Proceedings of the ASME 2019
Pressure Vessels & Piping Conference
PVP2019
July 14-19, 2019, San Antonio, TX, USA

PVP2019-93292

TUNABLE EOS MATERIAL MODEL IN THE SIMULATION OF PULSED MERCURY SPALLATION TARGET VESSEL

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ABSTRACT

A pulsed spallation target is subjected to very short (~1μs) but intense loads from repeated proton pulses. The effect of this pulsed loading on the stainless-steel target module that contains flowing mercury target material is difficult to predict. Different simulation approaches and material models for the mercury have been tried. To date the best matching simulation to the experimental data was obtained by an equation of state (EOS) material model with a specified tensile cutoff pressure, which simulates the cavitation threshold [1]. The inclusion of a threshold to represent cavitation was a key parameter in achieving successful predictions of stress waves triggered by the high energy pulse striking the mercury and vessel. However, recent measurements of strain responses of target modules showed that significant discrepancy between the measured strain and simulated value with the EOS mercury model still exists. These differences grow to irreconcilable values when non-condensable helium gas is intentionally injected into the flowing mercury. A novel EOS mercury model embedded into ABAQUS VUMAT has been investigated in this project, which introduces the concept of proportional, integral, and derivative (PID) control into the mercury EOS model. By tuning the new introduced PID parameters (Kp, Ki and Kd), we replace the specified cutoff pressure with an adjustable spring-damper-like material behavior which may better match the complex dynamics of the mercury and helium mixture. This approach is expected to reduce the gap between measured and simulated vessel strain responses. Primitive application of this tunable EOS mercury model on prototypic shape experimental target has demonstrated its capability and potential of improving mechanical behavior of EOS mercury with cutoff pressure considered.

Keywords: EOS, PID, material model, mercury spallation target, simulation, VUMAT, cavitation.

NOMENCLATURE

β	Hg volumetric expansion coefficient
ε	strain
ρ	Hg density
ρ_0	reference density
η	nominal volumetric compressive strain
η_{lim}	limiting compression
Γ	Grüneisen ratio
Γ_0	Grüneisen material constant
c_0	constant in Us-Up Hugoniot equation
e(t)	error between PID output and setpoint
$\dot{e}$	deviatoric part of strain rate
p	pressure in Mie-Grüneisen equation of state
p_{bv}	pressure due to bulk viscosity
p_H	Hugoniot pressure
r(t)	setpoint of PID loop
s	constant in Us-Up Hugoniot equation
t	time
u(t)	output of PID loop
Cv	Hg constant volume specific heat
E_H	specific energy (per unit mass)
E_m	internal energy per unit mass
Eshear	shear energy
K	Hg bulk modulus of elasticity
K_d	derivative coefficient
K_i	integral coefficient
K_p	proportional coefficient
P	Hg pressure
$\dot{Q}$	heat rate per unit mass
S	deviatoric stress tensor
Us	shock velocity
Up	particle velocity

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INTRODUCTION

In a sufficiently superheated liquid, the energy deposited by an energetic particle can cause local boiling that, after a short time, leads to a bubble of visible size. This effect was sought and observed in 1952 by Donald Glaser, during the course of his well-thought-out and persistent search for a new device that could reveal the tracks of high-energy particles [2, 3]. Since then the idea of bubble nucleation by the local formation of vapor evolved gradually. However, although a fundamental reason for the discrepancy was thus identified, quantitative agreement between the calculated and measured pressure threshold for bubble formation, although improved, was still very poor compared with the agreement achieved by Riepe and Hahn's bubble chamber results [2, 4].

Besides the theory development of local boiling and cavitation in superheated liquid, efforts of experimental measurements in this kind of superheated liquid has never stopped. Particularly for mercury, in 1953 Briggs measured the cavitation threshold of mercury in Pyrex glass using his spinner method [5]. Experiments by Taleyarkhan et al. and Moraga with mercury that had not been thoroughly degassed led to cavitation at less than 1 bar of negative pressure [6, 7]. These experimental studies in return provided more validation data for further development of mercury model [1, 2, 8-11].

