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Equation-of-State Test Suite for the DYNA3D Code

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This document describes the creation and implementation of a test suite for the Equation-of-State models in the DYNA3D code. A customized input deck has been created for each model, as well as a script that extracts the relevant data from the high-speed edit file created by DYNA3D. Each equation-of-state model is broken apart and individual elements of the model are tested, as well as testing the entire model. The input deck for each model is described and the results of the tests are discussed. The intent of this work is to add this test suite to the validation suite presently used for DYNA3D.

Executive Summary

All of the Equation-of-State models in DYNA3D now function as described in the DYNA3D users manual. This was not the case at the beginning of this effort to create a test suite for the EOS models and this will be discussed further below.

In general, pressure contributions from terms involving only the relative volume are typically accurate to better than one part in 10^{11}, i.e., accurate to the level of machine precision, while contributions from terms that in which the pressure is linear in the internal energy are typically accurate to a few parts in 10^7. The lower accuracy from terms involving a contribution to the pressure from the internal energy is a result of the use of a second order accurate operator to integrate the internal energy.

In comparing the results of Equation-of-State models 8, 12 and 14 to a theoretical model of these equations-of-state, a reduction in the accuracy of these models to the level of a few parts in 10^4 was observed during unloading/reloading events. This may warrant further investigation, as a minor change in the bulk unloading modulus used in the theoretical model (on the order of a few parts in 10^4) resulted in an improvement of 3 to 4 orders of magnitude between the code results and the theoretical model.

Similar reductions in accuracy are observed in the testing of Equation-of-State models 11 and 17. The reduced accuracy exhibited by these models has been traced to the use of cubic splines by DYNA3D to evaluate both the partially crushed and completely crushed response curves and the numerical technique used to represent the completely crushed response.

Evaluation of Equation-of-State model 13 is limited to the underlying JWL EOS and some aspects of the evolution equations. While the accuracy of the JWL portions of EOS model 13 are the same as those for EOS model 2 (a JWL model that exhibits the expected level of accuracy) in DYNA3D, lower accuracy has been observed in the testing of EOS model 13 due to the complex set of equations used to describe the evolution of the burn.

Equation-of-State models 4 and 5 can, under certain circumstances, also exhibit degraded accuracy. Equation-of-State model 4 is a Gruneisen model that is linear in the internal energy, but contains terms that are higher order in the excess compression. These higher order terms are not handled well by the second order accurate operator that performs the numerical integration of the internal energy. Therefore, if these higher order terms make a significant contribution to the pressure, the accuracy of EOS model 4 may be degraded and caution is advised. Equation-of-State model 5 is a ratio of polynomials that contains terms that are higher order than linear in the internal energy. The current solution algorithm used in EOS model 5 is consistently accurate only when the EOS is independent of the internal energy or linear in the internal energy, i.e., when these higher order terms are not important. Therefore, if these higher order polynomial terms make a significant contribution to the pressure, the accuracy of EOS model 5 may be degraded and extreme caution is advised.

These Equation-of-State test problems were added to the DYNA3D test suite (version 1.3380). All problems yield the same answers with that version of the code as the results discussed in this report.

Finally, creation of this test suite and subsequent evaluation of the EOS models uncovered coding bugs in Equation-of-State models 8, 9, 12, 13, 14, 16 and 17. These bugs were tracked to the appropriate sections of the source code and fixed. One of these was traced as far back as 1996, which is the oldest version of the source code in existence at LLNL. Another was the source of a long standing discrepancy between the results obtained with DYNA3D and those obtained using LS-DYNA and ALE3D. As a result of the testing and analysis performed during the creation of this test suite, EOS Form 16 was determined to be unnecessary and was removed from the code. The results of testing this EOS model have been moved to the end of this report as an appendix.

In conclusion, as a result of the creation and exercising of this test suite, all of the Equation-of-State models in DYNA3D now function as described in the DYNA3D users manual. Caution should be exercised in the use of Equation-of-State models 4 and 5 if the higher order terms in these models make a significant contribution to the pressure.

Introduction

This report describes the creation and implementation of a test suite for the Equation-of-State models in the DYNA3D code, using the latest developmental version of the code, which evolved as the test suite was created. Therefore, the version number used will be noted for each test.

Input files were derived from a template supplied by Jerry Lin. Each equation-of-state model has a custom input file, as well as a script that extracts the pressure from the DYNA3D high-speed edit file. Each equation-of-state model is decomposed into as many relevant terms as possible, and each of these terms is tested, as well as the implementation of the model itself. For instance, EOS Form 1 is a 7 term polynomial. The implementation of each of the 7 terms is tested, as is the sum of the first four terms and the last three terms (which is how the code actually handles the EOS), as will be discussed below. The number of cubes is modified in each test to accommodate the number of elements of the EOS model being tested.

The equation-of-state testing is based on a series of cubes, 1 cm on a side, with an initial density of 1 g/cm^3. This yields a simple initial volume and density. For many of the tests, each cube is hydrostatically compressed to approximately 94% of the original volume, released back to the original volume, hydrostatically expanded out to ~ 106% of the original volume and then released back to the original state. For other tests, the drive was modified to exercise the EOS model in an appropriate manner. The details of the drive used are given in each test.

This test suite serves two purposes. The first is to determine if the EOS models are in fact behaving as intended. The second is to provide a baseline of answers so that future code and/or compiler changes can be detected if they cause a difference in the code results.

In order to determine if the EOS models are implemented as intended, it is necessary to create an independent model that returns the expected answer. This was done in a spreadsheet for each EOS model. Due to the nature of the EOS models, there are two forms of expected answer. The first is a true theoretical answer in which the pressure is determined from the model equation and the internal energy is determined from a closed form integral. These results will be labeled *Theoretical* or *Closed Form* in the following discussion. Unfortunately, this situation is not obtained for all of the EOS models in DYNA3D.

For many of the EOS models in DYNA3D, the internal energy makes a contribution to the pressure and this prevents the generation of a closed form integral for the internal energy. In these cases, a numerical integration is performed in the spreadsheet model to provide, not a true theoretical answer, but a reference answer that has some uncertainty associated with it. The level of the uncertainty in these reference answers will be discussed. For some of these models, portions of the EOS model do allow the creation of a closed form integral even if the full model does not. In these cases, the closed form solution will be used for the portions of the EOS model to which they can be applied and the spreadsheet integration will be used for the rest of the model. These results will be labeled *Reference* in the following discussion to distinguish them from the theoretical results described in the previous paragraph.

As to the second purpose, these Equation-of-State test problems were added to the DYNA3D test suite (version 1.3380). All problems yield the same answers with that version of the code as the results discussed in this report.

Equation-of-State Form 1

The first model tested is Equation-of-State Form 1, a polynomial that is a function of the excess compression and is linear in the internal energy. The expression for EOS Form 1 is as follows:

$$p = C_0+C_1\mu+C_2\bar{\mu}^2+C_3\mu^3+(C_4+C_5\mu+C_6\bar{\mu}^2)E,$$

where p is the pressure, μ is the excess compression (related to the density by $\mu = \rho/\rho_0 - 1$), and E is the specific internal energy (energy per unit initial volume). The tension-limited excess compression, $\bar{\mu}$, is given by:

$$\bar{\mu} = \max(\mu,0).$$

Equation-of-State Form 1 was tested using 10 cubes, one for each of the coefficients (7 cubes), one for the sum of the first four terms, one for the sum of the last three terms (These two cubes are included because these are the quantities actually calculated by DYNA3D.) and one for the full equation-of-state model. The 10 cubes are compressed hydrostatically to approximately 94% of the original volume, released back to the original volume, hydrostatically expanded out to ~ 106% of the original volume and then released back to the original state.

Prior to discussing the calculations using EOS Form 1, a few code issues need to be addressed and these are not necessarily readily apparent to the user. First, because the sound speed looks like $dp/d\rho$ and μ is proportional to ρ, in order to avoid divide by zero issues in calculations using the sound speed, it is necessary that the C_1 coefficient not be zero, so an input value of 1.0e-20 was used for this coefficient when testing the other terms in the polynomial. Also, in order for the terms dependent on the internal energy to perform as expected, it is required to have an initial energy present in the simulation, so the initial internal energy was set to a value of 1.0e-3 in the cubes testing these terms (Cubes 5, 6, 7, 9 and 10). In the cubes testing the other coefficients (Cubes 1, 2, 3, 4 and 8), the initial internal energy was set to 1.0e-9. In addition, in order to eliminate issues with the work performed by the bulk viscosity, the two input coefficients for the bulk viscosity on the material card were set to 1.0e-20 in each of the 10 cubes. Failing to do so results in the work performed on the cube being dominated by contributions from the bulk viscosity. Finally, the code version used for this test was version 14.2.0 revision 1.3287.

Input coefficients for Equation-of-State Form 1 were developed for the purposes of this testing. The values were chosen so that the contribution from each term was of the same order of magnitude (with the exception of the first term, which is constant). The following values were used as input for the testing of the full implementation of EOS Form 1: C_0 = 1.0e-9, C_1 = 1.224e-4, C_2 = 1.2e-3, C_3 = 1.3e-2, C_4 = 1.1e-2, C_5 = 2.4e-4 and C_6 = 1.3. The following table gives the values of the coefficients for each of the 10 cubes in the test suite.

Table 1. Suite of test input coefficients for EOS Form 1

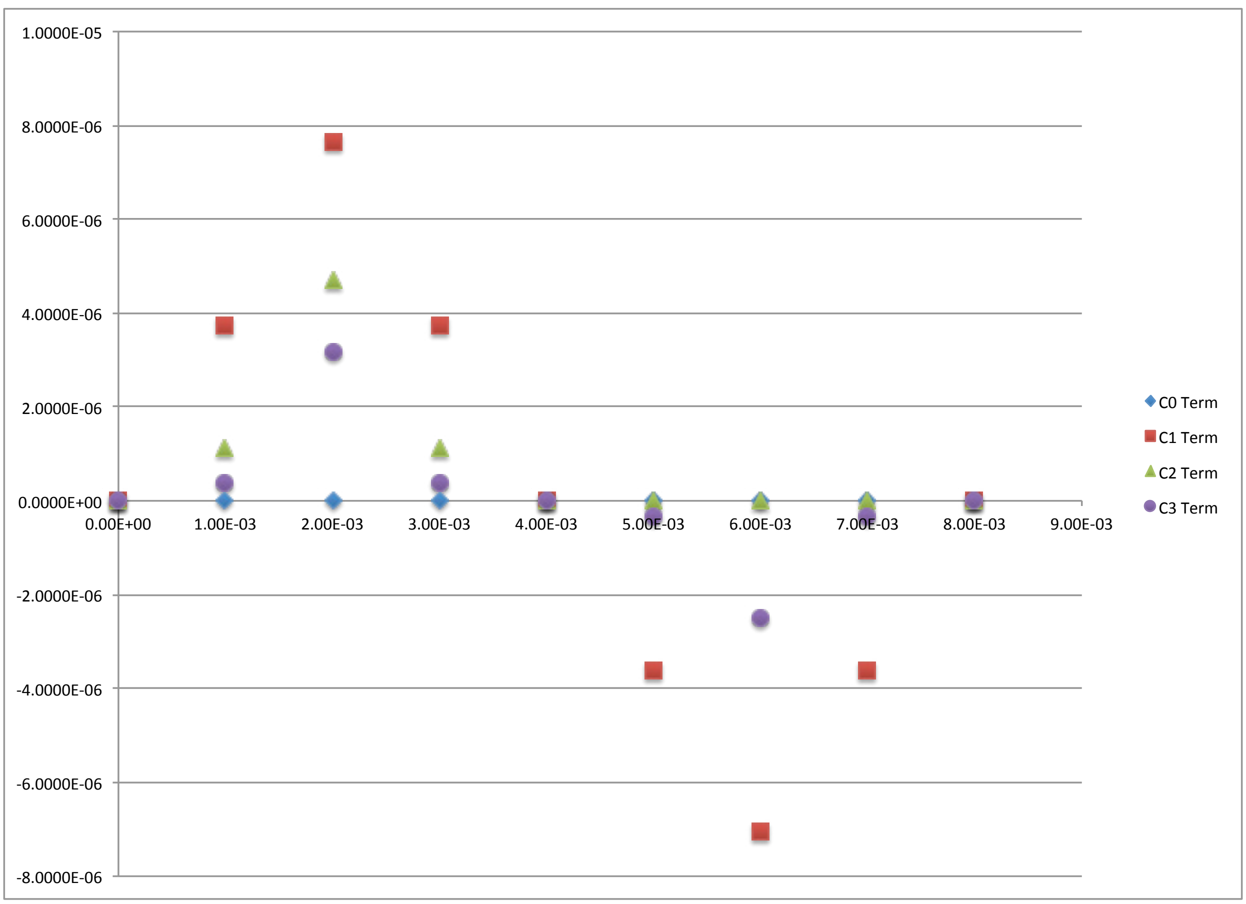
Cube	C_0	C_1	C_2	C_3	C_4	C_5	C_6
1	1.0e-9	1.0e-20	0	0	0	0	0
2	0	1.224e-4	0	0	0	0	0
3	0	1.0e-20	1.2e-3	0	0	0	0
4	0	1.0e-20	0	1.3e-2	0	0	0

5	0	1.0e-20	0	0	1.1e-2	0	0
6	0	1.0e-20	0	0	0	2.4e-4	0
7	0	1.0e-20	0	0	0	0	1.3
8	1.0e-9	1.224e-4	1.2e-3	1.3e-2	0	0	0
9	0	1.0e-20	0	0	1.1e-2	2.4e-4	1.3
10	1.0e-9	1.224e-4	1.2e-3	1.3e-2	1.1e-2	2.4e-4	1.3

As stated above, the intent of this test was to create a situation in which each term in the polynomial was making essentially an equal contribution to the final pressure (with the exception of the C_0 term, which represents a constant offset) and not to create a test that was reflective of any real material.

Each term in the polynomial was tested independently, then the sums of the first four terms and the last three terms, followed by testing of the EOS as a whole. The following plot contains the pressure from each of the first four terms in the polynomial, as returned by the code, as a function of time for this simulation.

Figure 1. Code pressures for the first four coefficients as a function of time



As the plot demonstrates, each of the terms depending on μ returns a peak pressure on the order of 10^{-6} in compression and on the order of -10^{-6} in tension. Note that the C_2 term depends on $\overline{\mu}$, not μ, and therefore makes no contribution to the pressure when the cube is in tension.

The following observations can be made from the code output. Coefficient 0 represents a constant pressure offset and was set to a value of 1.0e-9 in the first cube. To better than 1 part in 10^{12}, the cube remains at this pressure during the cycling of its volume. Coefficient 1 is linear in the excess compression. It should therefore return zero pressure when the compression is zero, return a positive value when the cube is compressed and should be negative when the cube is expanded, which is reflected in the code output. Coefficient 2 goes as the square of the tension-limited excess compression and should therefore only return positive pressures when the cube is compressed, which is what the code returns. Coefficient 3 is proportional to the cube of the excess compression. It should therefore return zero pressure when the compression is zero, return a positive value when the cube is compressed and should be negative when the cube is expanded, which is reflected in the code output. Therefore, the code output is behaving qualitatively as expected.

The agreement between the pressures for each of the first four terms as calculated using the theoretical expression and the results returned by the code is investigated in the following table. The level of agreement can be quantified by defining the normalized difference between the two as:

$$(\textit{Theoretical - Code})/\textit{Code} \tag{1}$$

where *Theoretical* is the result from the exact expression and *Code* is the code result. Using this definition, the agreement between the theoretical predictions and the code results is better than 1 part in 10^{11}, as illustrated by the following table for the C_3 coefficient.

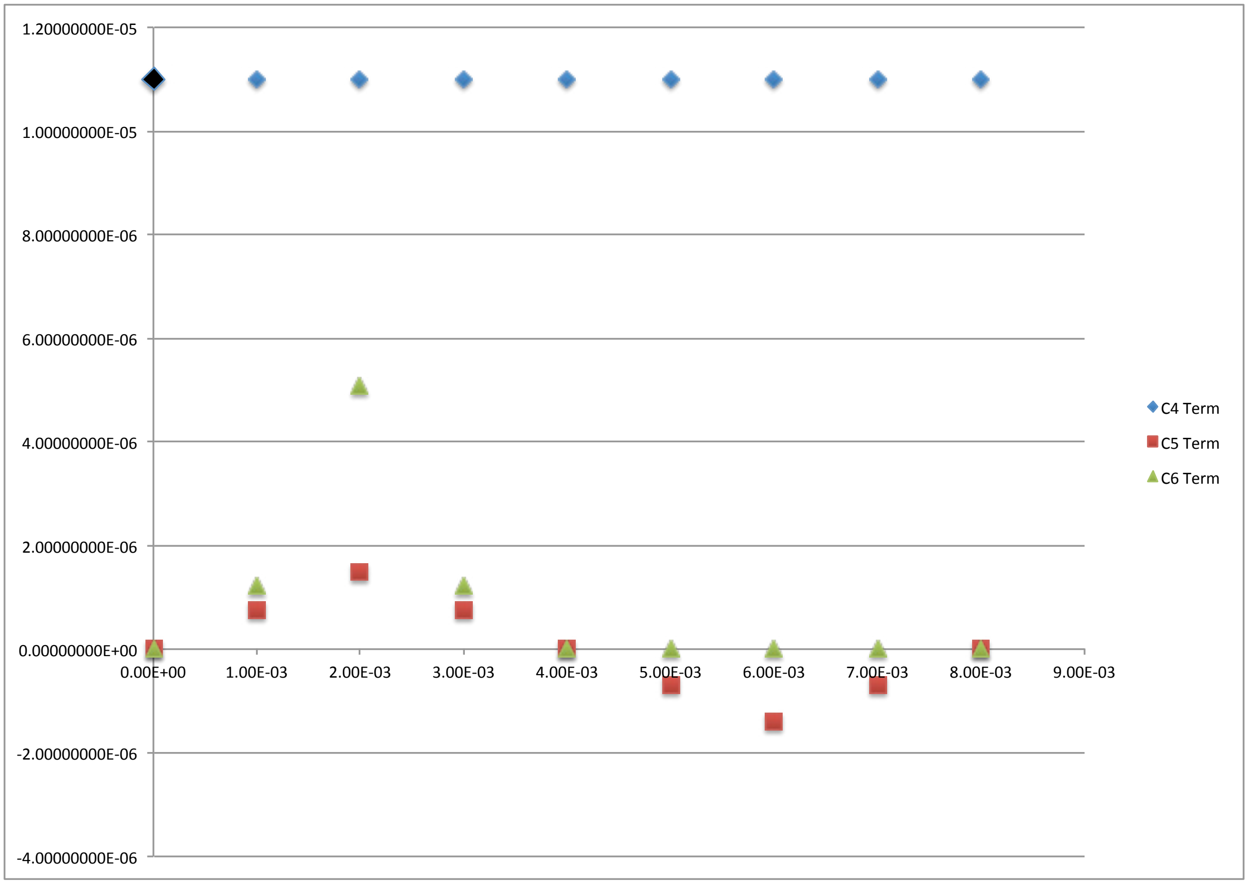
Table 2. Exact and Code Pressures for the C_3 Coefficient

Time	*Theoretical*	*Code*	*(Theoretical - Code)/Code*
0.00E+00	0.000000E+00	0.000000E+00	0.000000E+00
1.00E-03	3.728549E-07	3.728549E-07	3.309371E-12
2.00E-03	3.171158E-06	3.171158E-06	1.813912E-12
3.00E-03	3.728549E-07	3.728549E-07	4.049536E-12
4.00E-03	0.000000E+00	-1.265654E-34	0.000000E+00
5.00E-03	-3.306906E-07	-3.306906E-07	-1.685885E-12
6.00E-03	-2.494402E-06	-2.494402E-06	-1.928778E-13
7.00E-03	-3.306906E-07	-3.306906E-07	8.964921E-13
8.00E-03	0.000000E+00	-5.417888E-34	0.000000E+00

As the table clearly demonstrates, the predictions of theoretical expression and the code results are in excellent agreement. Note that the two differences representing the cube returning to its starting position have been artificially set to zero. Similar levels of agreement are exhibited between the theoretical expression and the code results for the C_0, C_1 and C_2 coefficient terms.

The next plot displays the pressure from each of the last three terms in the polynomial, as returned by the code, as a function of time for this simulation.

Figure 2. Code pressures for the last three coefficients as a function of time



As the plot demonstrates, the C_4 term, which depends only on the internal energy, makes a contribution on the order of 10^{-5}, while the C_5 term returns a peak pressure on the order of 10^{-6} in compression and on the order of -10^{-6} in tension. Note that the C_6 term depends on $\overline{\mu}$, not μ, and therefore makes no contribution to the pressure when the cube is in tension.

Coefficient 4 is proportional to the internal energy and should therefore return a value of 1.1e-5 when the cube is at its original volume, a value larger than this when compressed and a value smaller than this when expanded. This is again reflected in the code output, with the value at zero compression being equal to the expected value to better than 1 part in 10^{14}. Coefficient 5 is linear in both the excess compression and the internal energy. It should therefore return zero pressure when the compression is zero, return a positive value when the cube is compressed and should be negative when the cube is expanded, which is reflected in the code output. Coefficient 6 is linear in the internal energy and proportional to the square of the tension-limited excess Compression. It should therefore only return positive pressures when the cube is compressed, which is what the code returns. Therefore, the code output is behaving qualitatively as expected.

Using the earlier definition for the normalized difference, the agreement between the theoretical expression and the code result can be quantified as illustrated in the following table for the C_5 coefficient.

Table 3. Exact and Code Pressures for the C_5 Coefficient

Time	*Theoretical*	*Code*	*(Theoretical - Code)/Code*
0.00E+00	0.000000E+00	0.000000E+00	0.000000E+00
1.00E-03	7.346516E-07	7.346516E-07	9.205043E-13
2.00E-03	1.499644E-06	1.499644E-06	-4.319421E-08
3.00E-03	7.346516E-07	7.346516E-07	2.876522E-12
4.00E-03	0.000000E+00	-2.286171E-18	-1.000000E+00
5.00E-03	-7.058441E-07	-7.058441E-07	-2.835817E-12
6.00E-03	-1.384324E-06	-1.384324E-06	-1.464370E-12
7.00E-03	-7.058441E-07	-7.058441E-07	-4.219900E-12
8.00E-03	0.000000E+00	-3.495870E-18	-1.000000E+00

As was observed in the results from the first four coefficients, the agreement between the code results and the theoretical expression is better than 1 part in 10^{11}, with the exception of the point at peak compression. This is most likely due to the code output not being reported at exactly the peak of the compression. Similar levels of agreement are exhibited between the theoretical expression and the code results for the C_4 and C_6 coefficient terms.

Now that the behavior of each of the individual terms in the expression for Equation-of-State Form 1 has been investigated, the behavior of the full expression can be examined. The following plot contains the pressure returned by the code for the full equation-of-state as a function of time.

Figure 3. Code pressure for the full EOS as a function of time

Note that the pressure is behaving as one would expect, in that the pressure increases as the cube is compressed, decreases back to the starting value as the compression is released, further decreases as the cube is placed into tension and then relaxes back to the starting value as the tension is released.

The following table compares the pressure returned by the code as a function of time for the full equation-of-state to that predicted by the theoretical expression.

Table 4. Exact and Code Pressures for Equation-of-State Form 1

Time	*Code*	*Theoretical*	*(Theoretical - Code)/Code*
0.00E+00	1.100100000E-05	1.100100000E-05	0.000000E+00
1.00E-03	1.820305217E-05	1.820305106E-05	-6.094752E-08
2.00E-03	3.309979879E-05	3.309978426E-05	-4.387902E-07
3.00E-03	1.820305217E-05	1.820304720E-05	-2.732168E-07
4.00E-03	1.100100000E-05	1.100099501E-05	-4.538428E-07
5.00E-03	6.361980486E-06	6.361979934E-06	-8.665773E-08
6.00E-03	5.902921677E-08	5.902828883E-08	-1.572003E-05
7.00E-03	6.361980485E-06	6.361978144E-06	-3.680995E-07
8.00E-03	1.100100000E-05	1.100099678E-05	-2.930470E-07

As demonstrated in the table, the code result agrees with the theoretical expression to better than 5 parts in 10^7 across the range of pressures tested. An exception to these results occurs at the peak tension point. This is most likely due to the fact that this point involves the difference of two small numbers but could also be due to the code output not being reported at exactly the peak of the tension. These results establish confidence in the pressures returned by the implementation of Equation-of-State Form 1 in DYNA3D.

