experiments dealing with isolated fuel coolant interaction phenomena are needed to examine the accuracy of the modeling assumptions, especially in regard to droplet sizes and contact area.

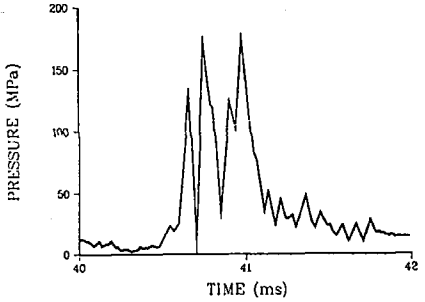
PBE-SG2 ANALYSIS

The PBE-SG2 carbide experiment utilized a 15% enriched UC-fuel pin which was failed with a single pulse in the ACPR. The radial average deposition at the axial peak was 2420 J/g. Because of uncertainties in the time of failure and in the thermodynamic state of the fuel at failure in the PBE-SG2 experiment, the analysis was performed parametrically. Figure 1 shows the SIMMER model constructed for this analysis. It has essentially the same configuration as the PBE-5S model. Initially, the fuel pin is filled with a uniform density of UC and the coolant channel with sodium. All materials excluding the fuel pin are initially at 770 K and 0.28 MPa. Three SIMMER calculations, each beginning at pin failure, were made using the PBE-SG2 model. Case 1 used a uniform initial fuel temperature of 6942 K and a corresponding fuel vapor pressure of 20 MPa. This temperature is based upon the peak energy deposition in the pin. For this calculation the top channnel boundary was assumed to be rigid. In cases 2 and 3 axial and radial temperature distributions based on EXPAND calculations were applied to the fuel at the time of failure. Also, the top boundary condition was changed to a free piston. In case 2 the initial peak fuel temperature was 6942 K and the initial fuel vapor pressure was 20 MPa. For case 3 failure was assumed to occur at 4.5 MPa fuel vapor pressure which corresponds to a peak fuel temperature of 6098 K. This pressure was chosen because a 4.5 MPa leading ramp was measured immediately before the major pressure events in the experiment. Case 3 included power generation in the fuel after failure. These initial conditions are summarized in Table I.

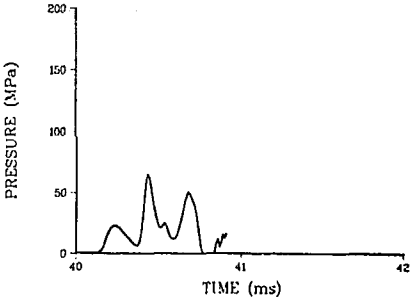
Experimental pressure traces for PBE-SC2 along with calculated results for cases 1, 2, and 3 are shown in Figure 3. A summary of experimental and calculated results is presented in Table III. At the bottom pressure transducer location the measured peak experimental pressure is approximately 190 MPa while the corresponding calculated pressure in case 1 is about 160 MPa. At the top pressure transducer location, the measured experimental peak is about 170 MPa while the calculated peak pressure in case 1 is approximately 175 MPa. These pressures are predominantly due to sodium vapor generation. The discrepancy in the ratio of top to bottom pressure peaks is a result of the rigid top boundary condition which exists in case 1.

In case 2 peak pressures calculated at both the top and bottom transducer locations are about half those in the experiment although peak pressures calculated in the interaction zone in the coolant channel at the break location are nearly the same for cases 1 and 2. Pressure generated in the interaction zone

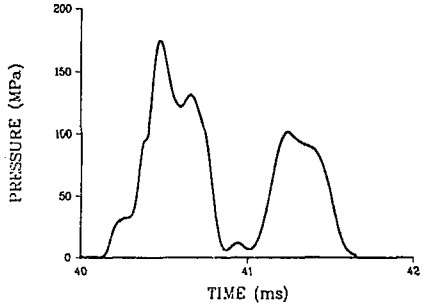
PBE-SG2 TOP PRESSURE TRACE



CALC. 2 TOP PRESSURE TRACE



CALC. 1 TOP PRESSURE TRACE



CALC. 3 TOP PRESSURE TRACE

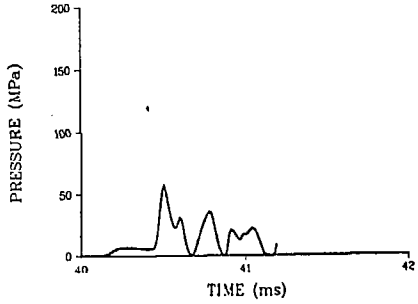
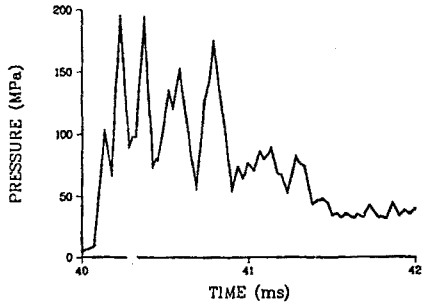