Pitting damage on target's inner vessel wall, which is caused by the mercury, has been noticed for a long time [8, 12]. To keep the structural integrity and extend the vessel life as long as possible, non-condensable helium gas is intentionally injected into the flowing mercury to relieve this damage. The injected helium gas, along with the bubbles in mercury, has complicated the liquid behavior and grown the differences between simulations and experimental measurements to irreconcilable value. The instinct change of target fluid from pure mercury to a mixture of mercury and gas requires a further development of material model, which can describe its complexity and help predict the response of this solid-fluid coupled target structure. A novel mercury material model introduced in this article will take an initial try, expecting to reduce the gap between measured and simulated vessel strain responses.

Novel Mercury Model Embedded in VUMAT

ABAQUS user subroutine VUMAT is used to define the mechanical constitutive behavior of a material [13]. In general, the Target model includes two materials, the stainless-steel vessel and the liquid mercury in the vessel. Challenges of dynamic simulation mainly come from the mercury material, due to the couple of complex physical response such as fluid dynamics, thermal hydraulics, cavitation, etc.

The beam tests on Prototypic-shape (PS) target were conducted during August 2000 [1]. Fig. 1 shows the outlook of the target main body constructed from type 304L stainless steel. Mercury flows inside the channels of the steel body, sending off neutron beams and taking away the heat deposited by the high energy proton beam. To investigate the response of this PS target that undergoes high frequency pressure pulses arising from the rapidly deposited proton beam energy, a quarter section, 3D finite element model of the PS target was developed using shell elements (ABAQUS element S4R) for the vessel walls and baffle and continuum elements (ABAQUS C3D8R) for the mercury and back flange [1]. Fig. 2 depicts this 3D finite element PS model, along with its boundary conditions. More details of the quarter symmetry PS model can be found in Ref [1].

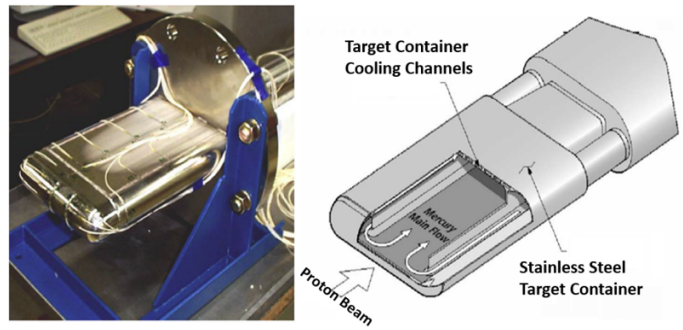

FIGURE 1: PROTOTYPIC-SHAPE TARGET WITH STRAIN SENSORS[1, 9]

The 3D PS target model employs only two materials: type 304L stainless steel and mercury. Material density and Young's Modulus were set as 8000 Kg/m3, 195.1 GPa respectively for 304L steel. For mercury a more complicated material model, the equation of state (EOS), has been introduced by considering its hydrodynamic material behavior. The EOS option is displacement/strain based and thus accounts for volume changes of the material. Here in ABAQUS the Linear Us–Up Hugoniot form was adopted in mercury's EOS material model. Mercury's initial density and wave speed are specified at ρ_0 = 13500 kg/m3 and c_0 = 1456 m/s. As no true shock phenomena are involved, the Grüneisen constant Γ_0 and particle speed coefficient ~~S~~ s are set to zero. Previous investigations have indicated that the practical onset of cavitation occurs at only a few bar tensile pressure [1]. A typical tensile failure value of 0.15 MPa was assigned in that PS model mercury material to achieve reasonable strain response when compared with experimental measurements from attached strain sensors.