The code results for the internal energy can also be examined for this equation-of-state. If one assumes that $C_0=C_1=C_2=C_3=0$, then a simple closed form solution for the internal energy resulting from the remaining terms can be derived[1]. The form of the solution is as follows:

$$E = \exp\{- (C_4(V-1) + C_5(\ln V - V + 1) + C_6(-1/V - 2\ln V + V)) + \ln E_0\}$$

where V is the final volume of the cube and E_0 is the initial specific internal energy. This solution takes advantage of the fact that the initial volume of the cube is 1 cm^3. Note also that the C_6 term contributes to the internal energy only when the tension-limited excess compression is non-zero.

Unfortunately, DYNA3D does not write the internal energy to the high-speed edit file, so GRIZ was used to extract the internal energy from the code results. This limits the accuracy of the comparison because the GRIZ output contains only 7 significant figures. A numerical integration (similar to that performed by DYNA3D) was performed using EXCEL as a check on both the results of the closed form solution and the internal energy as extracted using GRIZ.

The internal energy resulting from each of the three terms, extracted from the code output using GRIZ, was compared to the closed form solution. The following table displays the results for the internal energy resulting from the contribution of the C_5 term as a function of time.

[1]Ed Zywicz, private communication, November 2014.

Table 5. Exact and Code results for the Internal Energy from the C_5 term

Time	Code (GRIZ)	Closed Form	(Closed - GRIZ)/GRIZ
0.00E+00	1.00000000E-03	1.00000000E-03	0.00000000E+00
1.00E-03	1.00001100E-03	1.00001080E-03	-1.99758028E-07
2.00E-03	1.00004300E-03	1.00004320E-03	2.03851356E-07
3.00E-03	1.00001100E-03	1.00001080E-03	-1.99758028E-07
4.00E-03	1.00000000E-03	1.00000000E-03	2.16840434E-16
5.00E-03	1.00001100E-03	1.00001080E-03	-1.99760908E-07
6.00E-03	1.00004300E-03	1.00004320E-03	2.03759170E-07
7.00E-03	1.00001100E-03	1.00001080E-03	-1.99760908E-07
8.00E-03	1.00000000E-03	1.00000000E-03	2.16840434E-16

As expected, given the restrictions on the GRIZ output, agreement between the two numbers is at the level of a few parts in 10^7. This level of agreement is similar to that obtained for the C_4 and C_6 coefficients, as well.

The closed form solution for the internal energy resulting from the contribution for the three coefficients combined can also be compared to the code results, which is displayed in the following table.

Table 6. Exact and Code results for the Internal Energy from all 3 terms

Time	Code (GRIZ)	C_4 - C_6 Closed Form	(Closed - GRIZ)/GRIZ
0.00E+00	1.00000000E-03	1.00000000E-03	0.00000000E+00
1.00E-03	1.00034900E-03	1.00034945E-03	4.50177450E-07
2.00E-03	1.00078700E-03	1.00078689E-03	-1.06876630E-07
3.00E-03	1.00035000E-03	1.00034945E-03	-5.49473122E-07
4.00E-03	1.00000000E-03	1.00000000E-03	2.16840434E-16
5.00E-03	9.99677700E-04	9.99677541E-04	-1.58871608E-07
6.00E-03	9.99370200E-04	9.99370113E-04	-8.67579917E-08
7.00E-03	9.99677500E-04	9.99677541E-04	4.11928811E-08
8.00E-03	9.99999800E-04	1.00000000E-03	2.00000040E-07

As expected, the agreement between the two numbers is at the level of a few parts in 10^7, similar to the agreement displayed in the examination of the behavior of the individual coefficients and limited by the precision of the GRIZ output.

DYNA3D uses numerical integration for these calculations rather than a closed form solution. Therefore, a numerical integration was performed in EXCEL to check against the closed form solution, which should be exact. The following table compares the results for the internal energy from the numerical integration scheme to the closed form solution for the C_5 coefficient.

Table 7. Exact and Numerical Integration results for the Internal Energy from the C_5 term

Time	Numerical Int	Closed Form	(Closed - NI)/NI
0.00E+00	1.00000000E-03	1.00000000E-03	0.00000000E+00
1.00E-03	1.00001079E-03	1.00001080E-03	1.09090606E-08
2.00E-03	1.00004318E-03	1.00004320E-03	2.20412156E-08
3.00E-03	1.00001077E-03	1.00001080E-03	3.31736001E-08
4.00E-03	9.99999956E-04	1.00000000E-03	4.40828806E-08
5.00E-03	1.00001079E-03	1.00001080E-03	1.06932566E-08
6.00E-03	1.00004318E-03	1.00004320E-03	2.11773074E-08
7.00E-03	1.00001077E-03	1.00001080E-03	3.16611508E-08
8.00E-03	9.99999958E-04	1.00000000E-03	4.23541918E-08

As the table demonstrates, the agreement between the closed form solution and the EXCEL numerical integration is about an order of magnitude better than that exhibited by the closed form solution and the code results (as extracted using GRIZ). This is not surprising, as the GRIZ output is limited to 7 significant figures.

The level of agreement exhibited by the C_5 coefficient is also obtained for the C_6 coefficient, while the C_4 coefficient exhibits agreement between the numerical integration scheme and the closed form solution that is about 2 orders of magnitude better. As the contribution of the C_4 coefficient depends only on E (and not μ), this is not surprising.

The closed form solution for the internal energy resulting from the contribution for the three coefficients combined can also be compared to the results of the EXCEL numerical integration, which is displayed in the following table.

Table 8. Exact and Numerical Integration results for the Internal Energy from all 3 terms

Time	C_4 - C_6 Numerical Int	C_4 - C_6 Closed Form	(Closed - NI)/NI
0.00E+00	1.000000000E-03	1.00000000E-03	0.00000000E+00
1.00E-03	1.000349421E-03	1.00034945E-03	2.89911294E-08
2.00E-03	1.000786797E-03	1.00078689E-03	9.62788491E-08
3.00E-03	1.000349287E-03	1.00034945E-03	1.63580810E-07
4.00E-03	9.999998074E-04	1.00000000E-03	1.92584608E-07
5.00E-03	9.996775304E-04	9.99677541E-04	1.07451941E-08
6.00E-03	9.993700920E-04	9.99370113E-04	2.12760119E-08
7.00E-03	9.996775094E-04	9.99677541E-04	3.18066191E-08
8.00E-03	9.999999574E-04	1.00000000E-03	4.25515928E-08

As expected, the level of agreement exhibited in the table is, in general, a few parts in 10^8, similar to the level of agreement exhibited by the C_5 and C_6 coefficients.

Continuing with the closed form solution investigation, if one assumes that C_4=C_5=C_6=0, then a simple closed form solution for the internal energy due to the first four terms can be developed, which exhibits the following form:

$$E = -\{C_0(V-1) + C_1(\ln V - V + 1) + C_2(-1/V - 2\ln V + V) + C_3(-1/(2V^2) + 3/V + 3\ln V - V - 1.5)\} + E_0$$

where V is the final volume of the cube and E_0 is the initial internal energy. This solution takes advantage of the fact that the initial volume of the cube is 1 cm^3. Note that the C_2 term contributes to the internal energy only when the tension-limited excess compression is non-zero.

The internal energy resulting from each of the four terms, extracted from the code output using GRIZ, was compared to the results of the closed form solution. The following table displays the results for the internal energy resulting from the C_1 term as a function of time.

Table 9. Exact and Numerical Integration results for the Internal Energy from the C_1 term

Time	Code (GRIZ)	Closed Form	(Closed - GRIZ)/GRIZ
0.00E+00	1.0000000E-09	1.0000000E-09	0.0000000E+00
1.00E-03	5.6080920E-08	5.6080925E-08	9.6391507E-08
2.00E-03	2.2133490E-07	2.2133493E-07	1.2195607E-07
3.00E-03	5.6080920E-08	5.6080925E-08	9.6391507E-08
4.00E-03	1.0000000E-09	1.0000000E-09	0.0000000E+00
5.00E-03	5.6080910E-08	5.6080911E-08	1.2779578E-08
6.00E-03	2.2133450E-07	2.2133446E-07	-1.9498628E-07
7.00E-03	5.6080910E-08	5.6080911E-08	1.2779578E-08
8.00E-03	1.0000000E-09	1.0000000E-09	0.0000000E+00

The agreement between the code results and the closed form solution is better than 2 parts in 10^7 and is similar to the results from coefficients C_0, C_2 and C_3. These results are also similar to the level of agreement exhibited by the results for the last three terms of this EOS.

The internal energy resulting from the combination of the four terms, extracted from the code output using GRIZ, was compared to the results of the closed form solution. The following table displays these results as a function of time.

Table 10. Exact and Numerical Integration results for Internal Energy from the C_0 - C_3 terms

Time	Code (GRIZ)	Closed Form	(Closed - GRIZ)/GRIZ
0.00E+00	1.0000000E-09	1.0000000E-09	0.0000000E+00
1.00E-03	6.9793750E-08	6.9793744E-08	-8.5787025E-08
2.00E-03	3.5540810E-07	3.5540812E-07	4.7938045E-08
3.00E-03	6.9793750E-08	6.9793744E-08	-8.5787025E-08
4.00E-03	1.0000000E-09	1.0000000E-09	0.0000000E+00
5.00E-03	5.8600770E-08	5.8600763E-08	-1.1509280E-07
6.00E-03	2.6081650E-07	2.6081647E-07	-1.0994220E-07
7.00E-03	5.8600770E-08	5.8600763E-08	-1.1509280E-07
8.00E-03	1.0000000E-09	1.0000000E-09	0.0000000E+00

The agreement between the code results and the closed form solution is better than 2 parts in 10^7 and is similar to the level of agreement exhibited by the results for the last three terms of this

EOS. This established confidence in the numerical integration performed by the code to determine the internal energy.

Finally, a convergence study[2] was performed on the internal energy integration calculation for EOS Form 1. A series of seven simulations was run with successively smaller time-step values that varied between 5.0e-5 and 8.9e-11. Each simulation was run to the first peak in the compression. The final value of the internal energy for each of the first seven cubes was extracted using GRIZ. Using the energy from the simulation with the smallest time-step size as the "exact" answer, the error (difference in values) for each cube/term was calculated and examined as a function of the time-step size. For each term, the error looked like $error = C\,\Delta t^2$, where C is some constant and Δt is the time-step size. Therefore, the integration of the internal energy is second order accurate as the error is quadratic in Δt.

The pressure is the more important quantity being determined from the equation-of-state and the agreement between the code results and those obtained from the theoretical equation is better than 5 parts in 10^7, as exhibited earlier. This level of agreement is similar to that exhibited by the code results for the internal energy and the closed form solutions. Finally, as established by the convergence study, the agreement between the closed form solutions for the internal energy and the code results can be improved by decreasing the time step, which would also improve the agreement between the code predictions for the pressure and the theoretical result

This establishes the implementation of Equation-of-State Form 1 in DYNA3D. The equation-of-state is performing as expected, in that the pressure in the cubes increases as they are compressed and decreases as they are expanded. The behavior of each of the terms in the equation-of-state has been examined and found to be performing as expected and with good accuracy. The behavior of the equation-of-state as a whole has been examined and is performing as expected and with good accuracy.

[2] Ed Zywicz, e-mail communication, 1/13/2015.

Equation-of-State Form 2

The next model to be tested was Equation-of-State Form 2, a JWL expression often used for high-explosive detonation products. This EOS has the following form:

$$p = A(1 - \omega/(R_1 V)) \exp(-R_1 V) + B(1 - \omega/(R_2 V)) \exp(-R_2 V) + \omega E/V$$

where p is the pressure, V is the relative volume and E is the specific internal energy. A, B, ω, R_1 and R_2 are material dependent coefficients.

Equation-of-State Form 2 was tested using 4 cubes, one for each of the 'terms' and one for the full equation-of-state model. However, unlike Equation-of-State Form 1 which separated into terms easily, the manner in which each term of EOS Form 2 depends on ω prevents this equation-of-state model from being cleanly separated, unless ω is set to 0, in which case the dependence of the first two terms on the relative volume is modified. Therefore, the decision was made to test terms 1 and 3 with the first cube, terms 2 and 3 with the second cube and term 3 alone with the third cube. The full equation-of-state was tested using the fourth cube. The 4 cubes use the same compression and expansion as that used for the testing of EOS Form 1.

As it turns out, for the material coefficients chosen for this test of EOS Form 2, the contribution to the pressure from term 3 is orders of magnitude smaller than the contributions from terms 1 and 2, validating this testing choice. In addition, tests of this EOS with ω set to zero have already been conducted and discussed elsewhere[3]. While those tests were restricted to investigating only the pressure, the results exhibited good agreement between the theoretical model and the code (See Appendix A).

Prior to discussing the calculations using EOS Form 2, a few code issues need to be addressed and these are not necessarily readily apparent to the user. First, in order for the terms dependent on the internal energy to perform as expected, it is required to have an initial energy present in the simulation, so the initial internal energy was set to a value of 1.0e-3 in all of the cubes. In addition, in order to eliminate issues with the work performed by the bulk viscosity, the two input coefficients for the bulk viscosity on the material card were set to 1.0e-20 in each of the 4 cubes. Failing to do so results in the work performed on the cube being dominated by contributions from the bulk viscosity. Finally, the code version used for this test was version 14.2.0 revision 1.3293.

Input coefficients for Equation-of-State Form 2 for a typical material were taken from a 1973 paper by Lee, et. al.[4]. The following table gives the value of the input coefficients for each of the four cubes used in the test suite.

Table 11. Input coefficients for the testing of EOS Form 2

Cube	A	B	R_1	R_2	ω
1	8.684	0	4.6	1.25	0.25
2	0	1.8711e-1	4.6	1.25	0.25
3	0	0	4.6	1.25	0.25

[3] Benjamin, R.D., Informal report submitted to Jerry Lin and Robert Ferencz. The portion related to EOS Form 2 testing with ω=0 is included at the end of this report.

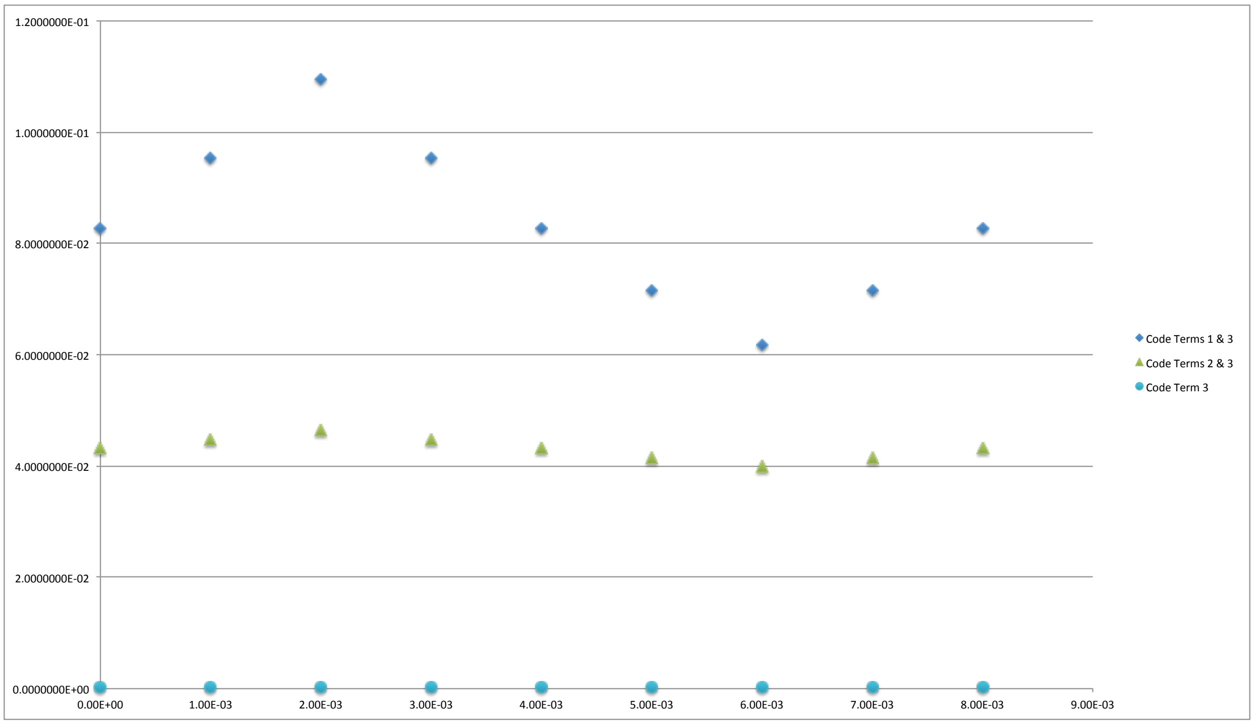
[4] Lee, Finger and Collins, UCID-16189, 1973.

4	8.684	1.8711e-1	4.6	1.25	0.25

Note that the R_1 and R_2 coefficients were set for each cube to avoid divide by zero problems in the code.

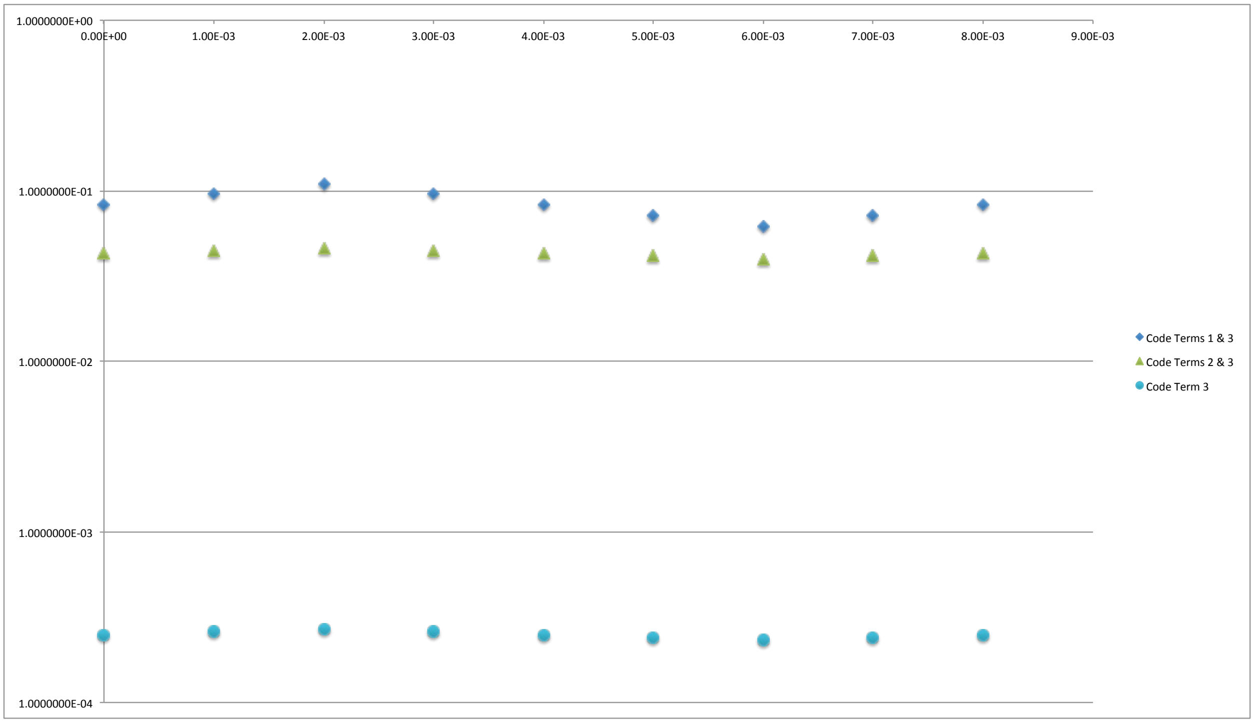
The following plot displays the pressure from each of the three individual terms tested for EOS Form 2, as returned by the code, as a function of time for this simulation.

Figure 4. Code pressure for the three terms as a function of time



As the plot demonstrates, the pressures returned by the first two terms differ by approximately a factor of two, while the contribution of the third term is orders of magnitude smaller. A log plot makes the difference between these terms more easily understood:

Figure 5. Code pressure for the three terms as a function of time



It is clear from this version of the plot that the contributions to the pressure from the first two terms (as tested) are approximately two orders of magnitude larger than the contribution from the third term.

The following observations may be made from the code output. In all of the cubes, the pressure increases as the cube is compressed and decreases as the cube is expanded, as expected. As asserted earlier, the pressure from Cube 3 (Term 3 only) is about 2 orders of magnitude smaller than the pressures resulting from Cubes 1 (Terms 1 and 3) and 2 (Terms 2 and 3). Finally, note that with this choice of input coefficients, the pressure appears to be positive definite.

Using the normalized difference defined by equation 1, the agreement between the pressures for each of the three 'terms' as calculated using the theoretical expression and the results returned by the code is demonstrated in the following table for the second 'term' as a function of time.

Table 12. Reference and Code Pressures for the second term of EOS Form 2

Time	*Reference Pressure*	*Code Pressure*	*(Reference - Code)/Code*
0.00E+00	4.3136330E-02	4.31363300E-02	9.65157754E-16
1.00E-03	4.4761805E-02	4.47618053E-02	-2.70069321E-09
2.00E-03	4.6401351E-02	4.64013505E-02	1.90932689E-09
3.00E-03	4.4761805E-02	4.47618053E-02	-2.70071119E-09
4.00E-03	4.3136330E-02	4.31363300E-02	-1.30296297E-14
5.00E-03	4.1527370E-02	4.15273695E-02	-2.06490702E-10
6.00E-03	3.9937214E-02	3.99372138E-02	-9.25914742E-10

7.00E-03	4.1527370E-02	4.15273695E-02	-2.06476165E-10
8.00E-03	4.3136330E-02	4.31363300E-02	-1.06167353E-14

As the table clearly demonstrates, the code pressures are in excellent agreement with the reference results, with the level of agreement being better than 3 parts in 10^9. This level of agreement is typical of the three individual terms tested in this simulation.

Now that the behavior of each of the individual terms in the expression for Equation-of-State Form 2 has been examined, the behavior of the full expression for this EOS can be investigated. The following plot displays the pressure as a function of time for EOS Form 2.

Figure 6. Code Pressure for EOS Form 2 as a function of time

Note that the pressure is behaving as one would expect, as the pressure increases when the cube is compressed, decreases as the cube is expanded and then returns to the initial pressure as the cube is relaxed back to its original configuration. Note also that with the present choice of input coefficients, the pressure returned by EOS Form 2 is positive definite.

The following table compares the reference pressure to the code results as a function of time.

Table 13. Reference and Code Pressures for Equation-of-State Form 2

Time	*Reference Pressure*	*Code Pressure*	*(Reference - Code)/Code*
0.00E+00	1.256824422E-01	1.256824422E-01	6.8460067E-15
1.00E-03	1.399047857E-01	1.399047857E-01	1.0924094E-10

2.00E-03	1.556900399E-01	1.556900400E-01	-8.1066458E-10
3.00E-03	1.399047857E-01	1.399047857E-01	1.0939826E-10
4.00E-03	1.256824422E-01	1.256824422E-01	7.8397819E-14
5.00E-03	1.128902140E-01	1.128902140E-01	1.8167009E-10
6.00E-03	1.014025564E-01	1.014025564E-01	3.6232252E-10
7.00E-03	1.128902140E-01	1.128902140E-01	1.8163468E-10
8.00E-03	1.256824422E-01	1.256824422E-01	-1.2057805E-13

As the table clearly demonstrates, the code predictions are again in excellent agreement with the theoretical results, with the level of agreement being better than 8 parts in 10^{10}. These results establish confidence in the pressures returned by the implementation of Equation-of-State Form 2 in DYNA3D.

The code results for the internal energy can also be investigated for this equation-of-state. Unfortunately, due to the form of this EOS (ω present in each term and E only in the third term), a simple closed form solution can only be generated for the third term, using the assumption that A=B=0. Making such an assumption leads to the following expression for the internal energy due to the third term:

$$E = \exp(-\omega \ln V + \ln E_0)$$

where V is the final volume of the cube and E_0 is the initial internal energy. This solution takes advantage of the fact that the initial volume of the cube is 1 cm^3.

The predictions of this closed form solution for the internal energy due to the third term can be compared to the code results as extracted using GRIZ, which again limits the comparison to 7 significant figures. This is done in the following table.