Figure 3. PBE-SG2 PRESSURE TRACES

PBE-SG2 BOTTOM PRESSURE TRACE



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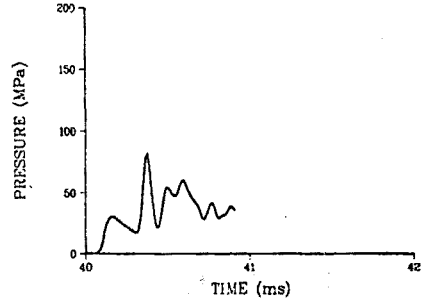

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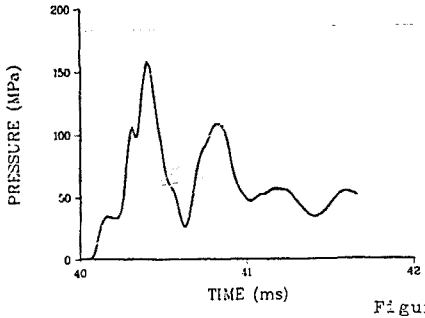

CALC. 3 BOTTOM PRESSURE TRACE

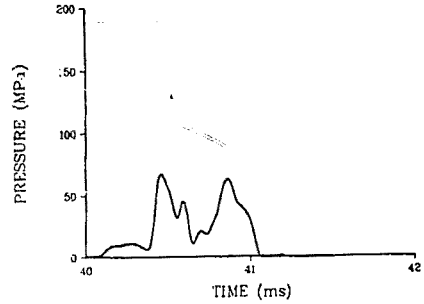

Figure 3 Continued

decays much more rapidly in case 2 than in case 1 which leads to a relief wave apparently catching the initial shock wave and preventing doubling upon reflection at the axial boundaries. The short duration of the initial pressure pulse in case 2 results from a smaller mass of fuel and sodium mixing than in case 1, a consequence of the initial variable temperature distribution. Although a variable temperature distribution more closely approximates reality, it adversely affects the agreement in these calculations. Case 3 results are about the same as case 2 except that peak pressures are somewhat lower. In cases 2 and 3, which include a piston model at the top boundary, the ratio of the amplitudes of the top and bottom pressure pulses agree reasonably well with the experiment. This ratio reflects the channel acoustics.

In all three SG2 calculations the interaction zone pressures are due to supercritical sodium and not to thermal expansion of subcooled liquid sodium. This is in contrast to the MURTI analysis presented at this meeting[9] which indicates that the pressure source is from nearly isochoric heating of cold single phase liquid. Calculated peak sodium temperatures are above 3000 K and the volume fraction of supercritical sodium in the pressure generating cells at the time of peak pressure is very high (80-90%). In the SIMMER calculations liquid fuel-sodium mixing occurs on a small scale (approximately the cell size of 2 mm), and it occurs in cells which are axially bounded on one side by cells filled with fuel vapor, liquid fuel and small amounts of sodium vapor, and on the other side by liquid sodium. The fuel-coolant interaction cells are partially voided before appreciable liquid fuel-sodium mixing occurs. This analysis probably underestimates mixing because SIMMER has no liquid-liquid slip.

CONCLUSIONS

The main conclusions that can be drawn from the analysis are as follows:

1. In the PBE-5S calculation there is no significant sodium vapor generation. The calculations suggest that the pressure source in the experiment is due to fuel vapor alone.

2. Compared to the PBE-5S experimental pressure traces, the SIMMER calculated pressure traces exhibit a different period and a different pulse width. These differences are probably a result of insufficient geometric detail in the SIMMER model.

3. In the SIMMER calculation of PBE-5S, attenuation of the pressure wave does not match the experiment. Among the modeling changes which might improve this result are a more detailed initial fuel pin temperature distribution and use of multicomponent condensation in SIMMER.

4. SIMMER analysis of PBE-SG2 suggests that the pressure source in the experiment is supercritical sodium and not thermal expansion of subcooled liquid sodium.

5. The PBE-SG2 analyses demonstrate that through the use of SIMMER (with its current standard heat transfer and hydrodynamic models) it is possible to generate FCI sodium pressures of the magnitude observed in the experiment, although the physical mechanisms for explosive FCIs are not represented accurately in the code.

In summary, although these preliminary SIMMER-II calculations were run only a few milliseconds into the PBE problems, they demonstrate that with model refinements SIMMER can become a valuable analysis tool for such experiments. Specific changes to SIMMER which would improve its ability to predict the thermal and hydrodynamic behavior in small scale experiments would be: (1) internodal conductive heat transfer, (2) temperature-dependent material properties, (3) relative liquid velocities and a fragmentation model, and (4) a pin model. Experiments dealing with isolated fuel coolant interaction (FCI) phenomena are needed to further develop FCI models in SIMMER.

ACKNOWLEDGMENT

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