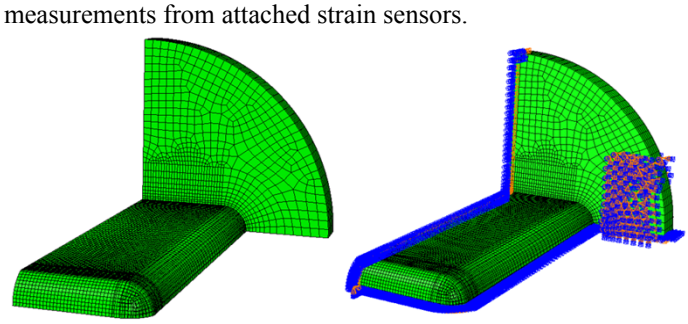

FIGURE 2: QUARTER MODEL OF PS TARGET AND ITS BOUNDARY CONDITIONS

Energy deposited from each proton pulse was transferred into initial stress field [1] that can be directly applied on the mercury elements. The proton pulse energy data is converted to incremental pressure by[10]:

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$$dP = Q \cdot \frac{\beta K}{\rho C_V} \qquad (1)$$

where

Q = volumetric energy deposition [J/m3]

β = Hg volumetric expansion coefficient = 183.0x10-6/°C

K = Hg bulk modulus of elasticity = 28.6 GPa

ρ = Hg density = 13500 Kg/m3

C_v = Hg constant volume specific heat = 140.0 J/Kg-K

In this simulation a total energy of 2.1 kJ was deposited from the proton beam pulse that happened in a short duration of no greater than 300 ns [10]. Distribution of the converted pressure field is illustrated in Fig. 3. A very short time duration (1ms) after the initial stress pulse was analyzed by using ABAQUS/Explicit to investigate the dynamic response of the Mercury-Steel integrated target structure.

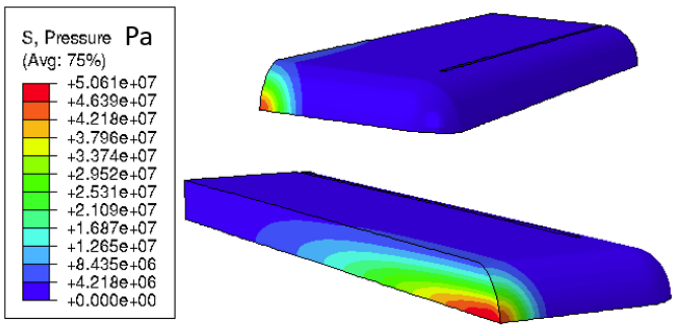

Figure 3: MERCURY'S INITIAL PRESSURE FIELD CONVERTED FROM PROTON PULSE

In previous simulations, the tensile cutoff stress played as a key parameter to improve the mercury's EOS Us-Up model when aligned with experimental sensor strains. It represents the cavitation in mercury flow under the proton pulse load, which significantly changes the speed of stress wave propagating through mercury and affected the response of steel vessel eventually. The selected failure mode was PRESSURE=DUCTILE along with ELEMENT DELETION=NO [10]. This provides a pressure – volume relationship that limits hydrostatic tension to a specified cutoff value, but regains stiffness once pressure tries to go above this value. Used with the EOS Us-Up behavior, mercury elements reaching this cutoff threshold acts an as impedance barrier. When pressure returns to above the cutoff pressure the nominal wave speed is restored. Therefore, this tensile failure cutoff tried to simulate the effect of mercury cavitation in terms of the wave speed change, rather than really create cavitated elements in mercury volume. This tensile failure behavior was homogeneously applied to all the mercury elements in the 3D model.

ABAQUS provides many inherited EOS material models, like the Us-Up model and the tensile failure behavior mentioned above, that can be implemented by configurating model parameters in its .inp file or through its CAE interface. These inherited models have prevented users from wasting a huge amount of efforts and cost in the development of unnecessary repeated wheels. In the meantime, ABAQUS opens up its user subroutine, i.e. VUMAT [13], to release even more freedom of integrating any user defined material behavior into its explicit solver.