Table 14. Exact and Code Internal Energies for the third term in EOS Form 2

Time	Code (GRIZ)	*Closed Form*	(*Closed* - GRIZ)/GRIZ
0.00E+00	1.00000000E-03	1.0000000E-03	0.000000E+00
1.00E-03	1.00756600E-03	1.0075662E-03	2.305122E-07
2.00E-03	1.01526700E-03	1.0152674E-03	3.984000E-07
3.00E-03	1.00756600E-03	1.0075662E-03	2.305122E-07
4.00E-03	1.00000000E-03	1.0000000E-03	2.168404E-16
5.00E-03	9.92565100E-04	9.9256503E-04	-7.150757E-08
6.00E-03	9.85257800E-04	9.8525778E-04	-2.430617E-08
7.00E-03	9.92565100E-04	9.9256503E-04	-7.150757E-08
8.00E-03	1.00000000E-03	1.0000000E-03	2.168404E-16

As expected, the agreement between the closed form solution for the third term and the code results is at the level of ~ 4 parts in 10^7, which is limited by the number of significant figures in the output provided by GRIZ.

Finally, the internal energy returned by the code for Equation-of-State Form 2 can be compared to a numerical integration performed using EXCEL to determine the sensitivity of this result to differences in the numerical integration scheme. This is done in the following table.

Table 15. Reference and Code Internal Energies for EOS Form 2

Time	Code (GRIZ)	*Reference Energy*	(*Reference* - GRIZ)/GRIZ
0.00E+00	1.00000000E-03	1.00000000E-03	0.000000E+00
1.00E-03	4.93969500E-03	4.93969415E-03	-1.712669E-07
2.00E-03	9.23689900E-03	9.23689620E-03	-3.026991E-07
3.00E-03	4.93969500E-03	4.93969592E-03	1.861780E-07
4.00E-03	1.00000000E-03	1.00000681E-03	6.809678E-06
5.00E-03	-2.61040300E-03	-2.61040235E-03	-2.471270E-07
6.00E-03	-5.91818900E-03	-5.91818634E-03	-4.489569E-07
7.00E-03	-2.61040300E-03	-2.61040365E-03	2.499197E-07
8.00E-03	1.00000000E-03	9.99994603E-04	-5.397370E-06

The agreement between these two numerical integration schemes is better than 5 parts in 10^7, except for the points representing the return of the cube to its original configuration, where the agreement is degraded by about a factor of 10. It is not clear at this time why these 2 points should exhibit a reduction in the level of agreement, but is likely due to the nodes not being returned to exactly their original locations.

Note that the changes in the internal energy are large compared to the initial value of the internal energy, so this comparison is not dominated by the initial value of the internal energy. Furthermore, the pressure is the more important quantity being determined from the equation-of-state and the agreement between the code results and those obtained from the theoretical model is better than 4 parts in 10^{10}, as exhibited earlier, which is better than the agreement exhibited by the internal energy results. The convergence study performed on the calculation of the internal energy for EOS Form 1 was not repeated for this EOS, as the same result is to be expected, which is that the internal energy calculation is expected to be second order accurate in Δt, the time step size for the simulation.

This establishes the implementation of Equation-of-State Form 2 in DYNA3D. The equation-of-state is performing as expected, in that the pressure in the cubes increases as they are compressed and decreases as they are expanded. The behavior of each of the terms in the equation-of-state has been examined and found to be performing as expected and with good accuracy. The behavior of the equation-of-state as a whole has been examined and is performing as expected and with good accuracy.

Equation-of-State Form 3

The next model to be tested was Equation-of-State Form 3, an equation-of-state developed by Seymour Sack to describe high-explosive detonation products and is an alternative to EOS Form 2. This EOS has the following form:

$$p = A_3/V^{A_1} \exp(-A_2V)\ (1 - B_1/V) + B_2E/V$$

where p is the pressure, V is the relative volume and E is the specific internal energy. A_1, A_2, A_3, B_1, and B_2 are material dependent coefficients. This EOS includes a tensile cap requiring that $p \geq 0$.

As there are two terms in the equation-of-state, Equation-of-State Form 3 was tested using 3 cubes, one for each of the two terms in the expression for EOS Form 3 and one for the full equation-of-state model. The 3 cubes use the same compression and expansion as that used for the testing of EOS Form 1.

Prior to discussing the calculations using EOS Form 3, a few code issues need to be addressed and these are not necessarily readily apparent to the user. First, in order for the term dependent on the internal energy to perform as expected, it is required to have an initial energy present in the simulation, so the initial internal energy was set to a value of 1.0e-3 in all of the cubes. In addition, in order to eliminate issues with the work performed by the bulk viscosity, the two input coefficients for the bulk viscosity on the material card were set to 1.0e-20 in each of the 3 cubes. Failing to do so results in the work performed on the cube being dominated by contributions from the bulk viscosity. Finally, the code version used for this test was version 14.2.0 revision 1.3297.

Input coefficients for Equation-of-State Form 3 were chosen such that the contribution to the pressure from the two terms was of the same order of magnitude as a function of time during the compression and expansion of the cubes. The following coefficients were used as input for the testing of the full implementation of EOS Form 3: $A_1 = 1.1$, $A_2 = 4.0$, $A_3 = 4.603$, $B_1 = 0.37$, $B_2 = 12.6$. The following table lists the values of the input coefficients for each of the cubes in the testing of EOS Form 3.

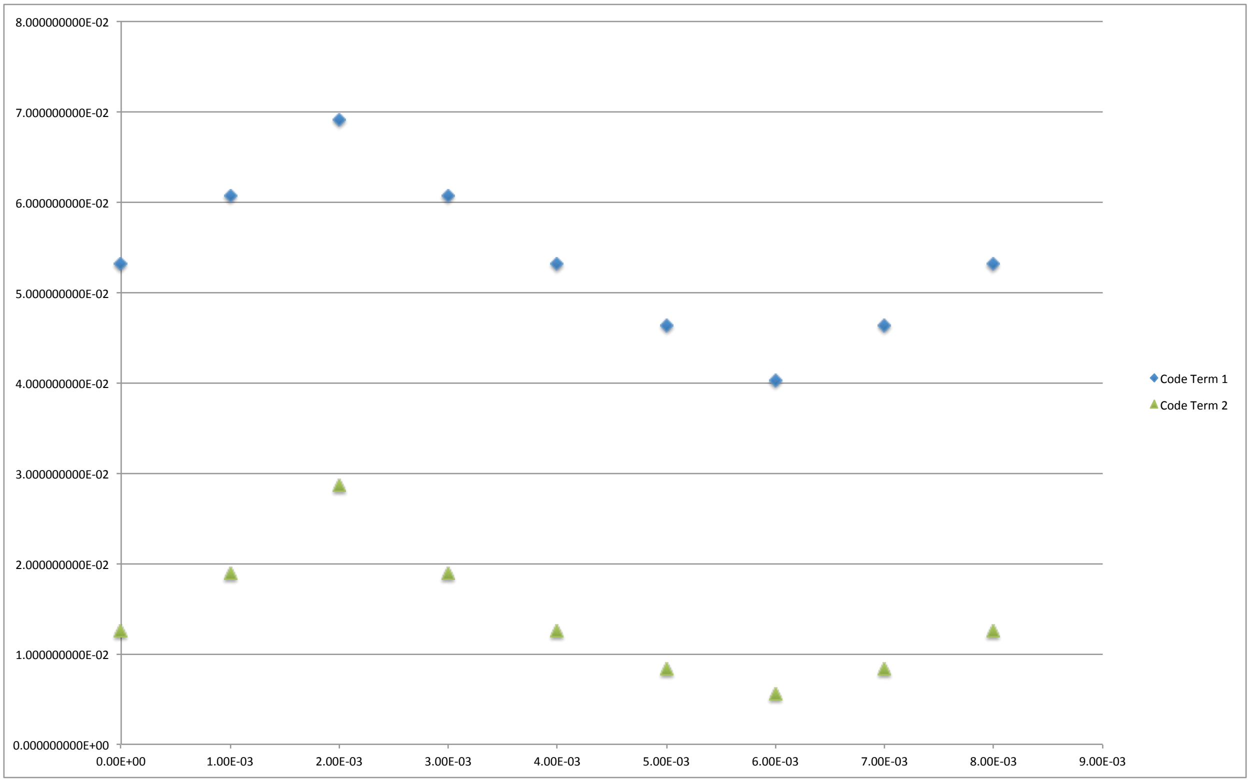
Table 16. Input coefficients for the testing of EOS Form 3

Cube	A_1	A_2	A_3	B_1	B_2
1	1.1	4.0	4.603	0.37	0
2	0	0	0	0	12.6
3	1.1	4.0	4.603	0.37	12.6

The initial specific energy was set to 1.0e-3 and the initial volume was 1.0 cm^3.

The two terms in the equation-of-state were tested independently, then the full equation-of-state model was tested. The following plot displays the pressures from the first two terms, as returned by the code, as a function of time for this simulation.

Figure 7. Code pressures for the two terms of EOS Form 3 as a function of time



As the plot demonstrates, both terms are contributing pressures on the order of 10^{-2} during cycling of the cubes.

The following observations may be made from the plot. Both terms contribute an increase in the pressure as the cubes are compressed and both exhibit a decrease in pressure as the cubes are expanded, as expected. In addition, both terms are positive definite during cycling of the cubes. Therefore, at least qualitatively, the code output is behaving as expected.

Using the normalized difference defined by equation 1, the agreement between the pressures for the two terms as calculated using the theoretical expression and the results returned by the code is demonstrated in the following table for the second term as a function of time.

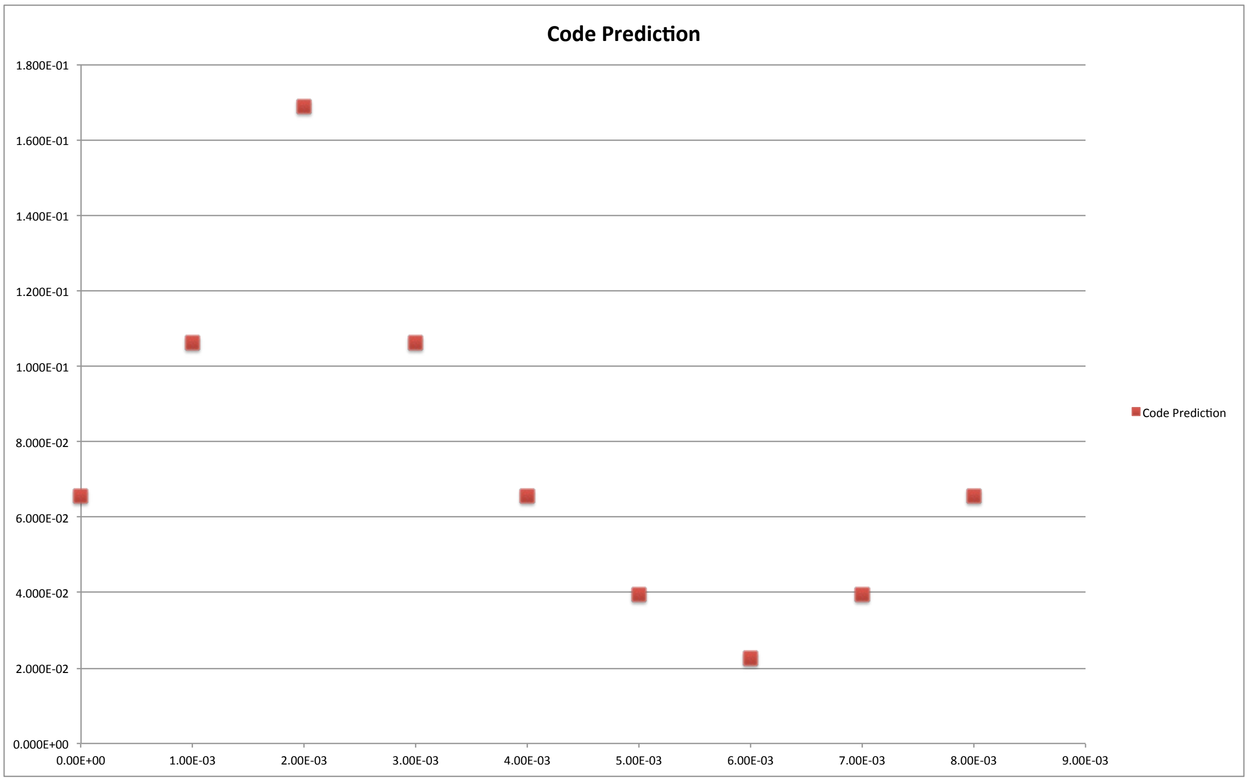
Table 17. Exact and Code Pressures for the second term of EOS Form 3

Time	*Theoretical Pressure*	*Code Pressure*	*(Theoretical - Code)/Code*
0.00E+00	1.260000000E-02	1.260000000E-02	1.3767646635E-16
1.00E-03	1.898692372E-02	1.898692380E-02	-4.3603550953E-09
2.00E-03	2.873072974E-02	2.873072995E-02	-7.3107502509E-09
3.00E-03	1.898692372E-02	1.898692380E-02	-4.3615349715E-09
4.00E-03	1.260000000E-02	1.260000000E-02	-4.5793533205E-11
5.00E-03	8.395730603E-03	8.395730551E-03	6.2878502149E-09
6.00E-03	5.616729867E-03	5.616729779E-03	1.5621260057E-08
7.00E-03	8.395730603E-03	8.395730551E-03	6.2521500466E-09
8.00E-03	1.260000000E-02	1.260000000E-02	-1.0185704241E-10

As the table demonstrates, the code pressures are in excellent agreement with the exact results, with the level of agreement being better than ~2 parts in 10^8. The level of agreement achieved in the testing of the first term of this EOS model is 3 - 4 orders of magnitude better than this (~ 1 part in 10^{12}).

Now that the behavior of the two individual terms in the expression for Equation-of-State Form 3 has been examined, the behavior of the full expression for this EOS may be investigated. The following plot displays the pressure returned by the code as a function of time for EOS Form 3.

Figure 8. Code pressures for EOS Form 3 as a function of time



Note that the pressure is behaving as one would expect, as the pressure increases when the cube is compressed, decreases as the cube is expanded and then returns to the initial pressure as the cube is relaxed back to its original configuration. Note also that the pressure returned by EOS Form 3 is positive definite.

The following table compares the reference pressures to the code results as a function of time for Equation-of-State Form 3. Reference pressures are used because there is no closed form solution for the internal energy for the full EOS model.

Table 18. Reference and Code Pressures for EOS Form 3

Time	*Reference Pressure*	*Code Pressure*	*(Reference - Code)/Code*
0.00E+00	6.571333806E-02	6.5713338057E-02	8.447470920E-16
1.00E-03	1.062837961E-01	1.0628379472E-01	1.287547442E-08
2.00E-03	1.688522055E-01	1.6885706298E-01	-2.876666795E-05

3.00E-03	1.062837961E-01	1.0628379472E-01	1.287409139E-08
4.00E-03	6.571333806E-02	6.5713338061E-02	-5.734206616E-11
5.00E-03	3.943319699E-02	3.9433197267E-02	-6.937270045E-09
6.00E-03	2.246573441E-02	2.2465187604E-02	2.433992539E-05
7.00E-03	3.943319699E-02	3.9433197269E-02	-6.986839961E-09
8.00E-03	6.571333806E-02	6.5713338065E-02	-1.278362110E-10

As the table clearly demonstrates, the code predictions are in excellent agreement with the reference results, with the level of agreement being better than 2 parts in 10^8. These results establish confidence in the pressures returned by the implementation of Equation-of-State Form 3 in DYNA3D.

Exceptions to the level of agreement between the theoretical expression and the code results exist at both the peak of the compression and the peak of the tension. The calculation of the theoretical pressure relies on a numerical integration of the internal energy performed in EXCEL. If the EXCEL result for the internal energy is replaced by the code reported internal energy (collected using GRIZ), the level of agreement improves by more than two orders of magnitude at each point. In addition, if the cube is slightly over-compressed in the EXCEL numerical integration (by a factor of 1.00000673) at the peak of the compression, the agreement also improves by more than two orders of magnitude. The cause of this failure of the EXCEL model to reproduce the code results for the full equation-of-state model is under study, as this methodology returned excellent results for the studies of both EOS Form 1 and EOS Form 2, as well as the individual terms of EOS Form 3.

The code results for the internal energy can also be investigated for this equation-of-state. A simple closed form solution can be generated for both terms individually, but not for the equation-of-state as a whole, as the internal energy appears in the second term but not the first. Assuming $B_2 = 0$, the following closed form solution for the first term was evaluated using Mathematica:

$$E = - \int A_3/V^{A_1} \exp(-A_2 V)\ (1 - B_1/V)\ dV$$

Assuming that $A_1=A_2=A_3=B_1=0$ leads to the following expression for the internal energy due to the second term:

$$E = \exp(-B_2 \ln V + \ln E_0)$$

where V is the final volume of the cube and E_0 is the initial internal energy. This solution takes advantage of the fact that the initial volume of the cube is 1 cm^3.

The predictions of the closed form solution for the internal energy due to the second term of EOS Form 3 can be compared to the code results as extracted using GRIZ, which again limits the comparison to 7 significant figures. This is done in the following table.

Table 19. Exact and Code Internal Energies for the second term in EOS Form 3

Time	Code (GRIZ)	*Closed Form*	(*Closed* - GRIZ)/GRIZ
0.00E+00	1.00000000E-03	1.0000000E-03	2.168404345E-16
1.00E-03	1.46214200E-03	1.4621423E-03	2.114283525E-07
2.00E-03	2.14612200E-03	2.1461217E-03	-1.559437627E-07
3.00E-03	1.46214200E-03	1.4621423E-03	2.114283525E-07
4.00E-03	1.00000000E-03	1.0000000E-03	2.168404345E-16
5.00E-03	6.86518200E-04	6.8651823E-04	3.658663042E-08
6.00E-03	4.73057000E-04	4.7305704E-04	7.855547160E-08
7.00E-03	6.86518200E-04	6.8651823E-04	3.658663042E-08
8.00E-03	1.00000000E-03	1.0000000E-03	2.168404345E-16

As expected, the agreement between the closed form solution for the second term and the code results is at the level of a couple of parts in 10^7. This level of agreement is also observed between the closed form solution for the first term and the code results.

Finally, the internal energy returned by the code for Equation-of-State Form 3 can be compared to a numerical integration performed using EXCEL to determine the sensitivity of this result to differences in the numerical integration scheme. This is done in the following table.

Table 20. Reference and Code Internal Energies for EOS Form 3

Time	Code (GRIZ)	*Reference*	(*Reference* - GRIZ)/GRIZ
0.00E+00	1.00000000E-03	1.000000000E-03	0.000000E+00
1.00E-03	3.50884400E-03	3.508844591E-03	1.683077E-07
2.00E-03	7.44446200E-03	7.444098806E-03	-4.878711E-05
3.00E-03	3.50884400E-03	3.508844591E-03	1.683077E-07
4.00E-03	1.00000000E-03	1.000000000E-03	0.000000E+00
5.00E-03	-5.62902800E-04	-5.629028257E-04	4.557229E-08
6.00E-03	-1.49941500E-03	-1.499369188E-03	-3.055337E-05
7.00E-03	-5.62902800E-04	-5.629028257E-04	4.557229E-08
8.00E-03	1.00000000E-03	1.000000000E-03	0.000000E+00

With the exception of the point at the peak of the tension, the agreement between these two numerical integration schemes is better than 4 parts in 10^7, indicating that these results are not very sensitive to the exact details of the numerical integration.

Exceptions to the level of agreement between the EXCEL numerical integration and the code results exist at both the peak of the compression and the peak of the tension. If the cube is slightly over-compressed in the EXCEL numerical integration (by a factor of 1.00000673) at the peak of the compression, the agreement improves by more than two orders of magnitude. The cause of this failure of the EXCEL model to reproduce the code results for the full equation-of-state model is under study, as this methodology returned excellent results for the studies of both EOS Form 1 and EOS Form 2, as well as the individual terms of EOS Form 3.

Note that the changes in the internal energy are large compared to the initial value of the internal energy, so this comparison is not dominated by the initial value of the internal energy. Furthermore, the pressure is the more important quantity being determined from the equation-of-state and the agreement between the code results and those obtained from the theoretical model is better than 4 parts in 10^8, as exhibited earlier, which is better than the agreement exhibited by the internal energy results. The convergence study performed on the calculation of the internal energy for EOS Form 1 was not repeated for this EOS, as the same result is to be expected, which is that the internal energy calculation is expected to be second order accurate in Δt, the time step size for the simulation.

This establishes the implementation of Equation-of-State Form 3 in DYNA3D. The equation-of-state is performing as expected, in that the pressure in the cubes increases as they are compressed and decreases as they are expanded. The behavior of each of the terms in the equation-of-state has been examined and found to be performing as expected and with good accuracy. The behavior of the equation-of-state as a whole has been examined and is performing as expected and with good accuracy.

Equation-of-State Form 4

The next model to be tested was Equation-of-State Form 4, the Gruneisen equation-of-state with cubic shock velocity-particle velocity. This EOS defines the pressure for compressed materials ($\mu > 0$) as:

$$p = \frac{\rho_0 C^2 \mu \left[1 + \left(1 - \frac{\gamma_0}{2}\right)\mu - \frac{a}{2}\mu^2\right]}{\left[1 - (S_1 - 1)\mu - S_2 \frac{\mu^2}{\mu + 1} - S_3 \frac{\mu^3}{(\mu + 1)^2}\right]^2} + (\gamma_0 + a\mu)E$$

and for expanded materials ($\mu < 0$) as:

$$p = \rho_0 C^2 \mu + (\gamma_0 + a\mu)E$$

where ρ_0 is the initial density, C is the intercept of the shock velocity vs. particle velocity (ν_s - ν_p) curve, S_1, S_2 and S_3 are the coefficients of the slope of the ν_s - ν_p curve, γ_0 is the Gruneisen gamma, and a is the first order volume correction to γ_0. The excess compression, μ, is related to the density by $\mu = \rho/\rho_0 - 1$. As in the testing of the other EOS models discussed earlier, ρ_0 = 1.0 and the initial volume, V_0 = 1.0.

While there are only two terms in the equation-of-state, Equation-of-State Form 4 was tested using 11 cubes in an attempt to deliver as much testing of the individual portions of the EOS model as possible. There are clean separations of the EOS for several choices of the input parameters and the manner in which the EOS is tested by these cubes is described below. The 11 cubes use the same compression and expansion as that used for the testing of EOS Form 1.

Prior to discussing the calculations using EOS Form 4, a few code issues need to be addressed and these are not necessarily readily apparent to the user. First, in order to eliminate issues with the work performed by the bulk viscosity, the two input coefficients for the bulk viscosity on the material card were set to 1.0e-20 in each of the 11 cubes. Failing to do so results in the work performed on the cube being dominated by contributions from the bulk viscosity. Next, C is related to the sound speed in the material and so to avoid divide by zero issues in calculations using the sound speed, it is necessary that this coefficient not be zero, so an input value of 1.0e-20 was used for this coefficient when eliminating contributions from the first term in both compression and expansion. Finally, the code version used for this test was version 14.2.0 revision 1.3297.

The input coefficients used for testing Equation-of-State Form 4 are for polystyrene (ρ_0 =1.046) and taken from Steinberg's paper[5], except that polystyrene has an accepted value of a=0.0. For testing purposes, a will be set to 0.1 to test the full implementation of the EOS model. The cubes are set up in the following manner:

Cube 1: C=1.0e-20, γ_0=0.67, a=0.1, S_1=1, S_2=0, S_3=0, E_0=1.0e-3 which tests the contribution of the $(\gamma_0 + a\mu)E$ term in both compression and expansion by making the contribution of the first term small in both compression and expansion and eliminates any possible contributions from the denominator in compression

[5] Steinberg, *Equation of State and Strength Properties of Selected Materials*, UCRL-MA-106439, Feb. 1996

Cube 2: C=0.189, γ_0=0, a=0, S_1=1, S_2=0, S_3=0, E_0=0 which tests the $\rho_0 C^2\mu$ term in expansion and a $\rho_0 C^2\mu(1+\mu)$ term in compression

Cube 3: C=0.189, γ_0=0.67, a=0, S_1=1, S_2=0, S_3=0, E_0=1.0e-3 which adds the contribution of the $(1-\gamma_0/2)\mu$ term in numerator of the first term in compression, but also adds $\gamma_0 E$ in both compression and expansion, so the splitting of the terms has become complicated

Cube 4: C=0.189, γ_0=0, a=0.1, S_1=1, S_2=0, S_3=0, E_0=1.0e-3 which adds the contribution of the $a\mu^2/2$ term in the numerator of the first term in compression, but also adds $a\mu E$ in both compression and expansion, so the splitting of the terms is again complicated

Cube 5: C=0.189, γ_0=0, a=0, S_1=2.965, S_2=0, S_3=0, E_0=0 which tests the contribution of the first term in the denominator in compression

Cube 6: C=0.189, γ_0=0, a=0, S_1=1, S_2=-4.609, S_3=0, E_0=0 which tests the contribution of the second term in the denominator in compression

Cube 7: C=0.189, γ_0=0, a=0, S_1=1, S_2=0, S_3=2.328, E_0=0 which tests the contribution of the third term in the denominator in compression

Cube 8: C=0.189, γ_0=0.0, a=0, S_1=2.965, S_2=-4.609, S_3=2.328, E_0=0 which tests the behavior of the full denominator in the EOS model

Cube 9: C=0.189, γ_0=0.67, a=0, S_1=2.965, S_2=-4.609, S_3=2.328, E_0=1.0e-3 which adds the contribution of the $(1-\gamma_0/2)\mu$ term in the numerator of the first term in compression with the full denominator, but also adds $\gamma_0 E$ in both compression and expansion, so the splitting of the terms has become complicated

Cube 10: C=0.189, γ_0=0, a=0.1, S_1=2.965, S_2=-4.609, S_3=2.328, E_0=1.0e-3 which adds the contribution of the $a\mu^2/2$ term in the numerator of the first term in compression with the full denominator, but also adds $a\mu E$ in both compression and expansion, so the splitting of the terms has become complicated

Cube 11: C=0.189, γ_0=0.67, a=0.1, S_1=2.965, S_2=-4.609, S_3=2.328, E_0=1.0e-3 which tests the implementation of the full EOS model

The following table summarizes these values for the input coefficients for the 11 cubes comprising this test suite.