A Mie-Grüneisen equation of state is linear in energy [13]. The most common form is

$$p - p_H = \Gamma\rho(E_m - E_H) \qquad (2)$$

where p_H and E_H are the Hugoniot pressure and specific energy (per unit mass) and are functions of density only. Γ is the Grüneisen ratio defined as

$$\Gamma = \Gamma_0\rho_0/\rho \qquad (3)$$

where Γ_0 is a material constant and ρ_0 is the reference density. The Hugoniot energy, E_H, is related to the Hugoniot pressure by

$$E_H = pH\eta/(2\rho_0) \qquad (4)$$

where $\eta = 1 - \rho_0/\rho$ is the nominal volumetric compressive strain. Elimination of Γ and E_H from the above equations yields

$$p = p_H(1 - \Gamma_0\eta/2) + \Gamma_0\,\rho_0\,E_m \qquad (5)$$

For linear Us-Up Hugoniot form:

$$p_H = \rho_0 c_0^2\,\eta/(1 - s\eta)^2 \qquad (6)$$

$$U_s = c_0 + sU_p \qquad (7)$$

$$p = \rho_0 c_0^2\,\eta(1 - \Gamma_0\eta/2)/(1 - s\eta)^2 + \Gamma_0\,\rho_0\,E_m \qquad (8)$$

where $\rho_0 c_0^2$ is equivalent to the elastic bulk modulus at small nominal strains, and s is the dimensionless coefficient for Us-Up model. There is a limiting compression given by the denominator of this form of the equation of state $\eta_{lim} = 1/s$.

The equation for conservation of energy equates the increase in internal energy per unit mass, E_m, to the rate at which work is being done by the stresses and the rate at which heat is being added. In the absence of heat conduction, the energy equation can be written as:

$$\rho\frac{\partial E_m}{\partial t} = (p - p_{bv})\frac{1\partial\rho}{\rho\partial t} + S{:}\dot{e} + \rho\dot{Q} \qquad (9)$$

where p_{bv} is the pressure due to bulk viscosity, S is the deviatoric stress tensor, $\dot{e}$ is the deviatoric part of strain rate and $\dot{Q}$is the heat rate per unit mass. Assuming no adiabatic heating and no bulk viscosity, Eq. (9) can be simplified as

$$\rho\frac{\partial E_m}{\partial t} = \frac{p\partial\rho}{\rho\partial t} + \frac{\partial E_{shear}}{\partial t} \qquad (10)$$

where E_{shear} is the shear energy. For each small time increment in VUMAT, if we consider p as the average for that short time duration, increment of E_m can be calculated through

$$\Delta E_m = (p + \Delta p/2)/\rho^2 + \Delta E_{shear} \qquad (11)$$

$$\Delta\rho = \rho\,\Delta\varepsilon \qquad (12)$$

The small increment of pressure at (t+1) time moment can be determined by differentiating Eq. 8, which is contributed by the change of density in Eq. 12 and the change of Em in Eq. 11 at its previous time moment (t).

$$\Delta p_{t+1} = f(p_t, \rho_t)\Delta\rho_t + g(E_{m_t})\,\Delta E_{m_t} \qquad (13)$$

The equation of state and the energy equation represent coupled equations for pressure and internal energy. All the pressure, strain, density and energy variables from Eq. 2 to Eq. 13 can be accessed from the VUMAT interface that ABAQUS provides. The additional material constants can be defined in USER MATERIAL section in ABAQUS's input file, which will be fed through the VUMAT interface and involve in the update of pressure, internal energy as well. The tensile failure cutoff of

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mercury can be defined as a constant in USER MATERIAL section to realize the same user experience as the EOS model ABAQUS has integrated. Instead, assigning the tensile failure cutoff value in VUMAT subroutine will provide additional benefit in case that the cutoff values must be inhomogeneously distributed among the mercury elements rather than an identical constant. In VUMAT when the elemental stress reaches or exceeds the tensile failure threshold, the cutoff value will take over and hold there for consecutive increments until a lower stress appears. Abaqus/Explicit solves these equations embedded in VUMAT simultaneously at each mercury material integration point and updates its elemental pressure and density at each time increment.

Employing the same material parameters as provided in reference [10], EOS model with tensile failure threshold implemented in VUMAT has achieved the same simulation results. Fig. 4 shows the comparison between the custom-developed VUMAT EOS and the previous implementation using EOS model ABAQUS has provided. At the time of 1.0e-5 s, both models produce equivalent distribution in either deformation or stress. The calculated maximum Von-Mises stresses of both simulations, which are located at the same shell steel elements near the front nose, match well with a difference of ~1%. Note that both Fig. 4 (a) and (b) plot out Von Mises stress of mercury elements as well, and the values are mostly close to zero (in blue color) due to their identical principal stress components and very small shear stress components.

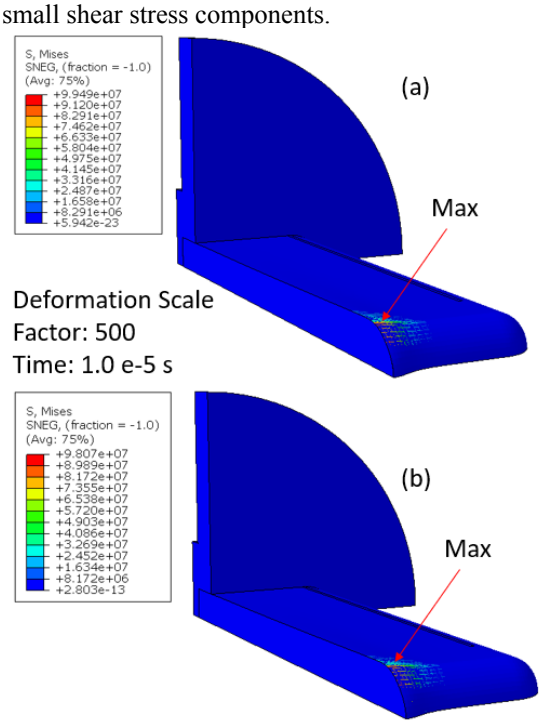

Figure 4: VON MISES STRESS DISTRIBUTION AND DEFORMATION OF PS TARGET MODELS, A) MERCURY USING ABAQUS'S INHERITED EOS MODEL; B) MERCURY USING EOS MODEL DEVELOPED IN VUMAT

PID Tuning on Tensile Failure Threshold

The in-house EOS subroutine implemented through VUMAT can replicate the full functionalities of existing EOS Us-Up model that ABAQUS/Explicit has provided. However, the reinventing of such an EOS model not only creates the opportunity of deeper customized material model, but more importantly paves the way to the final goal of this research. An identical tensile failure threshold for mercury material seems practical and efficient to reflect the overall cavitation or density variation on the change of stress wave speed. The recommended threshold value [10] produced a better match between simulations and experimental measurements but unneglectable gap between them still existed. These differences grow to irreconcilable values when non-condensable helium gas is intentionally injected into the flowing mercury. Seeking a further development of EOS Us-Up model with tensile failure cutoff considered, the following section introduces a Proportional-Integral-Derivative (PID) tuning mechanism to replace the unique tensile failure value. In principle the PID tuned cutoff value generates a dynamic effect that allows the tensile failure value varies in a wider range rather than a fixed constant. A typical PID equation can be expressed as [14]:

$$u(t) = K_p e(t) + K_i \int_0^t e(\tau) d\tau + K_d \frac{de}{dt} \qquad (14)$$

$u(t)$ is the output of signal constructed by three error components in form of proportion, integration and derivation respectively. *Kp, Ki* and *Kd* stand for proportional coefficient, integral coefficient and derivative coefficient of error *e*. In a feedback loop the output $u(t)$ is sent back to compare with setpoint $r(t)$ for the creation of new error, as shown in Fig. 5. Typical PID outputs in Fig. 6 show different responses when various combinations of *Kp, Ki* and *Kd* are adopted.

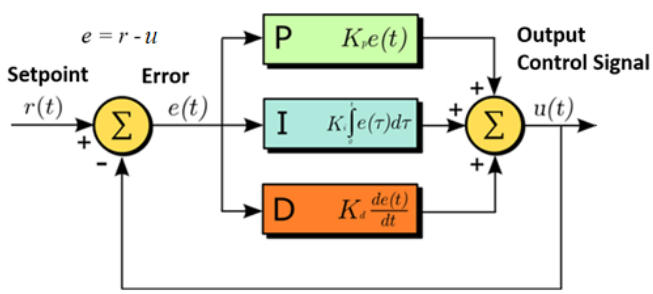

Figure 5: PID FEEDBACK LOOP[14]