Table 21. Input coefficients for the testing of EOS Form 4

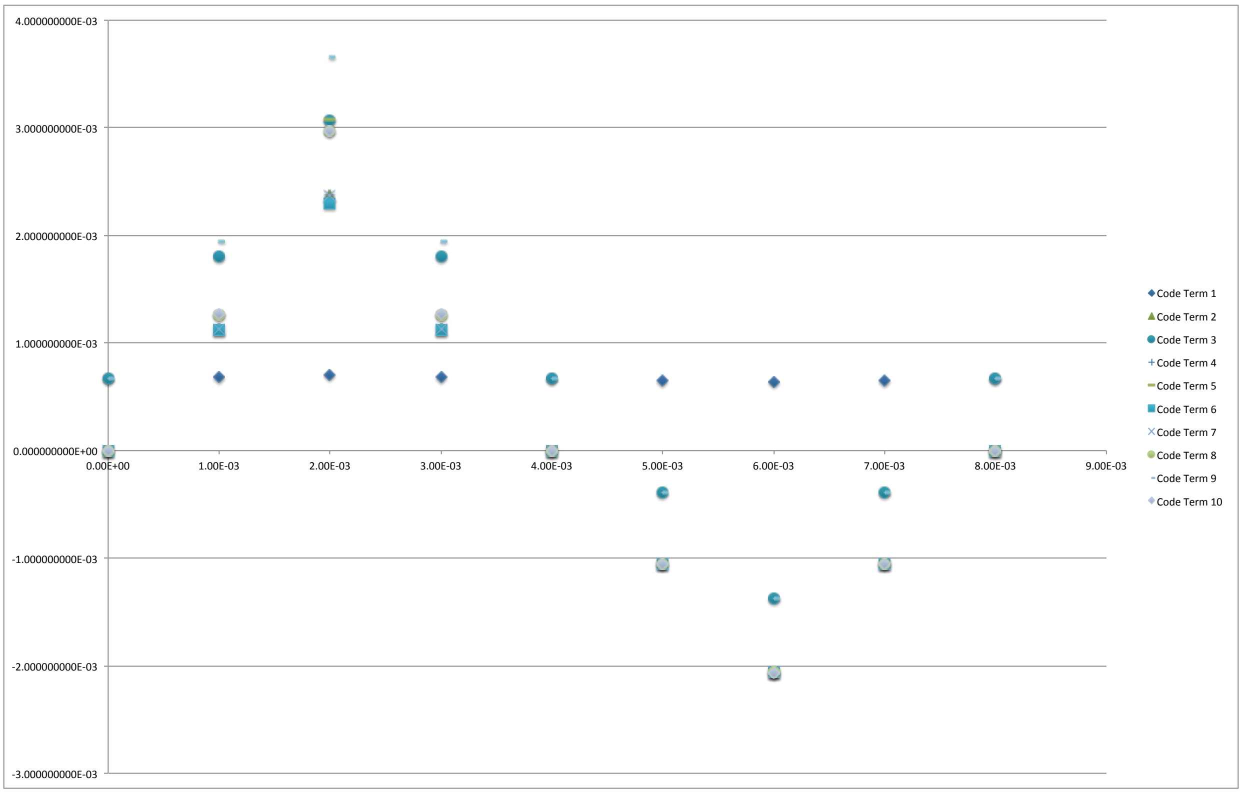
Cube	C	S_1	S_2	S_3	γ_0	a	E_0
1	1.0e-20	1	0	0	0.67	0.1	1.0e-3
2	0.189	1	0	0	0	0	0
3	0.189	1	0	0	0.67	0	1.0e-3
4	0.189	1	0	0	0	0.1	1.0e-3
5	0.189	2.965	0	0	0	0	0
6	0.189	1	-4.609	0	0	0	0
7	0.189	1	0	2.328	0	0	0
8	0.189	2.965	-4.609	2.328	0	0	0
9	0.189	2.965	-4.609	2.328	0.67	0	1.0e-3
10	0.189	2.965	-4.609	2.328	0	0.1	1.0e-3

11	0.189	2.965	-4.609	2.328	0.67	0.1	1.0e-3

As stated above, there is no clean way to separate this EOS model into all of its components, as γ_0 and *a* appear in both the first and second term in both compression and expansion, but the internal energy appears only in the second term in compression and expansion.

The following plot displays the pressure from each of the first 10 cubes as a function of time, as returned by the code.

Figure 9. Code pressures for the tested components of EOS Form 4 as a function of time



As the plot demonstrates, the pressure from each of the tested terms returned by the code is of the same order of magnitude for each of the cubes.

The following observations may be made from the code output. In all of the cubes, the pressure increases as the cube is compressed and decreases as the cube is expanded, which is the expected behavior. The contribution from Cube 1 is positive definite for the input coefficients that were chosen ($\gamma_0 > 0$, $a > 0$). Note that cube 9 is the actual Gruneisen EOS for polystyrene, an artifact of the method employed to break this EOS model into pieces. Note also that cube 9 returns the largest pressures in compression, but not in tension.

Using the normalized difference defined by equation 1, the agreement between the pressures for the fifth 'term' as calculated using the reference expression and the results returned by the code is demonstrated in the following table as a function of time.

Table 22. Reference and Code Pressures for the fifth term of EOS Form 4

Time	*Reference Pressure*	*Code Pressure*	*(Reference - Code)/Code*
0.00E+00	0.0000000E+00	0.000000000E+00	0.0000000000E+00

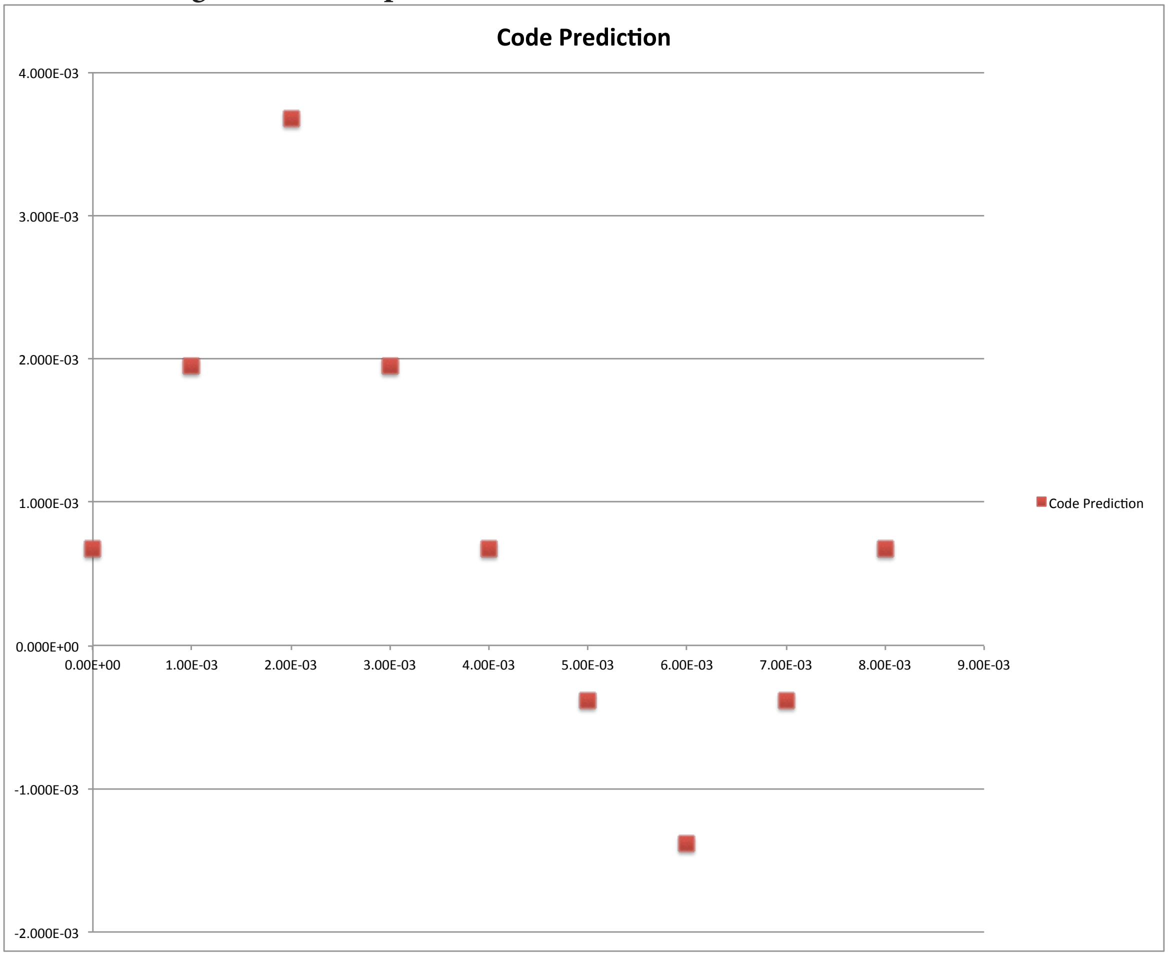
1.00E-03	1.2757496E-03	1.275749626E-03	-1.4240170041E-12
2.00E-03	3.0816590E-03	3.081659035E-03	-1.8432772597E-12
3.00E-03	1.2757496E-03	1.275749626E-03	-2.6075250489E-12
4.00E-03	0.0000000E+00	0.000000000E+00	0.0000000000E+00
5.00E-03	-1.0505493E-03	-1.050549326E-03	-5.8082849386E-13
6.00E-03	-2.0603039E-03	-2.060303888E-03	-7.1378394012E-13
7.00E-03	-1.0505493E-03	-1.050549326E-03	-6.1901373599E-13
8.00E-03	0.0000000E+00	0.000000000E+00	0.0000000000E+00

As the table clearly demonstrates, the code pressures are in excellent agreement with the reference results, with the level of agreement being better than 3 parts in 10^{12}. This level of agreement is typical of the individual 'terms' tested, with the exception of the results from Cubes 3 and 9.

The normalized differences from Cubes 3 and 9 are on the order of 10^{-8} in compression and 10^{-7} in tension. While this level of agreement between the reference result and the code result is still quite good, the fact that it is considerably lower than the agreement exhibited by the other cubes warranted further investigation. It was discovered that if the GRIZ reported internal energy, limited in accuracy to 7 digits when written to an output file, was replaced by a more accurate result available only internally in GRIZ (which differed from the written output in the 8^{th} digit and beyond), the agreement between the code results and the exact expression was improved by about an order of magnitude. This indicates that the conversion of the representation of the internal energy from a 64 bit number to a 32 bit number that occurs when GRIZ creates its written output file is affecting the accuracy of our results for this equation-of-state model. The level of difference between the written and internal representations of the internal energy indicates that this equation-of-state model, at least for the present choice of input coefficients, is very sensitive to the value of the internal energy, something that shall be encountered again.

Now that the behavior of each of the tested individual 'terms' in the expression for Equation-of-State Form 4 has been examined, the behavior of the full expression for this EOS can be investigated. The following plot displays the pressure as a function of time for EOS Form 4 as returned by the code.

Figure 10. Code pressures for EOS Form 4 as a function of time



Note that the pressure is behaving as one would expect, in that the pressure increases as the cube is compressed, decreases as the cube is expanded and returns to the initial pressure when the cube is returned to its original configuration. It is interesting to note that the pressures returned by the full implementation of EOS Form 4 closely resemble the results obtained from Cube 9.

The following table compares the reference pressure to the code results as a function of time.

Table 23. Reference and Code Pressures for Equation-of-State Form 4

Time	*Reference Pressure*	*Code Pressure*	*(Reference - Code)/Code*
0.00E+00	6.7000000E-04	6.700000000E-04	0.000000000E+00
1.00E-03	1.9505269E-03	1.951836391E-03	-6.709008253E-04
2.00E-03	3.6666304E-03	3.679715364E-03	-3.555985185E-03
3.00E-03	1.9505269E-03	1.951836391E-03	-6.708926974E-04
4.00E-03	6.7000015E-04	6.700000000E-04	2.198101937E-07
5.00E-03	-3.8621619E-04	-3.862162978E-04	-2.806375243E-07
6.00E-03	-1.3805138E-03	-1.380513983E-03	-1.528347745E-07
7.00E-03	-3.8621619E-04	-3.862162978E-04	-2.877481273E-07
8.00E-03	6.7000001E-04	6.700000000E-04	8.340091871E-09

As the table demonstrates, the code predictions in compression are no longer in excellent agreement with the reference results. This is similar to the results obtained from Cube 3 and Cube 9. However, replacing the 7 digit GRIZ written result for the internal energy with the more accurate internal representation available in GRIZ does not improve the agreement between the code pressure and the reference result, as it did in the testing of Cubes 3 and 9.

Further investigation revealed that if the GRIZ reported internal energy (the higher resolution internal representation) was decreased by 0.19% on the ramp up to maximum compression and the ramp back down to the initial configuration, the normalized agreement between the code reported pressure and the theoretical pressure improved from -6.71E-04 to -6.80E-10, an improvement of nearly six orders of magnitude. This is a further indication that, at least for the present choice of input coefficients, this equation-of-state model is very sensitive to the value of the internal energy.

Examination of the results obtained in this testing of Equation-of-State Form 4 indicate that this sensitivity to the value of the internal energy is obtained when both γ_0 is non-zero and C is large enough for the first term to contribute in compression, as revealed by Cubes 3, 9 and 11. It appears as if the trapezoidal rule implemented in the code to perform the numerical integration of the internal energy is not sufficiently converged for the higher order terms introduced by non-zero values of γ_0, at least for the present choice of input coefficients. Since the use of non-zero values for a introduces even higher order terms than γ_0, it is believed that if substantially larger values were tested for a, the behavior observed would be similar to that obtained for the γ_0 terms.

While the results obtained from the testing of Equation-of-State Form 4 are clearly not as good as the results obtained in testing the EOS models previously discussed in this document, these results do establish a degree of confidence in the implementation of Equation-of-State Form 4 in DYNA3D. However, the user should perhaps be warned that this EOS model is known to exhibit, under certain circumstances, a marked sensitivity to the value of the internal energy. Furthermore, while this sensitivity is relatively easy to test for in a constructed test suite such as is discussed here, such a sensitivity may prove far more difficult to diagnose in a real-world simulation.

Now that the pressures returned by the code have been discussed, the code results for the internal energy can be investigated. Given the manner in which the EOS model was split into 'terms' for testing purposes, closed form solutions for the internal energy can be derived for many of these 'terms'. For some cubes, closed form solutions exist in both compression and tension, while for others the closed form solution exists only in tension. For the cubes that exhibit a closed form solution only in tension, a numerical integration was performed in EXCEL to generate internal energies to be used for the reference calculation of the pressure. Closed form solutions for the internal energy for Cube 2 exist in both tension and compression. In tension, the internal energy solution has the following form:

$$E = -\rho_0 C^2(\ln V - V + 1)$$

where V is the final volume of the cube and the other coefficients are as before. In compression, this solution has the form:

$$\mathrm{E} = -\rho_0 C^2(-\ln V + 1 - 1/V)$$

where V is again the final volume of the cube and the other coefficients are as before. Both of these solutions take advantage of the fact that the initial volume of the cube is 1 cm^3 and that the initial internal energy for Cube 2 is 0.

The predictions of these closed form solutions for the internal energy in Cube 2 can be compared to the code results as extracted using GRIZ, which limits the comparison to 7 significant figures. The following table makes this comparison.

Table 24. Exact and Code Internal Energies for Cube 2 in Equation-of-State Form 4

Time	Code (GRIZ)	*Closed Form*	(*Closed* - GRIZ)/GRIZ
0.00E+00	0.0000000E+00	0.0000000E+00	0.000000000E+00
1.00E-03	1.6401100E-05	1.6401103E-05	1.895318702E-07
2.00E-03	6.6953550E-05	6.6953552E-05	3.411465412E-08
3.00E-03	1.6401100E-05	1.6401103E-05	1.895318702E-07
4.00E-03	3.8724100E-16	0.0000000E+00	0.000000000E+00
5.00E-03	1.6074710E-05	1.6074716E-05	3.596924472E-07
6.00E-03	6.4302020E-05	6.4302019E-05	-1.462639420E-08
7.00E-03	1.6074710E-05	1.6074716E-05	3.596924472E-07
8.00E-03	3.9116950E-16	0.0000000E+00	0.000000000E+00

As expected, the level of agreement between the closed form solution for Cube 2 and the code result is at the level of about 3.5 parts in 10^7. With the exception of Cube 8 in compression, this level of agreement is typical for all of the internal energy calculations, whether the code is being compared to a closed form solution or to the result of a numerical integration performed in EXCEL. The agreement between the closed form solution for Cube 8 and the code result in compression is about an order of magnitude lower than that exhibited by the other cubes and may be a result of higher order terms in μ causing an issue with the convergence of the numerical integration scheme, as was proposed earlier for the full EOS model results for the pressure.

While one might expect that Cubes 9 and 10 would also exhibit this tendency toward a reduced level of agreement for the internal energy in compression, neither cube does. This is most likely a result of the fact that closed form solutions for the internal energy do not exist for these two cubes in compression and the comparison is therefore made to the numerical integration performed in EXCEL.

Next, the internal energy returned by the code for Equation-of-State Form 4 can be compared to the result from a numerical integration performed using EXCEL, as no simple closed form solution for the internal energy from this EOS model exists. The following table makes this comparison, where the internal energy as extracted using GRIZ to a written output file has been replaced by the higher resolution representation available internally in GRIZ, so the comparison is not limited to 7 significant figures.

Table 25. Reference and Code Internal Energies for Equation-of-State Form 4

Time	Code (GRIZ)	*Reference*	(*Reference* - GRIZ)/GRIZ
0.00E+00	1.000000047497E-03	1.00000000000E-03	-4.749699778E-08

1.00E-03	1.037878333591E-03	1.03786906000E-03	-8.935141017E-06
2.00E-03	1.118558109738E-03	1.11838361237E-03	-1.560020549E-04
3.00E-03	1.037878333591E-03	1.03786908357E-03	-8.912432074E-06
4.00E-03	1.000000047497E-03	1.00000021981E-03	1.723126002E-07
5.00E-03	9.959134040400E-04	9.95913587433E-04	1.841460157E-07
6.00E-03	1.023421995342E-03	1.02342235407E-03	3.505135388E-07
7.00E-03	9.959134040400E-04	9.95913591548E-04	1.882771842E-07
8.00E-03	1.000000047497E-03	1.00000000834E-03	-3.915972438E-08

As the table demonstrates, the agreement between the two numerical integration schemes is quite good in tension, but not as good in compression. The degraded agreement in compression is most likely due to the presence of multiple higher order terms in μ in the expression for the internal energy and differences in convergence between the two integration schemes for these terms. Note that the availability of extra significant figures in the GRIZ extracted internal energy has not resulted in an improvement in the agreement.

This establishes the implementation of Equation-of-State Form 4 in DYNA3D. The equation-of-state is performing as expected, in that the pressure in the cubes increases as they are compressed and decreases as they are expanded. The behavior of each of the terms in the equation-of-state has been examined and found to be performing as expected and with good accuracy in most cases and reasonable accuracy in others (See results from Cubes 3 and 9). The behavior of the equation-of-state as a whole has been examined and is performing as expected and with good accuracy in tension and reasonable accuracy in compression.

The results obtained from the testing of Equation-of-State Form 4 are clearly not as good as the results obtained in testing the EOS models previously discussed in this document. In light of this result, the user should perhaps be warned that this EOS model is known to exhibit, under certain circumstances, a marked sensitivity to the value of the internal energy. Furthermore, while this sensitivity is relatively easy to test for in a constructed test suite such as is discussed here, such a sensitivity may prove far more difficult to diagnose in a real-world simulation.

Equation-of-State Form 5

The next model to be tested was Equation-of-State Form 5, an equation-of-state that defines the pressure as a ratio of two polynomials that are functions of both the excess compression, μ, and the internal energy, *E*. The form of the equation is as follows:

$$p = \frac{F_1 + F_2 E + F_3 E^2 + F_4 E^3}{F_5 + F_6 E + F_7 E^2}(1 + \alpha\mu)$$

where each of the F_i are polynomials of the excess compression, μ, with the following form:

$$F_i = \sum_{k=0}^{n} A_{ik}\mu^k$$

with n = 4 for F_1 and F_2 and n = 3 for F_3 through F_7. The excess compression, μ, is defined as usual:

$$\mu = \rho/\rho_0 - 1 = V_0/V - 1$$

where ρ is the density (ρ_0 the initial density) and *V* the volume (V_0 the initial volume). In tension ($\mu < 0$), the first term, F_1, is replaced by $F_1 + \beta\mu^2$. The polynomial form chosen for this equation-of-state model (use of multiple terms that are second order or higher in μ and/or *E*) is one that will cause problems for the determination of the internal energy in DYNA3D and, as the pressure depends on the internal energy, may therefore also cause issues with the determination of the pressure. ***It is therefore recommended that code users be warned against the use of this equation-of-state model until an improved method for determining the internal energy has been implemented.***

Equation-of-State Form 5 was tested using 11 cubes. The first cube comprised the simplest test, $p = 1 + \alpha\mu$ in compression and, using the required replacement, $p = (1 + \beta\mu^2)(1 + \alpha\mu)$ in tension. There are then 4 cubes testing each term in the numerator and an additional cube testing the sum of the 4 terms in the numerator. These are followed by three cubes testing each of the terms in the denominator and a cube testing the sum of the three terms in the denominator. Finally, there is a cube testing the full implementation of this equation-of-state model.

Prior to discussing the calculations using EOS Form 5, a few code issues need to be addressed and these are not necessarily readily apparent to the user. First, in order to eliminate issues with the work performed by the bulk viscosity, the two input coefficients for the bulk viscosity on the material card were set to 1.0e-20 in each of the 11 cubes. Failing to do so results in the work performed on the cube being dominated by contributions from the bulk viscosity. Finally, the code version used for this test was version 14.2.0 revision 1.3306.

The input coefficients used for testing Equation-of-State Form 5 are for hydrogen (ρ_0 =0.085) and taken from Steinberg's paper[6], except that hydrogen has an accepted value of β=0.0. For testing purposes, β will be set to 0.1 for Cube 1 and to test the full implementation of the EOS model (Cube 11). The cubes are set up in the following manner:

[6] Steinberg, *The Hydrodynamic Equations of State For the KOVEC code - Addendum 1*, Addendum 1 to UCID-17046-Rev 1, 1978.