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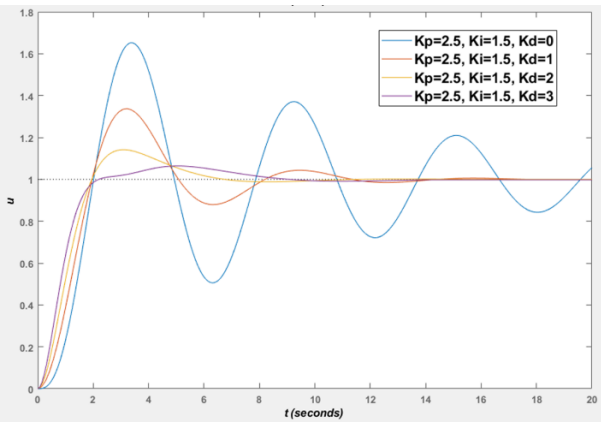

Figure 6: TYPICAL PID OUTPUT WITH SETPOINT =1[14]

The EOS Us-Up model implemented in VUMAT subroutine facilitates the integration of the PID controller into ABAQUS/Explicit solver in terms of tuning the tensile failure threshold. Treating elemental pressure as output variable $u(t)$ in Eq. 14 and using tensile failure threshold as setpoint r, VUMAT realizes this feedback loop through all mercury elements in each incremental calculation.

Primitive Application of PID-EOS Mercury on Prototypic Shape Target

Since ABAQUS calls VUMAT subroutine for each assigned element defined in USER MATERIAL section, this PID controller will be applied on every user defined mercury element. Thereafter it generates pressure response individually regarding to the PID parameters when elemental pressure grows beyond the threshold. In general, the combination of three PID parameters, *Kp, Ki* and *Kd* could be arbitrary and numerous, which ideally indicates abundant dynamic pressure responses can be simulated for mercury's tensile failure behavior. Practically not all the combinations in PID parameters space can lead to a job completion in ABAQUS/Explicit solver, due to the convergence errors such as highly distorted elements or overspeed problem [13]. Table 1 lists the 30 randomly selected groups PID parameter that have been explored in this investigation, 20 of them completed the simulations of 1 millisecond and the remaining 10 failed before that. Corresponding ranges of these parameters are: Kp [0.01, 0.99], Ki [0.03, 890000], and Kd [0.002, 0.9].

Table 1: COMBINATIONS OF PID PARAMETERS

Kp	*Ki*	*Kd*	*Completed*
1.00E-01	3.00E-02	2.00E-03	Yes
1.00E-01	3.00E-02	2.00E+01	No
1.00E-01	3.00E+01	2.00E-03	Yes
1.00E-02	3.00E-02	2.00E-03	Yes
1.00E+01	3.00E-02	2.00E-03	No
5.00E-01	3.00E-02	2.00E-03	Yes
8.00E-01	3.00E-02	2.00E-03	Yes
9.50E-01	3.00E-02	2.00E-03	Yes
9.90E-01	3.00E-02	2.00E-03	Yes
9.90E-01	3.00E-01	2.00E-03	Yes
9.90E-01	8.00E-01	2.00E-03	Yes
9.90E-01	8.00E+01	2.00E-03	Yes
9.90E-01	8.00E+02	2.00E-03	Yes
9.90E-01	8.00E+03	2.00E-03	Yes
9.90E-01	8.00E+04	2.00E-03	Yes
9.90E-01	8.00E+05	2.00E-03	Yes
9.90E-01	8.00E+06	2.00E-03	No
9.90E-01	2.00E+06	2.00E-03	No
9.90E-01	1.00E+06	2.00E-03	No
9.90E-01	9.00E+05	2.00E-03	No
9.90E-01	8.60E+05	2.00E-03	Yes
9.90E-01	8.90E+05	2.00E-03	Yes
9.90E-01	8.90E+05	2.00E-02	Yes
9.90E-01	8.90E+05	2.00E-01	Yes
9.90E-01	8.90E+05	2.00E+01	No
9.90E-01	8.90E+05	2.00E+00	No
9.90E-01	8.90E+05	8.00E-01	Yes
9.90E-01	8.90E+05	9.00E-01	Yes
9.90E-01	8.90E+05	1.10E+00	No
9.90E-01	8.90E-02	1.10E+00	No

The PID controller brings a spring-damper-like material behavior near the reference setpoint, i.e. the tensile failure cutoff value in EOS model. Fig. 7 shows this PID behavior by selecting one mercury element near the target nose for a better illustration. Pressure results from four different material models, the EOS model provided by ABAQUS, EOS model with tensile failure cutoff provided by ABAQUS, the EOS implemented in VUMAT with tensile cutoff considered, and the EOS implemented in VUMAT with PID (K_p=1.0e-1, K_i=3.0e-2, K_d=2.0e-3) controller around tensile cutoff value, are compared side by side. A tensile cutoff value, -1.5e5 Pa, is given to all applicable cases.

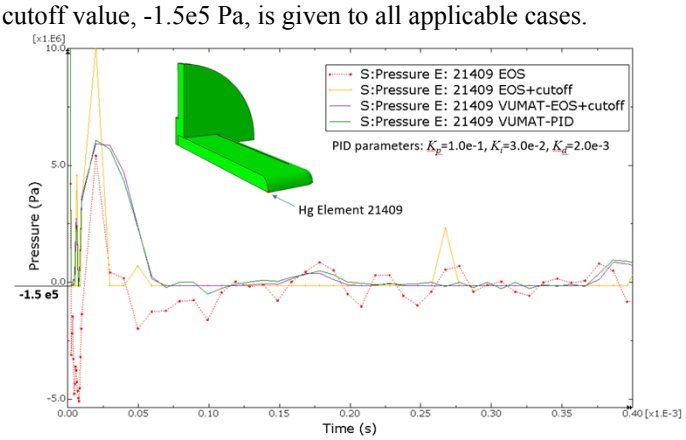

Figure 7: TYPICAL ELEMENTAL PRESSURE OF MERCURY MATERIAL, WITH OR WITHOUT TENSILE FAILURE CUTOFF REALIZED IN EOS OR VUMAT-EOS

Without considering tensile failure cutoff, the pressure of mercury element 21409 can go lower than -1.5e5 which means to sustain much more tensile stress. When tensile failure cutoff applied either in ABAQUS's EOS model or novel EOS model implemented in VUMAT, the pressure holds there for a while and recovers with compression. Pressure behavior of VUMAT with PID controller falls in between, that allows the pressure to go beyond the cutoff but return above threshold faster than the EOS model with cutoff excluded does. The PID controller tunes the mercury elements in pressure, leading to the change in density and speed of wave propagation. However, different combinations of PID parameters applied on mercury elements cause little variation of strain response on stainless steel wall. Fig.8 assembles elemental strain results from the 20 successful PID EOS runs listed in Table 1. The selected steel element locates at the target nose which is adjacent to the mercury element shown in Fig. 7.

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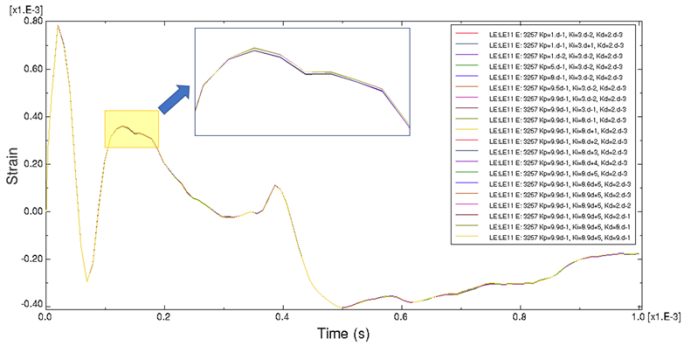

Figure 8: COMPARISON OF STRAIN RESPONSE OF ONE STEEL ELEMENT IN 20 COMPLETED PID RESULTS

DISCUSSION

ABAQUS/Explicit has provided inherited functionalities of EOS material models, including the Us-Up model and the others to describe complicated hydrodynamics behavior interacting with solid structures and environmental loads. Research work in this article tries to simulate the structural response after high energy proton pulse strikes on the stainless-steel pressure vessel and the fluid mercury contained inside in a very short time. Previous simulation results have shown that EOS Us-Up model, along with a suitable tensile failure threshold, fit with the behavior of fluid mercury particularly when a large amount of cavitation occurs due to the internal stress initiated by the proton pulse. However, the homogeneous assumption of mercury's tensile failure behavior and one-size-fit-all approach of tensile failure threshold might match the simulation results well with experimental measurements at some sensor locations, but not all of them.