Cube 1: $F_{11}=F_{51}=1.0$, $F_{2i}=F_{3i}=F_{4i}=F_{6i}=F_{7i}=0.0$, $\alpha=1$, $\beta=0.1$, $E_0=2.507\text{e-}3$ which tests the contribution of the $(1 + \alpha\mu)$ term in compression and $(1 + \alpha\mu)(1+\beta\mu^2)$ term in expansion by eliminating contributions from the polynomial terms

Cube 2: F_{1i} taken from Steinberg, $F_{51}=1.0$, $F_{2i}=F_{3i}=F_{4i}=F_{6i}=F_{7i}=0.0$, $\alpha=0$, $\beta=0$, $E_0=2.507\text{e-}3$ which tests the contribution of the first polynomial term in the numerator

Cube 3: F_{2i} taken from Steinberg, $F_{51}=1.0$, $F_{1i}=F_{3i}=F_{4i}=F_{6i}=F_{7i}=0.0$, $\alpha=0$, $\beta=0$, $E_0=2.507\text{e-}3$ which tests the contribution of the second polynomial term in the numerator

Cube 4: F_{3i} taken from Steinberg, $F_{51}=10.0$, $F_{1i}=F_{2i}=F_{4i}=F_{6i}=F_{7i}=0.0$, $\alpha=0$, $\beta=0$, $E_0=2.507\text{e-}3$ which tests the contribution of the third polynomial term in the numerator

Cube 5: F_{4i} taken from Steinberg, $F_{51}=100.0$, $F_{1i}=F_{2i}=F_{3i}=F_{6i}=F_{7i}=0.0$, $\alpha=0$, $\beta=0$, $E_0=2.507\text{e-}3$ which tests the contribution of the third polynomial term in the numerator

Cube 6: F_{1i}, F_{2i}, F_{3i}, F_{4i} taken from Steinberg, $F_{51}=100.0$, $F_{6i}=F_{7i}=0.0$, $\alpha=0$, $\beta=0$, $E_0=2.507\text{e-}3$ which tests the contribution of all of the polynomial terms in the numerator

Cube 7: F_{5i} taken from Steinberg, $F_{11}=1.0$, $F_{2i}=F_{3i}=F_{4i}=F_{6i}=F_{7i}=0.0$, $\alpha=0$, $\beta=0$, $E_0=2.507\text{e-}3$ which tests the contribution of the first polynomial term in the denominator

Cube 8: F_{6i} taken from Steinberg, $F_{11}=1.0$, $F_{2i}=F_{3i}=F_{4i}=F_{5i}=F_{7i}=0.0$, $\alpha=0$, $\beta=0$, $E_0=2.507\text{e-}3$ which tests the contribution of the second polynomial term in the denominator

Cube 9: F_{7i} taken from Steinberg and modified to eliminate time step crashes, $F_{11}=1.0$, $F_{2i}=F_{3i}=F_{4i}=F_{5i}=F_{6i}=0.0$, $\alpha=0$, $\beta=0$, $E_0=2.507\text{e-}3$ which tests the contribution of the third polynomial term in the denominator

Cube 10: F_{5i}, F_{6i}, F_{7i} taken from Steinberg, $F_{11}=1.0$, $F_{1i}=F_{2i}= F_{3i}=F_{4i} =0.0$, $\alpha=0$, $\beta=0$, $E_0=2.507\text{e-}3$ which tests the contribution of all of the polynomial terms in the denominator

Cube 11: F_{1i}, F_{2i}, F_{3i}, F_{4i}, F_{5i}, F_{6i},F_{7i} taken from Steinberg, $\alpha=1.0$, $\beta=0.1$, $E_0=2.507\text{e-}3$ which tests the implementation of the full EOS model

The following table summarizes these values for the input coefficients for the 11 cubes comprising this test suite.

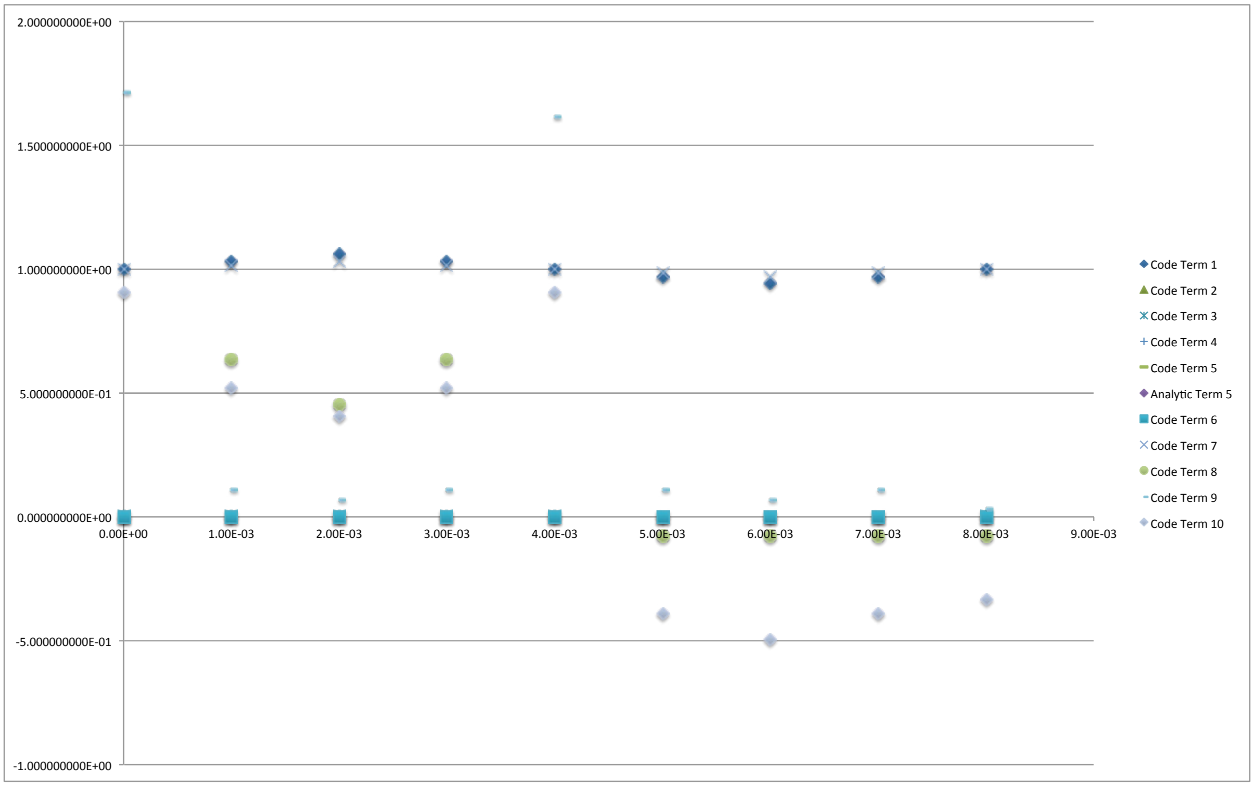
Table 26. Input coefficients for the testing of EOS Form 5

Cube	F_{1i}	F_{2i}	F_{3i}	F_{4i}	F_{5i}	F_{6i}	F_{7i}	α	β
1	$F_{11}=1$	0	0	0	$F_{51}=1$	0	0	1.0	0.1
2	F_{1i}	0	0	0	$F_{51}=1$	0	0	0	0
3	0	F_{2i}	0	0	$F_{51}=1$	0	0	0	0
4	0	0	F_{3i}	0	$F_{51}=10$	0	0	0	0
5	0	0	0	F_{4i}	$F_{51}=100$	0	0	0	0
6	F_{1i}	F_{2i}	F_{3i}	F_{4i}	$F_{51}=100$	0	0	0	0
7	$F_{11}=1$	0	0	0	F_{5i}	0	0	0	0
8	$F_{11}=1$	0	0	0	0	F_{6i}	0	0	0
9	$F_{11}=1$	0	0	0	0	0	F_{7i}	0	0
10	$F_{11}=1$	0	0	0	F_{5i}	F_{6i}	F_{7i}	0	0
11	F_{1i}	F_{2i}	F_{3i}	F_{4i}	F_{5i}	F_{6i}	F_{7i}	1.0	0.1

Entries in the table refer to the coefficients set for a particular cube, e.g., F_{1i} means that the F_{1i} coefficients were taken from the Steinberg paper and F_{11}=1 means that only the F_{11} coefficient was set for that cube and the remaining F_{1i} were equal to zero.

The following plot shows the pressures, as a function of time, for the 10 cubes that tested individual elements of Equation-of-State Form 5.

Figure 11. Code pressures for the tested elements of EOS Form 5 as a function of time



As the plot demonstrates, the contributions from the tested terms vary over several orders of magnitude.

Several observations may be made from the code output that are not readily apparent from the plot. In most cases, the pressure behaves as one would expect, increasing when the cube is compressed and decreasing when the cube is expanded. However, in Cubes 4 and 5, the code predicts the opposite behavior. This is not really alarming, as the equation-of-state model is not intended to be representative of reality when broken apart. A further illustration of this is given by Cubes 8, 9, and 10, in which the code predicted pressure decreases in both compression and expansion. Similar behavior is observed in the analytic modeling.

Using the normalized difference defined by equation 1, the agreement between the pressures calculated using the theoretical expression and the results returned by the code is illustrated in the following table for Cube 6, which is a test of the numerator, as a function of time.

Table 27. Reference and Code Pressures for the numerator of EOS Form 5

Time	*Reference Pressure*	*Code Pressure*	*(Reference - Code)/Code*
0.00E+00	2.7083239E-05	2.708323918E-05	1.8765102839E-15

1.00E-03	2.7488275E-05	2.748827479E-05	2.6488496623E-11
2.00E-03	2.7918291E-05	2.791784784E-05	1.5873820463E-05
3.00E-03	2.7488275E-05	2.748827479E-05	7.8862145166E-11
4.00E-03	2.7083239E-05	2.708323917E-05	1.0682935517E-10
5.00E-03	2.6701314E-05	2.670131429E-05	1.3580752944E-10
6.00E-03	2.6340796E-05	2.634079607E-05	1.6578885788E-10
7.00E-03	2.6701314E-05	2.670131429E-05	1.9255936954E-10
8.00E-03	2.7083239E-05	2.708323917E-05	2.1816921559E-10

As the table clearly demonstrates, for this portion of the testing, the code pressures are in excellent agreement with the reference results, with the level of agreement being better than about 2 parts in 10^{10}. An exception to this exists at the point of peak compression and is due to the code output not being reported at exactly the peak of the compression, which is used to perform the theoretical calculation.

Unfortunately, the level of agreement exhibited by the testing of Cube 6 is not observed in all of the testing of terms for this equation-of-state model. This is a result of the higher order terms being more important in some of the tests than in others. When these higher order terms become important, the code does not always return a good value for the internal energy. As the pressure is a strong function of the internal energy in this equation-of-state model, if the internal energy is incorrect, the pressure will be as well. An example of poor agreement between the code results and the reference calculation is shown in the following table for Brick 9, which tests the last term in the denominator.

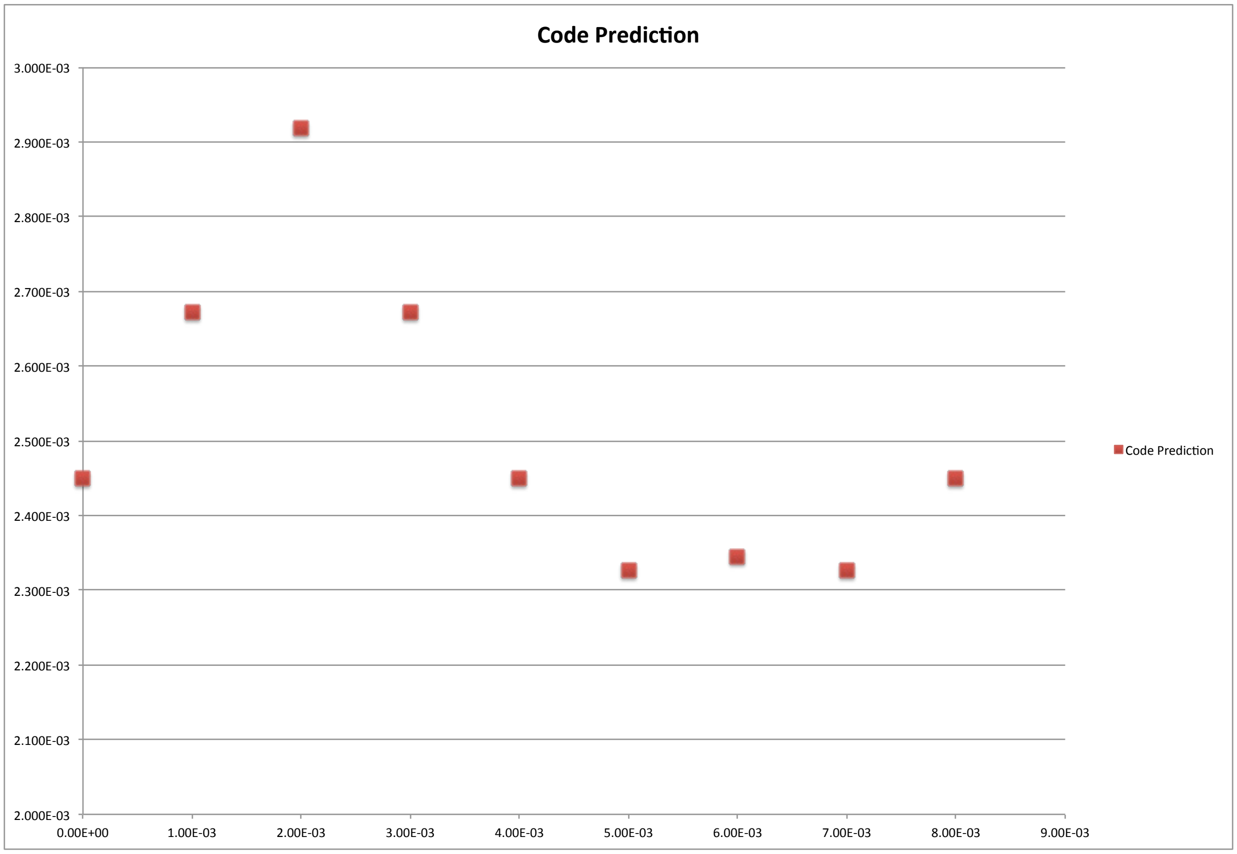
Table 28. Reference and Code Pressures for last term in the denominator of EOS Form 5

Time	*Reference Pressure*	*Code Pressure*	*(Reference - Code)/Code*
0.00E+00	1.7147079E+00	1.71470793E+00	1.8129177612E-15
1.00E-03	1.0946776E-01	1.09418103E-01	4.5379620746E-04
2.00E-03	6.9674221E-02	6.96782470E-02	-5.7778054135E-05
3.00E-03	1.0946776E-01	1.09402318E-01	5.9814336518E-04
4.00E-03	1.7147079E+00	1.61230584E+00	6.3512820559E-02
5.00E-03	1.1038900E-01	1.10407112E-01	-1.6403710074E-04
6.00E-03	6.8606631E-02	6.86094078E-02	-4.0479999142E-05
7.00E-03	1.1038900E-01	1.10389075E-01	-6.6727214041E-07
8.00E-03	1.7147079E+00	3.08933581E-02	5.4504096598E+01

As this table demonstrates, the results of testing this term are scattered and the worst agreement is exhibited by the return of the cube to its starting position. As will be demonstrated later, this poor agreement is a result of the inability of the code to determine the internal energy of the cube reliably. The results of the testing of Equation-of-State Form 5 are essentially split in half, with 5 of the cubes returning results similar to those exhibited in Table 27 and 5 cubes returning results more like those displayed in Table 28.

Now that the behavior of the tested terms has been examined, the behavior of the full expression for Equation-of-State Form 5 can be investigated. The following plot displays the pressure as a function of time for EOS Form 5 as tested in this simulation.

Figure 12. Code pressures for Equation-of-State Form 5 as a function of time



Note that the pressure returned by the code is behaving as one would expect, as the pressure is increasing when the cube is compressed and decreasing when the cube is expanded. A small exception to this should be noted at the peak of the tension, for which the code returns a pressure slightly greater than that on the ramp up to, and returning from, the peak. This same behavior is also observed in the reference calculations, as will be demonstrated below. Finally, for the choice of input coefficients tested, the pressure returned by EOS Form 5 is positive definite.

The following table compares the reference pressure to the code results as a function of time, relying on a numerical integration in EXCEL to provide the internal energy for the reference calculation of the pressure.

Table 29. Reference and Code Pressures for Equation-of-State Form 5

Time	*Reference Pressure*	*Code Pressure*	*(Reference - Code)/Code*
0.00E+00	2.4503574E-03	2.45035738E-03	-1.769867829E-16
1.00E-03	2.6719720E-03	2.67197158E-03	1.703316199E-07
2.00E-03	2.9193193E-03	2.91905698E-03	8.987659836E-05
3.00E-03	2.6719720E-03	2.67197052E-03	5.675207596E-07
4.00E-03	2.4503574E-03	2.45035546E-03	7.823089252E-07

5.00E-03	2.3258153E-03	2.32581311E-03	9.521792577E-07
6.00E-03	2.3449292E-03	2.34492680E-03	1.034749613E-06
7.00E-03	2.3258153E-03	2.32581230E-03	1.305629030E-06
8.00E-03	2.4503574E-03	2.45035371E-03	1.505292869E-06

As the table clearly demonstrates, the code results are in good agreement with the reference predictions, with the agreement being better than 2 parts in 10^6. This is not as good as the agreement exhibited by EOS Forms 1 and 2. It is more along the lines of the agreement exhibited by EOS Form 4, and it will be demonstrated below that this is largely due to the inability of the code to return a good value for the internal energy.

The code results for the internal energy can also be investigated for Equation-of-State Form 5. For the preset choice of input coefficients ($\alpha=\beta=0$ for most of the cubes), a closed form solution exists for the internal energy for Cubes 1, 2, 3, 4, 5, 7, 8 and 9. The following table compares the closed form solution for Cube 2 to the code results.

Table 30. Exact and Code Internal Energies for Cube 2 in Equation-of-State Form 5

Time	Code (GRIZ)	*Closed Form*	(*Closed* - GRIZ)/GRIZ
0.00E+00	2.50700000E-03	2.5070000E-03	0.000000000E+00
1.00E-03	2.50737300E-03	2.5073729E-03	-3.857733274E-08
2.00E-03	2.50851500E-03	2.5085167E-03	6.734626177E-07
3.00E-03	2.50737300E-03	2.5073729E-03	-3.857733274E-08
4.00E-03	2.50700000E-03	2.5070000E-03	0.000000000E+00
5.00E-03	2.50736100E-03	2.5073610E-03	-1.054155200E-08
6.00E-03	2.50842100E-03	2.5084212E-03	7.256319242E-08
7.00E-03	2.50736100E-03	2.5073610E-03	-1.054155200E-08
8.00E-03	2.50700000E-03	2.5070000E-03	0.000000000E+00

The level of agreement is generally better than a few parts in 10^7, which is a good as can be expected with the number of significant digits reported by GRIZ. Unfortunately, this level of agreement is not obtained for all of the testing, as shown in the following table for Cube 9, which tests the last term in the denominator.

Table 31. Exact and Code Internal Energies for Cube 9 in Equation-of-State Form 5

Time	Code (GRIZ)	*Closed Form*	(*Closed* - GRIZ)/GRIZ
0.00E+00	2.50700000E-03	2.5070000E-03	0.000000000E+00
1.00E-03	9.92093000E-03	9.9186792E-03	-2.268727143E-04
2.00E-03	1.24184100E-02	1.2418747E-02	2.712340686E-05
3.00E-03	9.92164500E-03	9.9186792E-03	-2.989210275E-04
4.00E-03	2.58538800E-03	2.5070000E-03	-3.031962707E-02
5.00E-03	-9.87666900E-03	-9.8774796E-03	8.207354988E-05
6.00E-03	-1.25175400E-02	-1.2517793E-02	2.021769191E-05

7.00E-03	-9.87747600E-03	-9.8774796E-03	3.658106403E-07
8.00E-03	1.86774200E-02	2.5070000E-03	-8.657737525E-01

Note that the level of agreement is now many orders of magnitude lower than that exhibited by Cube 2. Furthermore, the level of agreement exhibited by Cube 2 is observed only for Cubes 1, 2, 5 and 6. It is worth noting that Cube 6 does not have a simple closed form solution, but uses a numerical integration performed in EXCEL to provide the internal energy comparison. Finally, if the closed form solution internal energies for Cube 9 are replaced by the code calculated internal energies (as reported by GRIZ) in the calculation of the pressure, the agreement with the code results for the pressure improves by more than three orders of magnitude from that demonstrated in Table 28.

Finally, the internal energy returned by the code for Equation-of-State Form 5 can be compared to a numerical integration performed using EXCEL. This is done in the following table.

Table 32. Reference and Code Internal Energies for Equation-of-State Form 5

Time	Code (GRIZ)	*Reference Energy*	(*Reference* - GRIZ)/GRIZ
0.00E+00	2.50700000E-03	2.50700000000E-03	0.000000000E+00
1.00E-03	2.58299800E-03	2.58299842067E-03	1.628597286E-07
2.00E-03	2.66420700E-03	2.66429253436E-03	3.210499799E-05
3.00E-03	2.58299700E-03	2.58299842225E-03	5.506182842E-07
4.00E-03	2.50699800E-03	2.50700000291E-03	7.989285542E-07
5.00E-03	2.43505500E-03	2.43505723651E-03	9.184623474E-07
6.00E-03	2.36319600E-03	2.36319907158E-03	1.299757026E-06
7.00E-03	2.43505400E-03	2.43505724502E-03	1.332625882E-06
8.00E-03	2.50699600E-03	2.50700001975E-03	1.603412985E-06

Note that the level of agreement is now about an order of magnitude lower than that exhibited by Cube 2. Finally, if the numerically integrated internal energies for EOS Form 5 are replaced by the code calculated internal energies (as reported by GRIZ) in the calculation of the pressure, the agreement with the code results for the pressure improves by about an order of magnitude from that demonstrated in Table 29. This demonstrates the sensitivity of the pressure from this equation-of-state model to the internal energy result.

As these results demonstrate, it is possible to get good agreement between the code results for the internal energy and either the closed form solutions (when they exist) or a numerical integration, but there appears to be no way to guarantee success. Furthermore, even for a simple element such as hydrogen, this equation-of-state model returns questionable results. These results are easily examined in this simple test suite, but a real-world calculation, with complex geometries and more complex materials, would be expected to make such an analysis considerably more difficult. ***It is therefore recommended that code users be warned against the use of this equation-of-state model until an improved method for determining the internal energy has been implemented.***

Equation-of-State Form 6

The next model to be tested was Equation-of-State Form 6, a polynomial that is a function of the excess compression and is linear in the internal energy. The expression for EOS Form 6 is as follows:

$$p = C_0+C_1\mu+C_2\bar{\mu}^2+C_3\mu^3+(C_4+C_5\mu+C_6\bar{\mu}^2)E,$$

where p is the pressure, μ is the excess compression (related to the density by $\mu = \rho/\rho_0 - 1$), and E is the specific internal energy (energy per unit initial volume). The tension-limited excess compression, $\bar{\mu}$, is given by:

$$\bar{\mu} = \max(\mu,0).$$

Equation-of-State Form 6 differs from EOS Form 1 through the addition of a load curve that transfers internal energy into the material at a specified rate. This feature allows energy transfer mechanisms to be included in the modeling.

Equation-of-State Form 6 was tested in the same manner as EOS Form 1, using 10 cubes, one for each of the coefficients (7 cubes), one for the sum of the first four terms, one for the sum of the last three terms (These two cubes are included because these are the quantities actually calculated by DYNA3D.) and one for the full equation-of-state model. The 10 cubes are compressed hydrostatically to approximately 94% of the original volume, released back to the original volume, hydrostatically expended out to ~ 106% of the original volume and then released back to the original state.

Prior to discussing the calculations using EOS Form 6, a few code issues need to be addressed and these are not necessarily readily apparent to the user. First, because the sound speed looks like $dp/d\rho$ and μ is proportional to ρ, in order to avoid divide by zero issues in calculations using the sound speed, it is necessary that the C_1 coefficient not be zero, so an input value of 1.0e-20 was used for this coefficient when testing the other terms in the polynomial. In addition, in order to eliminate issues with the work performed by the bulk viscosity, the two input coefficients for the bulk viscosity on the material card were set to 1.0e-20 in each of the 10 cubes. Failing to do so results in the work performed on the cube being dominated by contributions from the bulk viscosity. Finally, the code version used for this test was version 14.2.0 revision 1.3306.

In order for the terms dependent on the internal energy to perform as expected, it is required to have an initial energy present in the simulation, so the initial internal energy was set to a value of 1.0e-3 in the cubes testing the terms dependent on the internal energy (Cubes 5, 6, 7, 9 and 10). In the cubes testing the other coefficients (Cubes 1, 2, 3, 4 and 8), the initial internal energy was set to 1.0e-9. Two load curves were used in this simulation to add internal energy to the cubes. The first load curve used a constant rate of 1.0e-6 to add energy to the material in Cubes 1, 2, 3, 4 and 8, while the second load curve used a constant rate of 1.0e-1 to add energy to Cubes 5, 6, 7, 9 and 10.

Input coefficients for Equation-of-State Form 6 were developed for the purposes of this testing and are the same as used for testing EOS Form 1. The values were chosen so that the contribution from each term was of the same order of magnitude (with the exception of the first term, which is constant). The following values were used as input for the testing of the full implementation of EOS Form 1: C_0 = 1.0e-9, C_1 = 1.224e-4, C_2 = 1.2e-3, C_3 = 1.3e-2, C_4 = 1.1e-2, C_5

= 2.4e-4 and C_6 = 1.3. The following table gives the values of the coefficients for each of the 10 cubes in the test suite.

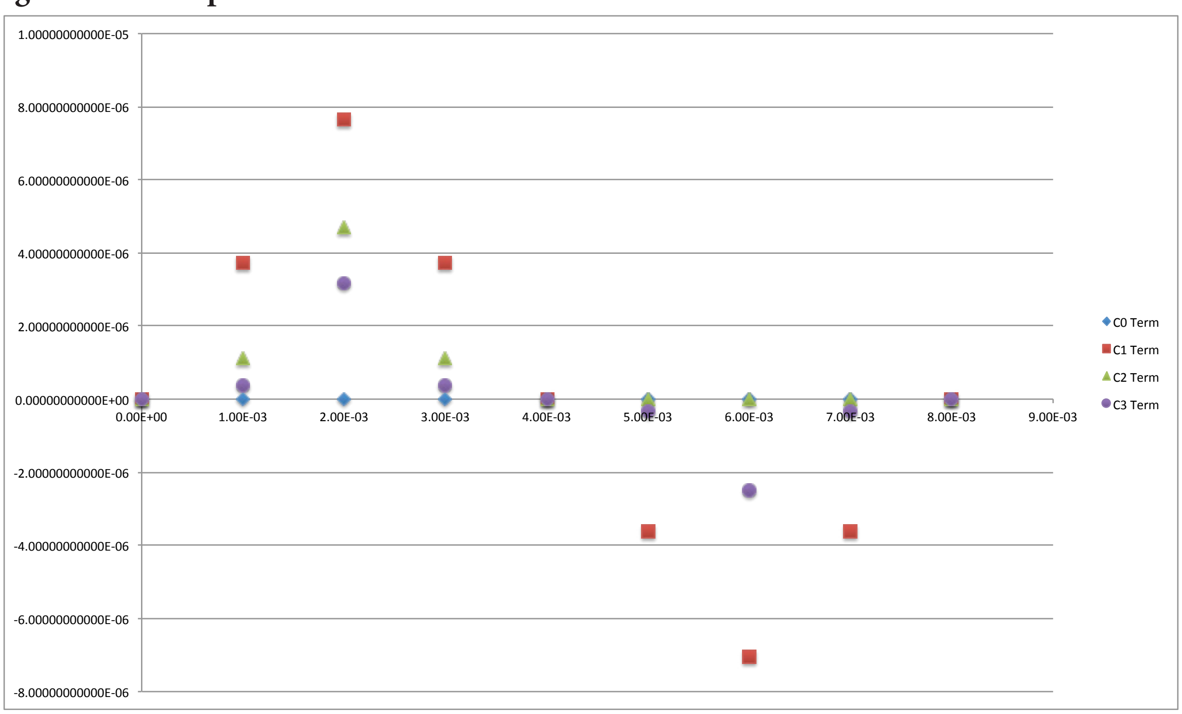
Table 33. Suite of test input coefficients for EOS Form 6

Cube	C_0	C_1	C_2	C_3	C_4	C_5	C_6
1	1.0e-9	1.0e-20	0	0	0	0	0
2	0	1.224e-4	0	0	0	0	0
3	0	1.0e-20	1.2e-3	0	0	0	0
4	0	1.0e-20	0	1.3e-2	0	0	0
5	0	1.0e-20	0	0	1.1e-2	0	0
6	0	1.0e-20	0	0	0	2.4e-4	0
7	0	1.0e-20	0	0	0	0	1.3
8	1.0e-9	1.224e-4	1.2e-3	1.3e-2	0	0	0
9	0	1.0e-20	0	0	1.1e-2	2.4e-4	1.3
10	1.0e-9	1.224e-4	1.2e-3	1.3e-2	1.1e-2	2.4e-4	1.3

As stated above, the intent of this test was to create a situation in which each term in the polynomial was making essentially an equal contribution to the final pressure (with the exception of the C_0 term, which represents a constant offset) and not to create a test that was reflective of any real material.

Each term in the polynomial was tested independently, then the sums of the first four terms and the last three terms, followed by testing of the EOS as a whole. The following plot contains the pressure from each of the first four terms in the polynomial, as returned by the code, as a function of time for this simulation.

Figure 13. Code pressures for the first four coefficients of EOS Form 6 as a function of time



As the plot demonstrates, each of the terms depending on μ returns a peak pressure on the order of 10^{-6} in compression and on the order of -10^{-6} in tension. Note that the C_2 term depends on $\overline{\mu}$, not μ, and therefore makes no contribution to the pressure when the cube is in tension. These results, for the first four coefficients, bear a striking resemblance to the results obtained from the testing of the first four coefficients of EOS Form 1, which is to be expected, as the pressures returned by these terms do not depend on the internal energy.

The following observations can be made from the code output. Coefficient 0 represents a constant pressure offset and was set to a value of 1.0e-9 in the first cube. To better than 1 part in 10^{12}, the cube remains at this pressure during the cycling of its volume. Coefficient 1 is linear in the excess compression. It should therefore return zero pressure when the compression is zero, return a positive value when the cube is compressed and should be negative when the cube is expanded, which is reflected in the code output. Coefficient 2 goes as the square of the tension-limited excess compression and should therefore only return positive pressures when the cube is compressed, which is what the code returns. Coefficient 3 is proportional to the cube of the excess compression. It should therefore return zero pressure when the compression is zero, return a positive value when the cube is compressed and should be negative when the cube is expanded, which is reflected in the code output. Therefore, the code output is behaving qualitatively as expected.

Using the normalized difference defined by equation 1, the agreement between the pressures calculated using the theoretical expression and the results returned by the code is illustrated in the following table for Cube 4, which is a test of the C_3 coefficient, as a function of time.

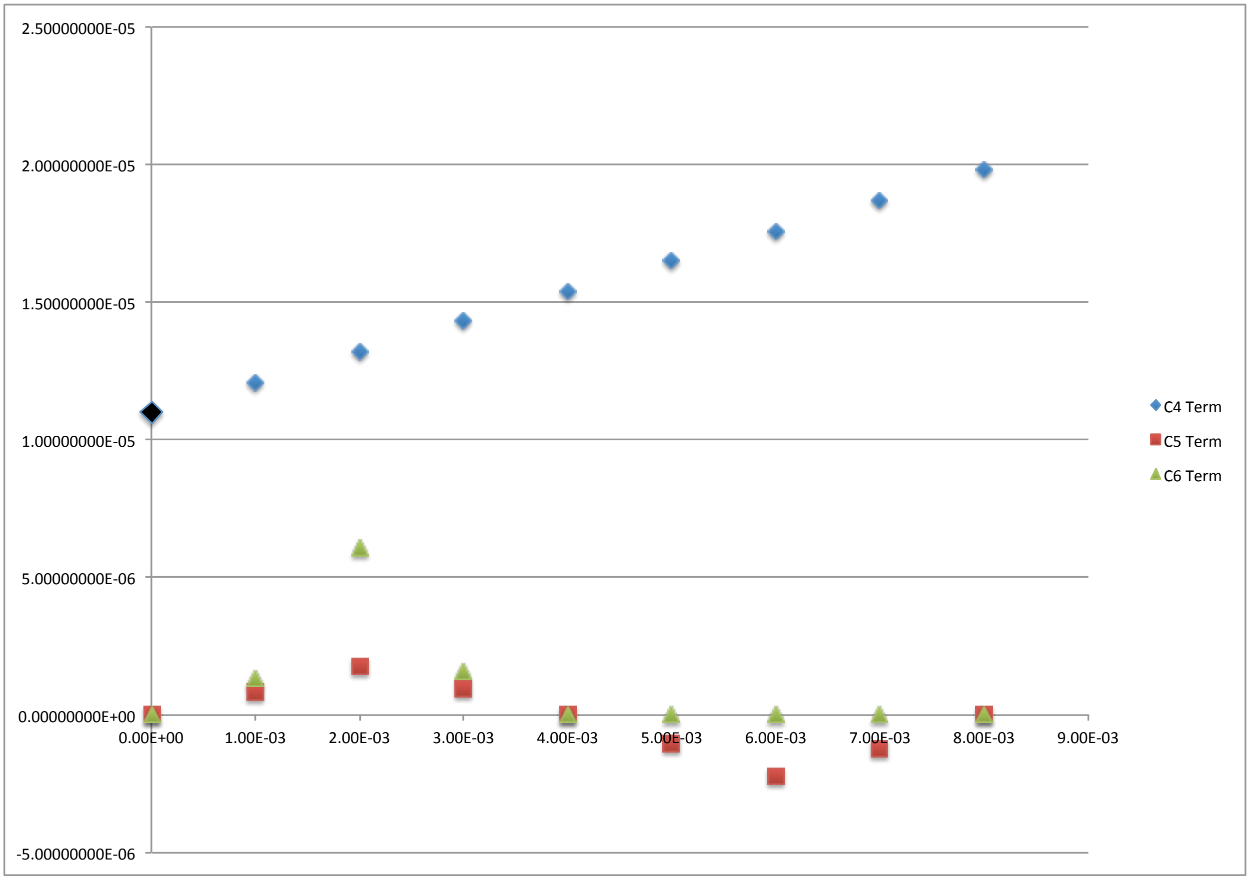
Table 34. Exact and Code pressures for the C_3 coefficient of EOS Form 6

Time	*Theoretical Pressure*	*Code Pressure*	*(Theoretical - Code)/Code*
0.00E+00	0.00000000E+00	0.0000000000E+00	0.0000000000E+00
1.00E-03	3.72854867E-07	3.7285486684E-07	3.3093714355E-12
2.00E-03	3.17115814E-06	3.1711581418E-06	1.8139116650E-12
3.00E-03	3.72854867E-07	3.7285486684E-07	4.0495358981E-12
4.00E-03	0.00000000E+00	0.0000000000E+00	0.0000000000E+00
5.00E-03	-3.30690617E-07	-3.3069061706E-07	-1.6858854446E-12
6.00E-03	-2.49440158E-06	-2.4944015822E-06	-1.9287780984E-13
7.00E-03	-3.30690617E-07	-3.3069061706E-07	8.9649211755E-13
8.00E-03	0.00000000E+00	0.0000000000E+00	0.0000000000E+00

As the table clearly demonstrates, the predictions of theoretical expression and the code results are in excellent agreement. Note that the two differences representing the cube returning to its starting position have been artificially set to zero. Similar levels of agreement are exhibited between the theoretical expression and the code results for the C_0, C_1 and C_2 coefficient terms. In fact, the results of testing these coefficients appears to be identical to the results obtained from the testing of EOS Form 1.

Given that the pressure returned by non-zero values of coefficients C_4 though C_6 is dependent on the internal energy, and this equation-of-state model includes a mechanism for moving energy into the material, it is expected that the results of testing these next terms will differ from the results obtained in testing EOS Form 1. The next plot displays the pressure from each of the last three terms in the polynomial, as returned by the code, as a function of time for this simulation.

Figure 14. Code pressures for the last three coefficients of EOS Form 6 as a function of time



Differences in these results are immediately apparent, as the C_4 term, which depends only on the internal energy and was nearly constant in the results of testing EOS Form 1, increases linearly with time as energy is added to Cube 5. While the C_5 term returns a peak pressure on the order of 10^{-6} in compression and on the order of -10^{-6} in tension and does not appear dramatically different, it is also affected by the additional energy. Note that the C_6 term depends on $\overline{\mu}$, not μ, and therefore makes no contribution to the pressure when the cube is in tension.

Coefficient 4 is linearly proportional to the internal energy and exhibits a straight line behavior as time progresses, as expected. Coefficient 5 is linear in both the excess compression and the internal energy. It should therefore return zero pressure when the compression is zero, return a positive value when the cube is compressed and should be negative when the cube is expanded, which is reflected in the code output. Coefficient 6 is linear in the internal energy and proportional to the square of the tension-limited excess compression. It should therefore only return positive pressures when the cube is compressed, which is what the code returns. Therefore, the code output is behaving qualitatively as expected.

Using the earlier definition for the normalized difference, the agreement between the reference expression and the code result can be quantified as illustrated in the following table for the

C_5 coefficient.

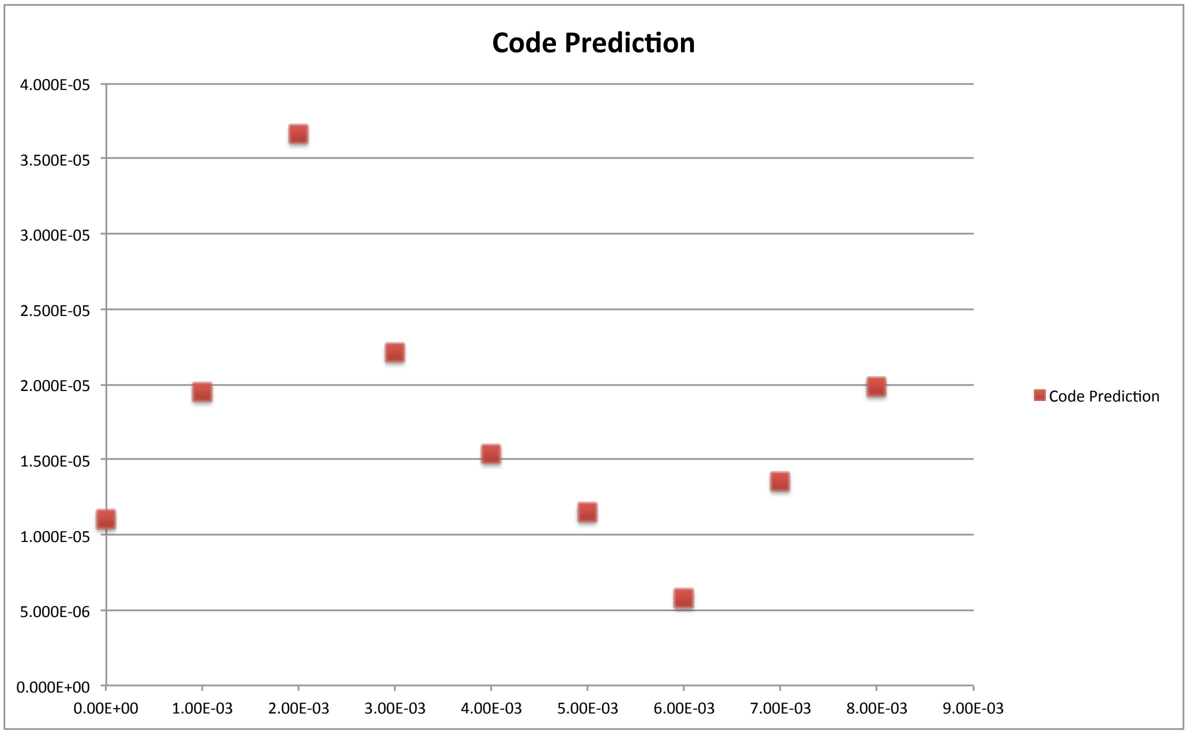
Table 35. Reference and Code pressures for the C_5 coefficient of EOS Form 6

Time	*Reference Pressure*	*Code Pressure*	*(Reference - Code)/Code*
0.00E+00	0.00000000E+00	0.0000000E+00	0.000000E+00
1.00E-03	8.08116471E-07	8.0811648E-07	-1.090474E-08
2.00E-03	1.79956849E-06	1.7995685E-06	-2.201588E-08
3.00E-03	9.55043065E-07	9.5504309E-07	-2.977672E-08
4.00E-03	0.00000000E+00	-3.2006266E-18	0.000000E+00
5.00E-03	-1.05876174E-06	-1.0587618E-06	-4.596441E-08
6.00E-03	-2.21490596E-06	-2.2149061E-06	-5.425837E-08
7.00E-03	-1.19992697E-06	-1.1999270E-06	-6.029304E-08
8.00E-03	0.00000000E+00	-6.2925262E-18	0.000000E+00

Note that the agreement between the code and reference results, while still quite good, is orders of magnitude lower than that achieved from the testing of EOS Form 1 and from the testing of the first four coefficients reported in Table 34. This is clearly the result of the added internal energy, and while this should not present an issue, no attempt was made to ensure that the analytical model handles the additional energy in exactly the same manner as the code. Similar levels of agreement are exhibited between the reference expression and the code results for the C_4 and C_6 coefficient terms.

Now that the behavior of each of the individual terms in the expression for Equation-of-State Form 6 has been investigated, the behavior of the full expression can be examined. The following plot contains the pressure returned by the code for the full equation-of-state as a function of time.

Figure 15. Code pressures for EOS Form 6 as a function of time



Note that the pressure is behaving as one would expect, in that the pressure increases as the cube is compressed, decreases as the compression is released, further decreases as the cube is placed into tension and then increases as the tension is released. However, due to the energy being added to the cube as time progresses, the pressure does not return to the initial value when the cube returns to its starting position.

The following table compares the pressure returned by the code as a function of time for the full equation-of-state to that predicted by the reference expression.

Table 36. Reference and Code pressures for EOS Form 6

Time	*Reference Pressure*	*Code Pressure*	*(Reference - Code)/Code*
0.00E+00	1.100100000E-05	1.100100000E-05	0.000000E+00
1.00E-03	1.949855427E-05	1.949855591E-05	-8.373007E-08
2.00E-03	3.661624915E-05	3.661625574E-05	-1.799905E-07
3.00E-03	2.208855308E-05	2.208856067E-05	-3.436272E-07
4.00E-03	1.539939128E-05	1.539939881E-05	-4.892684E-07
5.00E-03	1.150606417E-05	1.150607182E-05	-6.653925E-07
6.00E-03	5.824045126E-06	5.824053120E-06	-1.372600E-06
7.00E-03	1.356521395E-05	1.356522374E-05	-7.219220E-07
8.00E-03	1.980079570E-05	1.980080720E-05	-5.811605E-07

As demonstrated in the table, the code results agree with the reference expression to better than 5 parts in 10^7 across the range of pressures tested. Note that these results are strikingly similar to those obtained from the testing of EOS Form 1. These results establish confidence in the pressures returned by the implementation of Equation-of-State Form 6 in DYNA3D.

An exception to these results occurs at the peak tension point. This is most likely due to the fact that this point involves the difference of two small numbers but could also be due to the code output not being reported at exactly the peak of the tension.

The code results for the internal energy can also be examined for this equation-of-state. A simple, closed form solution for the internal energy can be realized for the first four coefficients, while the addition of a term that feeds energy into the cubes prevents the creation of such a solution for the last three coefficients, as well as the full equation-of-state model. The following table compares the code result for the internal energy in Cube 2 (the C_1 term) with the closed form solution for this term.

Table 37. Exact and Code Internal Energies for Cube 2 in Equation-of-State Form 6

Time	Code (GRIZ)	*Closed Form*	(*Closed* - GRIZ)/GRIZ
0.00E+00	1.00000000E-09	1.000000000E-09	0.000000000E+00
1.00E-03	5.70809200E-08	5.708092541E-08	9.470282503E-08
2.00E-03	2.23334900E-07	2.233349270E-07	1.208639386E-07
3.00E-03	5.90809300E-08	5.908092541E-08	-7.776241206E-08
4.00E-03	5.00000000E-09	5.000000000E-09	0.000000000E+00
5.00E-03	6.10809100E-08	6.108091072E-08	1.173345964E-08
6.00E-03	2.27334500E-07	2.273344568E-07	-1.898400420E-07
7.00E-03	6.30809100E-08	6.308091072E-08	1.136144663E-08
8.00E-03	9.00000000E-09	9.000000000E-09	1.838179139E-16

The agreement between the code results and the closed form solution is better than 2 parts in 10^7 and is similar to the results obtained from coefficients C_0, C_2 and C_3. These results are also similar to those obtained from the testing of EOS Form 1 and are limited by the accuracy of the GRIZ output.

As stated above, the addition of a source term for the internal energy precludes the creation of a simple, closed form solution for the internal energy for the last three coefficients in this equation-of-state model. The following table compares the code result for the internal energy due to the C_5 coefficient (Cube 6) to the result of a numerical integration performed in EXCEL.

Table 38. Reference and Code Internal Energies for Cube 6 in EOS Form 6

Time	Code (GRIZ)	*Reference Energy*	(*Reference* - GRIZ)/GRIZ
0.00E+00	1.00000000E-03	1.00000000E-03	0.000000E+00
1.00E-03	1.10001200E-03	1.10001151E-03	-4.470303E-07
2.00E-03	1.20004900E-03	1.20004894E-03	-5.165814E-08
3.00E-03	1.30000900E-03	1.30000860E-03	-3.066255E-07
4.00E-03	1.39999400E-03	1.39999419E-03	1.335316E-07
5.00E-03	1.50001000E-03	1.50001001E-03	7.457681E-09
6.00E-03	1.60006000E-03	1.60006040E-03	2.491204E-07

7.00E-03	1.70000700E-03	1.70000710E-03	5.734309E-08
8.00E-03	1.79998800E-03	1.79998836E-03	1.994603E-07

As expected, agreement between the two numbers is at the level of a few parts in 10^7. This level of agreement is similar to that obtained for the C_4 and C_6 coefficients, as well. These results are also similar to those obtained from the testing of EOS Form 1, which exhibited a closed form solution for these coefficients.

The internal energy of the full EOS model can also be investigated through the numerical integration in EXCEL and the following table compares the code results to those of the EXCEL integration.

Table 39. Reference and Code Internal Energies for EOS Form 6

Time	Code (GRIZ)	*Reference Energy*	(*Reference* - GRIZ)/GRIZ
0.00E+00	1.00000000E-03	1.00000000E-03	0.000000E+00
1.00E-03	1.10043600E-03	1.10043602E-03	1.873293E-08
2.00E-03	1.20122600E-03	1.20122556E-03	-3.671769E-07
3.00E-03	1.30039500E-03	1.30039394E-03	-8.168234E-07
4.00E-03	1.39985400E-03	1.39985375E-03	-1.769220E-07
5.00E-03	1.49944500E-03	1.49944389E-03	-7.377377E-07
6.00E-03	1.59917100E-03	1.59916962E-03	-8.611637E-07
7.00E-03	1.69947600E-03	1.69947470E-03	-7.677262E-07
8.00E-03	1.79998300E-03	1.79998143E-03	-8.739916E-07

As expected, agreement between the two numbers is, in general, at the level of a few parts in 10^7. These results are also similar to those obtained from the testing of EOS Form 1, which combined the closed form solution for the C_4, C_5 and C_6 coefficients with a numerical integration of the contribution from the C_0, C_1, C_2 and C_3 coefficients.

This establishes the implementation of Equation-of-State Form 6 in DYNA3D. The equation-of-state is performing as expected, in that the pressure in the cubes increases as they are compressed and decreases as they are expanded. The addition of a source term for the internal energy has been tested and found to be performing as expected. The behavior of each of the terms in the equation-of-state has been examined and found to be performing as expected and with good accuracy. The behavior of the equation-of-state as a whole has been examined and is performing as expected and with good accuracy.

Equation-of-State Form 7

Equation-of-State Form 7 has been superseded by EOS Form 13.

Equation-of-State Form 9

The next model to be tested was Equation-of-State Form 9. Testing will move slightly out of numerical order because although EOS Form 8 is appears to be an extension of EOS Form 9, EOS Form 9 is actually a simplified version of EOS Form 8. In either case, it makes sense logically to test EOS Form 9 first.

Equation-of-State Form 9 is a tabulated equation-of-state that is linear in the internal energy. The form of the equation for the pressure, p, is

$$p = C(\varepsilon_v) + \gamma T(\varepsilon_v)E$$

where E is the internal energy and ε_v is the volumetric strain, defined by $\varepsilon_v=\ln(V)$, where V is the relative volume. The $C(\varepsilon_v)$ and $T(\varepsilon_v)$ represent function evaluations from the tabulated data and the input $C_i(\varepsilon_v)$ therefore have the units of pressure. As there are two terms in EOS Form 9, this equation-of-state model will be tested with 3 cubes, one for each term (2 cubes) and one for the full equation-of-state model. The 3 cubes use the same compression and expansion as that used for the testing of EOS Form 1.

Prior to discussing the calculations using EOS Form 9, a few code issues need to be addressed and these are not necessarily readily apparent to the user. First, in order for the term dependent on the internal energy to perform as expected, it is required to have an initial energy present in the simulation, so the initial internal energy was set to a value of 1.0e-3 in all of the cubes. In addition, in order to eliminate issues with the work performed by the bulk viscosity, the two input coefficients for the bulk viscosity on the material card were set to 1.0e-20 in each of the 3 cubes. Failing to do so results in the work performed on the cube being dominated by contributions from the bulk viscosity. Also, in order to correctly calculate the sound speed, it is necessary to use non-zero values for the $C(\varepsilon_v)$ coefficients, so these were set to very small values for the testing of the second term using Cube 2. Finally, the code version used for this test was version 14.2.0 revision 1.3312b.