In order to introduce more flexibility into the EOS Us-Up model, or the tensile failure threshold if being more specifically, an equivalent EOS model has been implemented in ABAQUS's VUMAT subroutine. Result shows that the Us-Up model realized in VUMAT subroutine reproduces the same material behavior as ABAQUS's existing EOS model does. Based on that the PID controller integrated in the VUMAT goes further to turn the important feature of EOS Us-Up model, the tensile failure threshold tunable by giving combinations of three parameters *Kp, Ki* and *Kd*.

Primitive exploring of PID parameters space indicates that these three parameters can complete the simulation in replacing a fixed tensile failure threshold value, though some combinations may lead to uncompleted jobs. The tensile failure threshold added in the EOS Us-Up model was designated to include the bubble cavitation behavior inside mercury triggered by the high energy proton pulse. Regarding to that purpose it effectively avoided the overshot of bubble tension and reflected the change of wave propagation speed, but might be too rigid with one fixed constant. The PID controller changes the mercury behavior after reaching cutoff threshold, physically responses the tension like a spring to hold the pressure back rather than simply staying at the plateau for a while. Fig. 7 shows this effect.

Instead of using a fixed tensile failure threshold, the tunable PID feedback mechanism involves three parameters along with the setpoint of that threshold value, which seems to complicate the EOS Us-Up material model. However, the PID controller enables the possibility of optimizing mercury's cavitation behavior, i.e. the tensile failure, in a broader range of parameters space. When integrating with accelerated high performance computing (HPC) hardware and advanced scientific tools like machine learning, this tunable model would be more suitable to bridge the interfaces.

Initial results of using different PID parameters in VUMAT EOS model also show that the pressure variation in mercury elements brings limited effect on the strain response of steel vessel, due to steel's large Young's Modulus.

CONCLUSIONS

To date the best match of simulation results to experimental data in the investigation of target vessel which contains flowing mercury was obtained with an equation of state (EOS) material model with a specified tensile cutoff pressure threshold. The inclusion of a threshold to represent cavitation was a key parameter in achieving successful predictions of stress waves triggered by the high energy pulse striking the mercury and vessel. However, recent measurements of strain responses of target modules show that significant differences between the measured strain and the strain simulated with EOS mercury model still exist. These differences grow to irreconcilable values when non-condensable helium gas is intentionally injected into the flowing mercury. A novel EOS mercury model embedded into ABAQUS VUMAT has been investigated in this project, which introduces the concept of proportional, integral, and derivative (PID) control into the mercury EOS model. By tuning the new introduced PID parameters (*Kp, Ki* and *Kd*), we replace the mercury's specified tensile failure cutoff pressure with an adjustable spring-damper-like material behavior which may better match the complex dynamics of the mercury and helium mixture. Initial investigation of this tunable EOS mercury model on prototypic shape experimental target has shown its capability and potentiality of improving mechanical behaviors of EOS mercury with cutoff pressure considered. Meanwhile, the instinct change of target fluid from pure mercury to a mixture of mercury and gas requires a further development of material model. The mixture of mercury and bubbles might release significant pressure spikes once the bubbles collapse, which was considered as a major source of pitting damage on stainless steel vessel wall [8]. As mentioned in this article, existing EOS Us-Up model with cutoff pressure included can't fully describe these bubbles' behavior in mercury and their pressure emission directly. In order to reduce the discrepancy between measured and simulated vessel strain responses, further development of material model is needed to bridge the gap.

ACKNOWLEDGEMENTS

The authors are grateful for the support from Mark W. Wendel through the investigation of this work. Special thanks go to Bernie W. Riemer for providing the original PS target model and experimental strain response data. This material is based upon work supported by the U.S. Department of Energy, Office

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