Input coefficients for Equation-of-State Form 9 were chosen such that the contribution to the pressure from the two terms was of the same order of magnitude as a function of time during the compression and expansion of the cubes. The input coefficients were also chosen to be linear in the volumetric strain and are in fact just scaled by multiples of 10 from each other. The following table lists the (truncated) values of the input coefficients for each of the cubes in the testing of EOS Form 9.

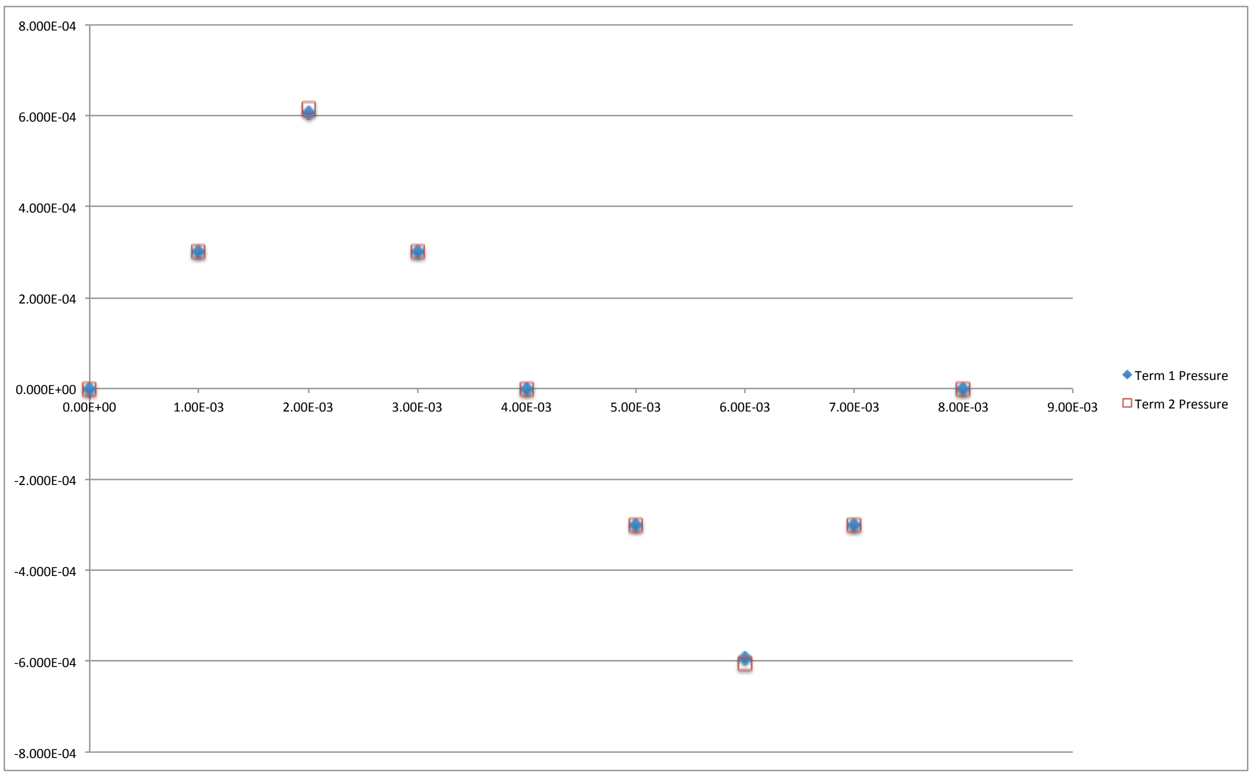
Table 40. Suite of test input coefficients for EOS Form 9

Cube									
1	ε_v	-6.19e-2	-4.08e-2	-2.02e-2	0.00	1.98e-2	3.92e-2	5.83e-2	7.70e-2
1	$C(\varepsilon_v)$	6.19e-4	4.08e-4	2.02e-4	0.00	-1.98e-4	-3.92e-4	-5.83e-4	-7.70e-4
1	$T(\varepsilon_v)$	61.9	40.8	20.2	0.00	-19.8	-39.2	-58.3	-77.0
1	γ	0.0							
2	ε_v	-6.19e-2	-4.08e-2	-2.02e-2	0.00	1.98e-2	3.92e-2	5.83e-2	7.70e-2

2	$C(\varepsilon_v)$	6.19e-10	4.08e-10	2.02e-10	0.00	-1.98e-10	-3.92e-10	-5.83e-10	-7.70e-10
2	$T(\varepsilon_v)$	61.9	40.8	20.2	0.00	-19.8	-39.2	-58.3	-77.0
2	γ	0.01							
3	ε_v	-6.19e-2	-4.08e-2	-2.02e-2	0.00	1.98e-2	3.92e-2	5.83e-2	7.70e-2
3	$C(\varepsilon_v)$	6.19e-4	4.08e-4	2.02e-4	0.00	-1.98e-4	-3.92e-4	-5.83e-4	-7.70e-4
3	$T(\varepsilon_v)$	61.9	40.8	20.2	0.00	-19.8	-39.2	-58.3	-77.0
3	γ	0.01							

The two terms in the equation-of-state were tested (almost) independently, given the requirement on the $C(\varepsilon_v)$ coefficients, then the full equation-of-state model was tested. The following plot displays the pressures from the first two terms, as returned by the code, as a function of time for this simulation.

Figure 16. Code pressures for the two terms of EOS Form 9 as a function of time



As the plot demonstrates, not only are both terms contributing pressures on the order of 6x10^{-4} at the peaks during cycling of the cubes, but the contributions of the two terms are nearly identical.

The following observations may be made from the plot. Both terms contribute an increase in the pressure as the cubes are compressed and both exhibit a decrease in pressure as the cubes are expanded, as expected. In addition, given the choice of input coefficients, the pressure of both cubes should be zero when the cube is in its original configuration and this behavior is also observed. Therefore, at least qualitatively, the code output is behaving as expected.

Using the normalized difference defined by equation 1, the agreement between the pressures for the two terms as calculated using the theoretical expression and the results returned by the code is demonstrated in the following table for the second term as a function of time.

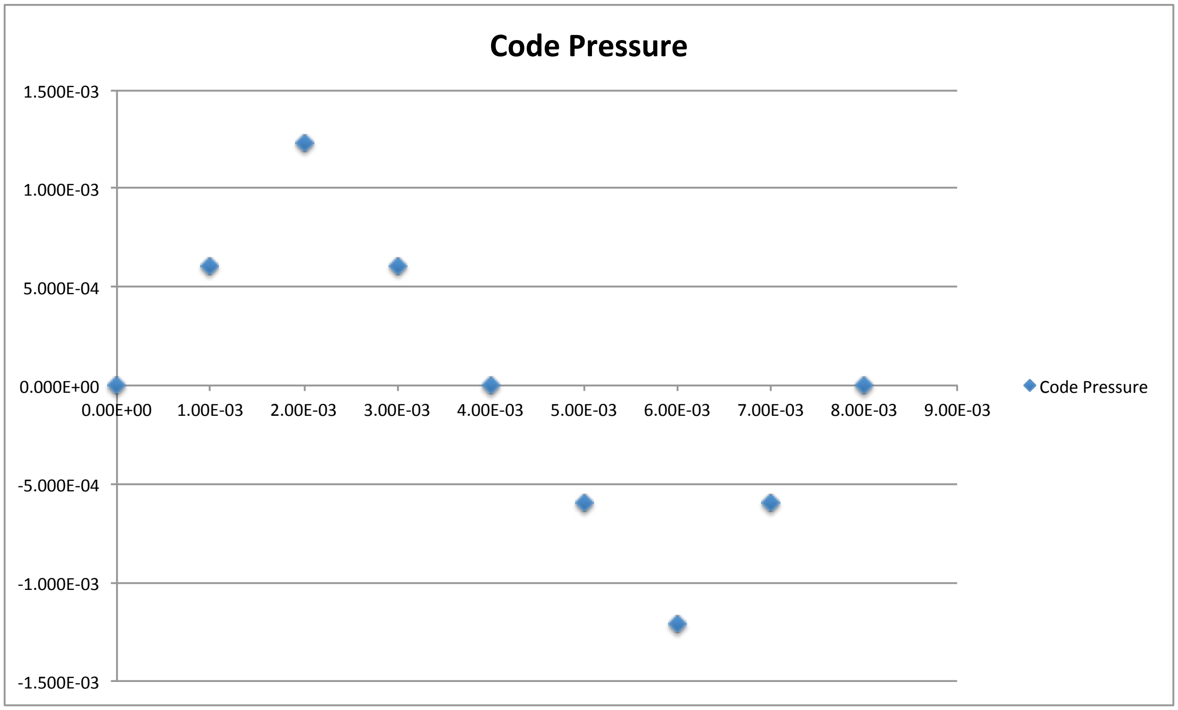
Table 41. Exact and Code pressures for the second term of EOS Form 9

Time	*Theoretical Pressure*	*Code Pressure*	*(Theoretical - Code)/Code*
0.00E+00	0.00000000E+00	3.552716264E-20	0.0000000000E+00
1.00E-03	3.02856624E-04	3.028566253E-04	-5.1001852331E-09
2.00E-03	6.16868695E-04	6.168687065E-04	-1.7863979875E-08
3.00E-03	3.02856624E-04	3.028566253E-04	-5.0991782019E-09
4.00E-03	0.00000000E+00	-3.996806885E-16	0.0000000000E+00
5.00E-03	-2.99870062E-04	-2.998700631E-04	-3.6520505671E-09
6.00E-03	-6.05088168E-04	-6.050881791E-04	-1.8600190099E-08
7.00E-03	-2.99870062E-04	-2.998700631E-04	-3.6520505671E-09
8.00E-03	0.00000000E+00	-2.975400681E-16	0.0000000000E+00

As the table demonstrates, the agreement between the theoretical results and the code predictions is better than 2 parts in 10^8, representing very good agreement. The level of agreement observed for this term is 4 to 5 orders of magnitude lower than the agreement exhibited for the first term in EOS Form 9, which is most likely due to the numerical integration of the internal energy, as will be demonstrated below. Note that since the pressure due to the first term is not dependent on the internal energy, it is unaffected by the code's determination of the internal energy.

Now that the behavior of the pressure resulting from each of the individual terms in the expression for Equation-of-State Form 9 has been investigated, the behavior of the full expression can be examined. The following plot displays the pressure returned by the code as a function of time for EOS Form 9.

Figure 17. Code pressures for EOS Form 9 as a function of time



Note that the pressure is behaving as one would expect, in that the pressure increases as the cube is compressed, decreases as the compression is released, further decreases as the cube is placed into tension and then increases as the tension is released. In addition, the pressure returns to the initial value when the cube returns to its starting position.

The following table compares the pressure returned by the code as a function of time for the full expression for Equation-of-State Form 9 to that predicted by the reference expression.

Table 42. Exact and Code pressures for EOS Form 9

Time	*Reference Pressure*	*Code Pressure*	*(Reference - Code)/Code*
0.00E+00	0.000000E+00	6.2632191100E-20	0.0000000000E+00
1.00E-03	6.057126E-04	6.0571264468E-04	-1.3607855291E-08
2.00E-03	1.233736E-03	1.2337361791E-03	-1.0491887991E-07
3.00E-03	6.057127E-04	6.0571264468E-04	3.9923632596E-08
4.00E-03	0.000000E+00	-1.3056222768E-15	0.0000000000E+00
5.00E-03	-5.997395E-04	-5.9973952672E-04	-1.3270471878E-08
6.00E-03	-1.210175E-03	-1.2101751477E-03	-1.1150687237E-07
7.00E-03	-5.997396E-04	-5.9973952672E-04	4.4551669176E-08
8.00E-03	0.000000E+00	-9.1482377220E-16	0.0000000000E+00

As the table demonstrates, the agreement between the reference results and the code predictions is better than 2 parts in 10^7, representing very good agreement. The level of agreement observed for the pressures resulting from EOS Form 9 is similar to the level of agreement between observed between an EXCEL numerical integration of the internal energy and the code prediction for the internal energy. Therefore, the level of agreement exhibited by the pressure for EOS Form 9 is most likely due to the numerical integration of the internal energy, as will be demonstrated below.

The code results for the internal energy can also be examined for this equation-of-state model. As the pressure for the first term is independent of the internal energy, we shall only report that the agreement between the closed form solution and the code prediction for the internal energy due to this term is better than 2 parts in 10^7, which is basically what is expected given the limitations of the GRIZ output used to acquire the internal energy. If one ignores the small contribution from the $C(\varepsilon_v)$ coefficients, the following expression gives the closed form solution for the internal energy due to the second term of EOS Form 9.

$$E = \exp(1000\gamma(V\ln V - V + 1) + \ln E_0)$$

The following table compares the closed form solution for the internal energy to the code prediction for the second term of EOS Form 9.

Table 43. Exact and Code Internal Energies for the second term of EOS Form 9

Time	Code (GRIZ)	*Closed Form*	(*Closed* - GRIZ)/GRIZ
0.00E+00	1.00000000E-03	1.00000000E-03	2.168404E-16
1.00E-03	1.00446500E-03	1.00446501E-03	1.369026E-08
2.00E-03	1.01779800E-03	1.01779773E-03	-2.653158E-07
3.00E-03	1.00446500E-03	1.00446501E-03	1.369026E-08
4.00E-03	1.00000000E-03	1.00000000E-03	2.168404E-16
5.00E-03	1.00455500E-03	1.00455542E-03	4.174679E-07
6.00E-03	1.01853100E-03	1.01853080E-03	-1.979068E-07
7.00E-03	1.00455500E-03	1.00455542E-03	4.174679E-07
8.00E-03	1.00000000E-03	1.00000000E-03	2.168404E-16

As the table demonstrates, the level of agreement between the closed form solution and the code results for the internal energy is better than 2 parts in 10^7, which then represents the limit with which the code can match the theoretical expression for the pressure, which uses the closed form solution for the internal energy to determine the pressure. The fact that the code results for the pressure resulting from this term actually exhibit somewhat better agreement with the theoretical pressure than this is not immediately explainable.

Due to the form of the equation-of-state model, there is no simple closed form solution for the internal energy due to the full expression for the equation-of-state. A numerical integration was performed in EXCEL to compare against the code results. The following table gives the result of that comparison.

Table 44. Reference and Code Internal Energies for EOS Form 9

Time	Code (GRIZ)	*Reference Energy*	(*Reference* - GRIZ)/GRIZ
0.00E+00	1.00000000E-03	1.000000E-03	0.000000E+00

1.00E-03	1.00893000E-03	1.008930E-03	8.452814E-10
2.00E-03	1.03559500E-03	1.035595E-03	2.383265E-07
3.00E-03	1.00893000E-03	1.008930E-03	1.074310E-07
4.00E-03	1.00000000E-03	1.000000E-03	2.150828E-07
5.00E-03	1.00911100E-03	1.009111E-03	-1.871172E-07
6.00E-03	1.03706200E-03	1.037061E-03	-6.073641E-07
7.00E-03	1.00911100E-03	1.009111E-03	-7.199445E-08
8.00E-03	1.00000000E-03	1.000000E-03	2.288180E-07

As the table demonstrates, the level of agreement between the EXCEL numerical integration and the code results for the internal energy is better than 6 parts in 10^7, which then represents a limit with which the code can match the reference expression for the pressure, which uses the EXCEL numerical integration for the internal energy to determine the reference pressure. A factor of two improvement in the normalized difference can be explained by the fact that the pressure due to the first term is calculated essentially exactly by the code. This is approximately the difference between the two tables, except for two of the points under tension, and so the improvement in agreement is not readily understood.

This establishes the implementation of Equation-of-State Form 9 in DYNA3D. The equation-of-state is performing as expected, in that the pressure in the cubes increases as they are compressed and decreases as they are expanded. The behavior of each of the terms in the equation-of-state has been examined and found to be performing as expected and with good accuracy. The behavior of the equation-of-state as a whole has been examined and is performing as expected and with good accuracy.

Author's Note: Two things were revealed in the testing of Equation-of-State Form 9. The first is that if the pressure returned by the code is dominated by the contribution of the second term, which depends on the internal energy, the accuracy of the code suffers somewhat due to the dependence on the numerical integration to find the internal energy. This can be compensated for by using smaller time steps and is easily observed in a simple test such as this. Determining if such a situation exists in a real world calculation may be somewhat more difficult.

The second item of note is that testing of this equation-of-state revealed an error in the code for this EOS model. The error, which involved the manner in which γ was handled inside subroutines, was found to exist in code versions dating back to 1996 (the oldest code versions easily obtainable). Therefore, for perhaps more than 20 years, this equation-of-state model has not been performing correctly within DYNA3D. As of code version 14.2.0 revision 1.3312b, this issue has been corrected.

Equation-of-State Form 8

The next model to be tested was Equation-of-State Form 8. Although EOS Form 8 is appears to be an extension of EOS Form 9, EOS Form 9 was actually put into DYNA3D as a simplified version of EOS Form 8.

Equation-of-State Form 8 is a tabulated equation-of-state that is linear in the internal energy. The form of the equation for the pressure, *p*, is

$$p\left(\varepsilon_v,\tilde{\varepsilon}_v\right)=C\left(\tilde{\varepsilon}_v\right)+\gamma T\left(\tilde{\varepsilon}_v\right)E+K\left(\tilde{\varepsilon}_v\right)\times\left(\tilde{\varepsilon}_v-\varepsilon_v\right)$$

where E is the internal energy and ε_v is the volumetric strain, defined by $\varepsilon_v=\ln(V)$, where V is the relative volume. $C(\varepsilon_v)$, $T(\varepsilon_v)$ and $K(\varepsilon_v)$ represent function evaluations from the tabulated data and the input $C(\varepsilon_v)$ therefore have the units of pressure. The minimum volumetric strain, $\tilde{\varepsilon}_v$, is given by the following expression:

$$\tilde{\varepsilon}_v\left(t\right)=\min\left[\varepsilon_v(\tau)\right],0\le\tau\le t$$

Note that the pressure is positive in compression and the volumetric strain is positive in tension. Also, the code expects the material to become stiffer with increasing compression and will issue a warning if the unloading bulk moduli do not fulfill this requirement.

It is important to note that in this equation-of-state model unloading occurs along a line using the interpolated value of the unloading bulk modulus that corresponds to the most compressive volumetric strain experienced by the system. To put this bluntly, the system unloads at the point at which the compression is relieved and unloads along a path that is probably different than the loading line and may not be linear if the contribution from the second term in the equation is important because the internal energy continues to evolve along the unloading/reloading path.

As there are really only two terms in EOS Form 8, this equation-of-state model will be tested with 3 cubes, one for each term (2 cubes) and one for the full equation-of-state model. However, due to the unloading/reloading behavior introduced by the bulk unloading moduli, the cubes do not use the same drive that has been used in all the previous tests. Instead, the cubes are compressed by moving all 8 nodes in 0.004 cm, releasing the nodes back to 0.001 cm, moving the nodes in 0.007 cm, releasing back to 0.001 cm, moving in to 0.01 cm, releasing back to 0.005 cm and then compressing back to 0.01 cm. This series of compressions and releases tests the unloading/reloading behavior introduced into this equation-of-state model.

Prior to discussing the calculations using EOS Form 8, a few code issues need to be addressed and these are not necessarily readily apparent to the user. First, in order for the term dependent on the internal energy to perform as expected, it is required to have an initial energy present in the simulation, so the initial internal energy was set to a value of 1.0e-3 in all of the cubes. In addition, in order to eliminate issues with the work performed by the bulk viscosity, the two input coefficients for the bulk viscosity on the material card were set to 1.0e-20 in each of the 3 cubes. Failing to do so results in the work performed on the cube being dominated by contributions from the bulk viscosity. Also, in order to correctly calculate the sound speed, it is necessary to use non-zero values for the $C(\varepsilon_v)$ coefficients, so these were set to very small values for the testing of the second term using Cube 2. Finally, the code version used for this test was version 15.2.0 revision 1.3377.

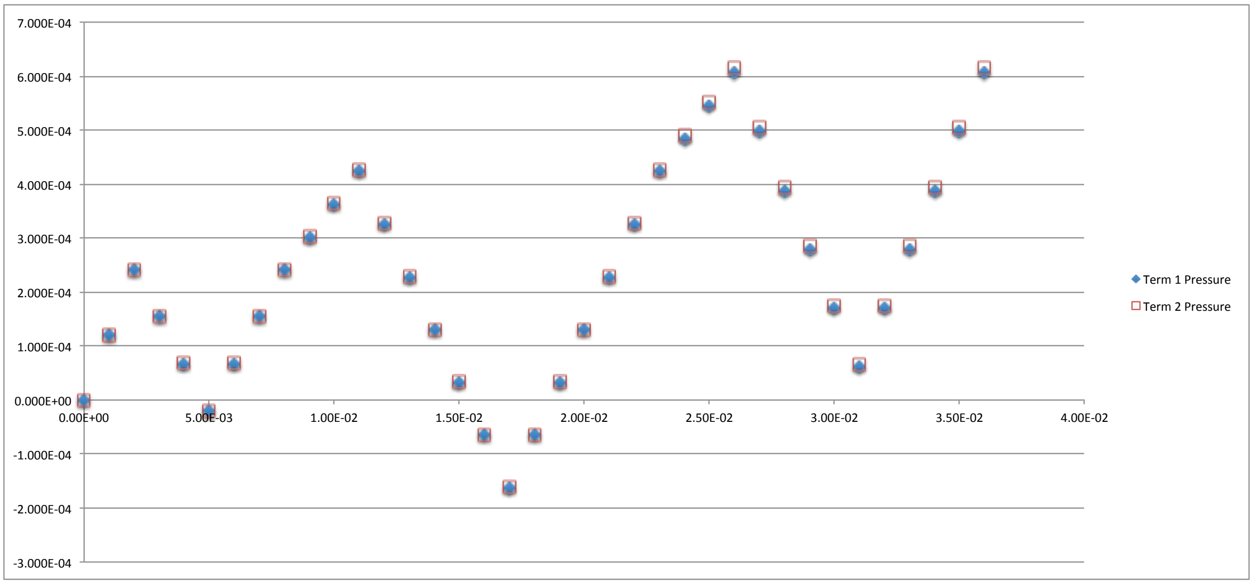
The input coefficients for Equation-of-State Form 8 chosen were the same as those used for the testing of EOS Form 9 and are such that the contribution to the pressure from the two terms was of the same order of magnitude as a function of time during the compression and expansion of the cubes. The input coefficients were also chosen to be linear in the volumetric strain and are in fact just scaled by multiples of 10 from each other. The additional unloading bulk moduli were chosen to be linear in the relative volume. The following table lists the (truncated) values of the input coefficients for each of the cubes in the testing of EOS Form 8.

Table 45. Suite of test input coefficients for EOS Form 8

Cube									
1	ε_v	-6.19e-2	-4.08e-2	-2.02e-2	0.00	1.98e-2	3.92e-2	5.83e-2	7.70e-2
1	$C(\varepsilon_v)$	6.19e-4	4.08e-4	2.02e-4	0.00	-1.98e-4	-3.92e-4	-5.83e-4	-7.70e-4
1	$T(\varepsilon_v)$	61.9	40.8	20.2	0.00	-19.8	-39.2	-58.3	-77.0
1	γ	0.0							
1	$K(\varepsilon_v)$	0.018	0.016	0.014	0.012	0.010	0.008	0.006	0.004
2	ε_v	-6.19e-2	-4.08e-2	-2.02e-2	0.00	1.98e-2	3.92e-2	5.83e-2	7.70e-2
2	$C(\varepsilon_v)$	6.19e-10	4.08e-10	2.02e-10	0.00	-1.98e-10	-3.92e-10	-5.83e-10	-7.70e-10
2	$T(\varepsilon_v)$	61.9	40.8	20.2	0.00	-19.8	-39.2	-58.3	-77.0
2	γ	0.01							
2	$K(\varepsilon_v)$	0.018	0.016	0.014	0.012	0.010	0.008	0.006	0.004
3	ε_v	-6.19e-2	-4.08e-2	-2.02e-2	0.00	1.98e-2	3.92e-2	5.83e-2	7.70e-2
3	$C(\varepsilon_v)$	6.19e-4	4.08e-4	2.02e-4	0.00	-1.98e-4	-3.92e-4	-5.83e-4	-7.70e-4
3	$T(\varepsilon_v)$	61.9	40.8	20.2	0.00	-19.8	-39.2	-58.3	-77.0
3	γ	0.01							
3	$K(\varepsilon_v)$	0.018	0.016	0.014	0.012	0.010	0.008	0.006	0.004

The two terms in the equation-of-state were tested (almost) independently, given the requirement on the $C(\varepsilon_v)$ coefficients, then the full equation-of-state model was tested. The following plot displays the pressures from the first two terms, as returned by the code, as a function of time for this simulation.

Figure 18. Code pressures for the two terms of EOS Form 8 as a function of time



As the plot demonstrates, not only are both terms contributing pressures on the order of $6x10^{-4}$ at the peak of the compression, but the contributions of the two terms are nearly identical.

The following observations may be made from the plot. Both terms contribute an increase in the pressure as the cubes are compressed and both exhibit a decrease in pressure as the cubes are expanded, as expected. In addition, given the choice of input coefficients, the pressure of both cubes should be zero at the beginning of the simulation and this behavior is also observed. Finally, although not obvious from the plot, the slope of the unloading/reloading lines differ from the slope of the monotonic path, which is expected given the choice of input coefficients. Therefore, at least qualitatively, the code output is behaving as expected.

Using the normalized difference defined in by equation 1, the agreement between the pressures for the second term as calculated using the reference expression and the results returned by the code is demonstrated in the following table as a function of time, using the expected value for the bulk unloading modulus.

Table 46. Reference and Code Pressures for the second term of EOS Form 8

Time	*Reference Pressure*	*Code Pressure*	*(Reference - Code)/Code*
0.00E+00	0.00000000E+00	0.00000000E+00	0.0000000000E+00
1.00E-03	1.20327020E-04	1.20327020E-04	-1.2115993482E-09
2.00E-03	2.41654811E-04	2.41654812E-04	-3.4828064011E-09
3.00E-03	1.54479117E-04	1.54498242E-04	-1.2379129097E-04
4.00E-03	6.76014835E-05	6.76396958E-05	-5.6493873144E-04
5.00E-03	-1.89782172E-05	-1.89209564E-05	3.0263133254E-03
6.00E-03	6.76014835E-05	6.76396958E-05	-5.6494005193E-04
7.00E-03	1.54479117E-04	1.54498242E-04	-1.2379186936E-04
8.00E-03	2.41654812E-04	2.41654812E-04	-1.8056829056E-09
9.00E-03	3.02856625E-04	3.02856625E-04	-1.8324738773E-09

1.00E-02	3.64504043E-04	3.64504044E-04	-1.9310947902E-09
1.10E-02	4.26662669E-04	4.26662670E-04	-2.0768385747E-09
1.20E-02	3.27605963E-04	3.27614326E-04	-2.5526606022E-05
1.30E-02	2.28989226E-04	2.29005934E-04	-7.2957346934E-05
1.40E-02	1.30812541E-04	1.30837576E-04	-1.9134643134E-04
1.50E-02	3.30759852E-05	3.31093311E-05	-1.0071439287E-03
1.60E-02	-6.42203652E-05	-6.41787258E-05	6.4880388985E-04
1.70E-02	-1.61076437E-04	-1.61026521E-04	3.0998623003E-04
1.80E-02	-6.42203655E-05	-6.41787258E-05	6.4880868975E-04
1.90E-02	3.30759840E-05	3.31093311E-05	-1.0071810769E-03
2.00E-02	1.30812538E-04	1.30837576E-04	-1.9136754777E-04
2.10E-02	2.28989221E-04	2.29005934E-04	-7.2978759574E-05
2.20E-02	3.27605955E-04	3.27614326E-04	-2.5549953667E-05
2.30E-02	4.26662658E-04	4.26662670E-04	-2.7847823843E-08
2.40E-02	4.89398502E-04	4.89398521E-04	-3.7561261000E-08
2.50E-02	5.52778113E-04	5.52778140E-04	-4.9069065170E-08
2.60E-02	6.16868668E-04	6.16868706E-04	-6.2470786642E-08
2.70E-02	5.05542241E-04	5.05549532E-04	-1.4422050299E-05
2.80E-02	3.94820409E-04	3.94834938E-04	-3.6795436668E-05
2.90E-02	2.84703298E-04	2.84725047E-04	-7.6388726198E-05
3.00E-02	1.75191019E-04	1.75219975E-04	-1.6525569023E-04
3.10E-02	6.62836757E-05	6.63198228E-05	-5.4504252767E-04
3.20E-02	1.75191018E-04	1.75219975E-04	-1.6525961971E-04
3.30E-02	2.84703295E-04	2.84725047E-04	-7.6398390889E-05
3.40E-02	3.94820403E-04	3.94834938E-04	-3.6811101536E-05
3.50E-02	5.05542230E-04	5.05549532E-04	-1.4443778398E-05
3.60E-02	6.16868651E-04	6.16868706E-04	-9.0265217497E-08

As the table demonstrates, the agreement between the reference expression and the code results is very good along the monotonic portion of the loading line, where the agreement is better than about 6 parts in 10^8. However, the agreement along the unloading/reloading lines is dramatically poorer, with the agreement being as poor as 1 part in 10^3. This appears to be due to the code using a slightly different value for the bulk unloading modulus than was used in the theoretical model, since if the differences along the unloading/reloading lines are minimized in the reference model, the agreement improves dramatically, as demonstrated in the following table.

Table 47. Reference and Code Pressures for the second term of EOS Form 8 using min K(ε_v)

Time	*Reference Pressure*	*Code Pressure*	*(Reference - Code)/Code*
0.00E+00	0.00000000E+00	0.000000000E+00	0.0000000000E+00
1.00E-03	1.20327020E-04	1.203270205E-04	-1.2115993482E-09

2.00E-03	2.41654811E-04	2.416548123E-04	-3.4828064011E-09
3.00E-03	1.54498242E-04	1.544982425E-04	-2.1207611175E-09
4.00E-03	6.76396955E-05	6.763969583E-05	-4.5556469891E-09
5.00E-03	-1.89209567E-05	-1.892095642E-05	1.5251717985E-08
6.00E-03	6.76396954E-05	6.763969583E-05	-5.8761359170E-09
7.00E-03	1.54498242E-04	1.544982425E-04	-2.6991511352E-09
8.00E-03	2.41654812E-04	2.416548123E-04	-1.8056829056E-09
9.00E-03	3.02856625E-04	3.028566253E-04	-1.8324738773E-09
1.00E-02	3.64504043E-04	3.645040439E-04	-1.9310947902E-09
1.10E-02	4.26662669E-04	4.266626697E-04	-2.0768385747E-09
1.20E-02	3.27614326E-04	3.276143256E-04	9.6767795464E-10
1.30E-02	2.29005936E-04	2.290059340E-04	7.9467833049E-09
1.40E-02	1.30837580E-04	1.308375763E-04	2.7699564625E-08
1.50E-02	3.31093368E-05	3.310933106E-05	1.7311030581E-07
1.60E-02	-6.41787176E-05	-6.417872575E-05	-1.2688650479E-07
1.70E-02	-1.61026510E-04	-1.610265211E-04	-6.7450180838E-08
1.80E-02	-6.41787179E-05	-6.417872575E-05	-1.2208660378E-07
1.90E-02	3.31093356E-05	3.310933106E-05	1.3596209228E-07
2.00E-02	1.30837577E-04	1.308375763E-04	6.5831344026E-09
2.10E-02	2.29005931E-04	2.290059340E-04	-1.3465857263E-08
2.20E-02	3.27614318E-04	3.276143256E-04	-2.2379966360E-08
2.30E-02	4.26662658E-04	4.266626697E-04	-2.7847823843E-08
2.40E-02	4.89398502E-04	4.893985208E-04	-3.7561261000E-08
2.50E-02	5.52778113E-04	5.527781405E-04	-4.9069065170E-08
2.60E-02	6.16868668E-04	6.168687065E-04	-6.2470786642E-08
2.70E-02	5.05549503E-04	5.055495323E-04	-5.6958723309E-08
2.80E-02	3.94834919E-04	3.948349376E-04	-4.6523276620E-08
2.90E-02	2.84725040E-04	2.847250473E-04	-2.5480303485E-08
3.00E-02	1.75219980E-04	1.752199750E-04	2.5959840084E-08
3.10E-02	6.63198399E-05	6.631982281E-05	2.5699262522E-07
3.20E-02	1.75219979E-04	1.752199750E-04	2.2030358603E-08
3.30E-02	2.84725037E-04	2.847250473E-04	-3.5144994853E-08
3.40E-02	3.94834913E-04	3.948349376E-04	-6.2188144903E-08
3.50E-02	5.05549493E-04	5.055495323E-04	-7.8686822775E-08
3.60E-02	6.16868651E-04	6.168687065E-04	-9.0265217497E-08

As this table demonstrates, the agreement along the unloading/reloading portions of the curves has improved dramatically, with the agreement now being better than 3 parts in 10^7, an improvement of nearly four orders of magnitude and representing very good agreement. This improvement is achieved by changing the value used for the bulk unloading modulus along the unloading/reloading curves by the amounts given in the following table.

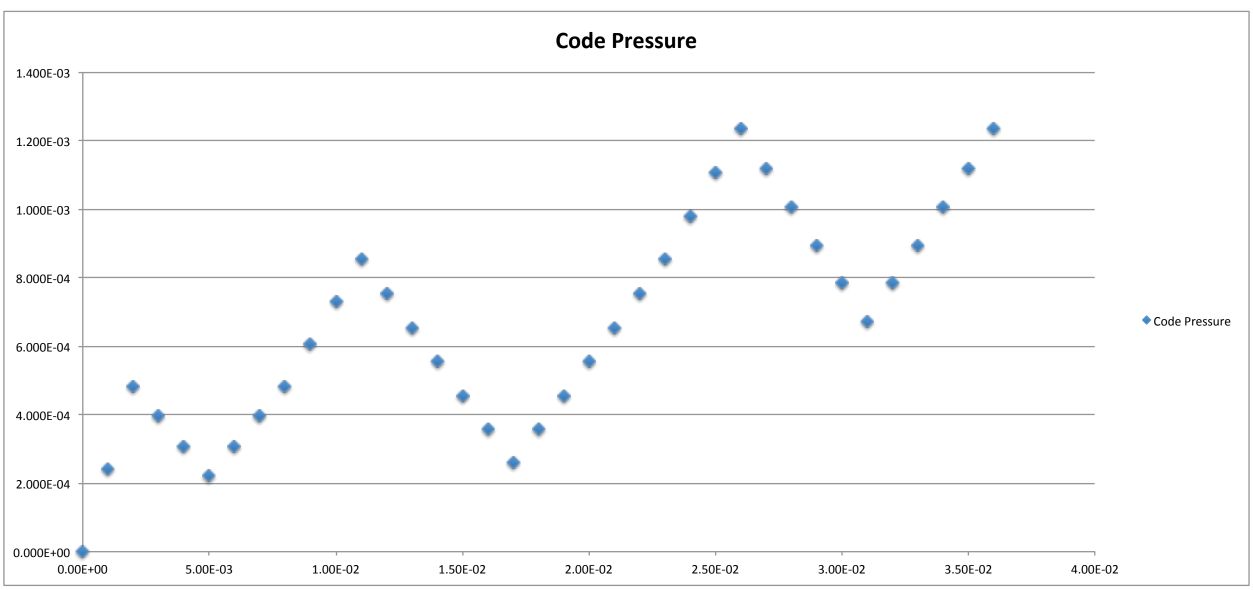
Table 48. Expected and minimizing values of $K(\varepsilon_v)$ for the second term of EOS Form 8

Expected $K(\varepsilon_v)$	Minimizing $K(\varepsilon_v)$	(Min - Expected)/Expected
0.014381	0.014377686	-2.20100E-04
0.016141	0.016140099	-8.52305E-05
0.017881	0.017879613	-6.64053E-05

As the table demonstrates, a small change in the value of the bulk unloading modulus (less than 3 parts in 10^4) results in a dramatic improvement in the agreement between the reference pressures and the code results. This implies that even though the input to the code was chosen such that the unloading points corresponded to input values of $K(\varepsilon_v)$, the interpolation routine returned values for the bulk unloading modulus that differed slightly from the input values. A difference this small in the returned value from an interpolation routine is not surprising. It is worth noting that as in the testing of EOS Form 9, the agreement between the theoretical expression and the code results for the first term is significantly better than that exhibited by the second term (approximately 5 orders of magnitude better), which is most likely due to the numerical integration of the internal energy, as will be demonstrated below. Note that since the pressure due to the first term is not dependent on the internal energy, it is unaffected by the code's determination of the internal energy.

Now that the behavior of the pressure resulting from each of the individual terms in the expression for Equation-of-State Form 8 has been investigated, the behavior of the full expression can be examined. The following plot displays the pressure returned by the code as a function of time for EOS Form 8.

Figure 19. Code pressures for EOS Form 8 as a function of time



Note that the pressure is behaving as one would expect, in that the pressure increases as the cube is compressed and decreases as the compression is released. In addition, the initial pressure is zero, as expected from the choice of input coefficients.

The following table compares the pressure returned by the code as a function of time for the full expression for Equation-of-State Form 8 to that predicted by the reference expression.

Table 49. Reference and Code Pressures for Equation-of-State Form 8

Time	*Reference Pressure*	*Code Pressure*	*(Reference - Code)/Code*
0.00E+00	0.00000000E+00	0.000000000E+00	0.0000000000E+00
1.00E-03	2.40653800E-04	2.406538002E-04	-7.7816160037E-10
2.00E-03	4.83309140E-04	4.833091412E-04	-3.1083177674E-09
3.00E-03	3.95789183E-04	3.958083093E-04	-4.8323114882E-05
4.00E-03	3.08566392E-04	3.086046058E-04	-1.2382623941E-04
5.00E-03	2.21640643E-04	2.216979044E-04	-2.5828754250E-04
6.00E-03	3.08566392E-04	3.086046058E-04	-1.2382623784E-04
7.00E-03	3.95789183E-04	3.958083093E-04	-4.8322888258E-05
8.00E-03	4.83309140E-04	4.833091412E-04	-2.9214461696E-09
9.00E-03	6.05712643E-04	6.057126447E-04	-3.0090906391E-09
1.00E-02	7.29007356E-04	7.290073586E-04	-3.1488754796E-09
1.10E-02	8.53324483E-04	8.533244860E-04	-3.3276475225E-09
1.20E-02	7.53214264E-04	7.532226286E-04	-1.1105637546E-05
1.30E-02	6.53542357E-04	6.535590671E-04	-2.5568135356E-05
1.40E-02	5.54308861E-04	5.543338994E-04	-4.5169011763E-05
1.50E-02	4.55513871E-04	4.555472209E-04	-7.3209466256E-05
1.60E-02	3.57157479E-04	3.571991242E-04	-1.1658852143E-04
1.70E-02	2.59239776E-04	2.592896993E-04	-1.9253995917E-04
1.80E-02	3.57157479E-04	3.571991242E-04	-1.1658852059E-04
1.90E-02	4.55513871E-04	4.555472209E-04	-7.3209464196E-05
2.00E-02	5.54308861E-04	5.543338994E-04	-4.5169009140E-05
2.10E-02	6.53542357E-04	6.535590671E-04	-2.5568132650E-05
2.20E-02	7.53214264E-04	7.532226286E-04	-1.1105635530E-05
2.30E-02	8.53324483E-04	8.533244860E-04	-3.3252027059E-09
2.40E-02	9.78796059E-04	9.787960626E-04	-3.5336743364E-09
2.50E-02	1.10555517E-03	1.105555175E-03	-3.7816508393E-09
2.60E-02	1.23373617E-03	1.233736179E-03	-4.0668114088E-09
2.70E-02	1.12025471E-03	1.120261979E-03	-6.4864718879E-06
2.80E-02	1.00737662E-03	1.007391138E-03	-1.4406825494E-05
2.90E-02	8.95102082E-04	8.951238276E-04	-2.4293129106E-05
3.00E-02	7.83431247E-04	7.834602100E-04	-3.6967746837E-05
3.10E-02	6.72364270E-04	6.724004355E-04	-5.3785758955E-05

3.20E-02	7.83431247E-04	7.834602100E-04	-3.6967745212E-05
3.30E-02	8.95102082E-04	8.951238276E-04	-2.4293126298E-05
3.40E-02	1.00737662E-03	1.007391138E-03	-1.4406821645E-05
3.50E-02	1.12025471E-03	1.120261979E-03	-6.4864675405E-06
3.60E-02	1.23373617E-03	1.233736179E-03	-4.0618882190E-09

As might have been expected, given the analysis of the second term for this EOS model, the agreement between the reference expression and the code results is very good along the monotonic portion of the loading line, where the agreement is better than about 4 parts in 10^9. However, the agreement along the unloading/reloading lines is dramatically poorer, with the agreement being as poor as ~ 3 parts in 10^4. This appears to be due to the code using a slightly different value for the bulk unloading modulus than was used in the theoretical model, since if the differences along the unloading/reloading lines are minimized in the reference model, the agreement improves dramatically, as demonstrated in the following table.

Table 50. Reference and Code Pressures for EOS Form 8 using min K(ε_v)

Time	*Reference Pressure*	*Code Pressure*	*(Reference - Code)/Code*
0.00E+00	0.00000000E+00	0.0000000000E+00	0.0000000000E+00
1.00E-03	2.40653800E-04	2.4065380021E-04	-7.7816160037E-10
2.00E-03	4.83309140E-04	4.8330914117E-04	-3.1083177674E-09
3.00E-03	3.95808308E-04	3.9580830927E-04	-1.9578857155E-09
4.00E-03	3.08604606E-04	3.0860460578E-04	1.2647401992E-10
5.00E-03	2.21697905E-04	2.2169790443E-04	3.4346421479E-09
6.00E-03	3.08604606E-04	3.0860460578E-04	1.2803916852E-10
7.00E-03	3.95808309E-04	3.9580830927E-04	-1.7312619502E-09
8.00E-03	4.83309140E-04	4.8330914117E-04	-2.9214461696E-09
9.00E-03	6.05712643E-04	6.0571264467E-04	-3.0090906391E-09
1.00E-02	7.29007356E-04	7.2900735856E-04	-3.1488754796E-09
1.10E-02	8.53324483E-04	8.5332448596E-04	-3.3276475225E-09
1.20E-02	7.53222626E-04	7.5322262856E-04	-2.7745158129E-09
1.30E-02	6.53559066E-04	6.5355906707E-04	-2.0552618007E-09
1.40E-02	5.54333899E-04	5.5433389939E-04	-1.0802587590E-09
1.50E-02	4.55547221E-04	4.5554722087E-04	3.1404070025E-10
1.60E-02	3.57199125E-04	3.5719912421E-04	2.4698277104E-09
1.70E-02	2.59289701E-04	2.5928969934E-04	6.2422089412E-09
1.80E-02	3.57199125E-04	3.5719912421E-04	2.4706598345E-09
1.90E-02	4.55547221E-04	4.5554722087E-04	3.1610106584E-10
2.00E-02	5.54333899E-04	5.5433389939E-04	-1.0776359443E-09
2.10E-02	6.53559066E-04	6.5355906707E-04	-2.0525561023E-09
2.20E-02	7.53222626E-04	7.5322262856E-04	-2.7724999081E-09

2.30E-02	8.53324483E-04	8.5332448596E-04	-3.3252027059E-09
2.40E-02	9.78796059E-04	9.7879606261E-04	-3.5336743364E-09
2.50E-02	1.10555517E-03	1.1055551752E-03	-3.7816508393E-09
2.60E-02	1.23373617E-03	1.2337361790E-03	-4.0668114088E-09
2.70E-02	1.12026198E-03	1.1202619794E-03	-2.9759809524E-09
2.80E-02	1.00739114E-03	1.0073911380E-03	-1.6459059152E-09
2.90E-02	8.95123828E-04	8.9512382760E-04	1.1395871527E-11
3.00E-02	7.83460212E-04	7.8346020999E-04	2.1326707415E-09
3.10E-02	6.72400439E-04	6.7240043552E-04	4.9431116921E-09
3.20E-02	7.83460212E-04	7.8346020999E-04	2.1342955359E-09
3.30E-02	8.95123828E-04	8.9512382760E-04	1.4204232873E-11
3.40E-02	1.00739114E-03	1.0073911380E-03	-1.6420559627E-09
3.50E-02	1.12026198E-03	1.1202619794E-03	-2.9716335441E-09
3.60E-02	1.23373617E-03	1.2337361790E-03	-4.0618882190E-09

As this table demonstrates, the agreement along the unloading/reloading portions of the curves has improved dramatically, with the agreement now being better than ~ 6 parts in 10^9, an improvement of nearly five orders of magnitude and representing very good agreement. This improvement is achieved by changing the value used for the bulk unloading modulus in the reference model along the unloading/reloading curves by the amounts given in the following table.

Table 51. Expected and minimizing values of $K(\varepsilon_v)$ for EOS Form 8

Expected $K(\varepsilon_v)$	Minimizing $K(\varepsilon_v)$	(Min - Expected)/Expected
0.014381	0.014377686	-2.201078290E-04
0.016141	0.016140099	-8.522772443E-05
0.017881	0.017879612	-6.641397873E-05

As the table demonstrates, a small change in the value of the bulk unloading modulus (less than 3 parts in 10^4) results in a dramatic improvement in the agreement between the theoretical pressures and the code results. This implies that even though the input to the code was chosen such that the unloading points corresponded to input values of $K(\varepsilon_v)$, the interpolation routine returned values for the bulk unloading modulus that differed slightly from the input values. A difference this small in the returned value from an interpolation routine is not surprising. It is also worth noting that the values used for the full expression of EOS Form 8 are essentially identical to those used for the analysis of the second term of this equation-of-state model. This is not a surprise, as the non-linear behavior along the unloading/reloading curve is due to the evolution of the internal energy and this term is the same in both cubes.

The code results for the internal energy can also be examined for this equation-of-state model. As the pressure for the first term is independent of the internal energy, we shall concentrate on the behavior of the second term and the full expression for this EOS model. Given the form for the pressure along the unloading/reloading lines, there is no simple closed form solution for the internal energy along these lines and so the code results will be compared to those obtained from a simple numerical integration performed in EXCEL. The following table makes this comparison for the second term in EOS Form 8 using the minimized value for K(ε_v).

Table 52. Reference and Code Internal Energies for the second term of EOS Form 8

Time	Code (GRIZ)	*Reference Energy*	(*Reference* - GRIZ)/GRIZ
0.00E+00	1.00000000E-03	1.00000000E-03	0.000000E+00
1.00E-03	1.00071700E-03	1.00071738E-03	3.792183E-07
2.00E-03	1.00286100E-03	1.00286108E-03	7.576553E-08
3.00E-03	1.00168900E-03	1.00168952E-03	5.180359E-07
4.00E-03	1.00103000E-03	1.00103007E-03	7.280449E-08
5.00E-03	1.00088500E-03	1.00088511E-03	1.129468E-07
6.00E-03	1.00103000E-03	1.00103007E-03	7.243395E-08
7.00E-03	1.00168900E-03	1.00168952E-03	5.176653E-07
8.00E-03	1.00286100E-03	1.00286108E-03	7.744132E-08
9.00E-03	1.00446500E-03	1.00446502E-03	1.693503E-08
1.00E-02	1.00642300E-03	1.00642294E-03	-5.954257E-08
1.10E-02	1.00873500E-03	1.00873474E-03	-2.546050E-07
1.20E-02	1.00653100E-03	1.00653077E-03	-2.253067E-07
1.30E-02	1.00489800E-03	1.00489786E-03	-1.407871E-07
1.40E-02	1.00383800E-03	1.00383808E-03	8.431918E-08
1.50E-02	1.00335400E-03	1.00335352E-03	-4.789139E-07
1.60E-02	1.00344600E-03	1.00344621E-03	2.124156E-07
1.70E-02	1.00411800E-03	1.00411820E-03	1.970439E-07
1.80E-02	1.00344600E-03	1.00344621E-03	2.116899E-07
1.90E-02	1.00335400E-03	1.00335352E-03	-4.818122E-07
2.00E-02	1.00383800E-03	1.00383808E-03	7.781202E-08
2.10E-02	1.00489800E-03	1.00489785E-03	-1.523238E-07
2.20E-02	1.00653100E-03	1.00653076E-03	-2.432729E-07
2.30E-02	1.00873500E-03	1.00873472E-03	-2.803757E-07
2.40E-02	1.01140100E-03	1.01140064E-03	-3.511650E-07
2.50E-02	1.01442100E-03	1.01442131E-03	3.092989E-07
2.60E-02	1.01779800E-03	1.01779768E-03	-3.099844E-07
2.70E-02	1.01455800E-03	1.01455769E-03	-3.020956E-07
2.80E-02	1.01194800E-03	1.01194812E-03	1.226989E-07
2.90E-02	1.00997100E-03	1.00997067E-03	-3.235266E-07
3.00E-02	1.00862700E-03	1.00862701E-03	9.807755E-09
3.10E-02	1.00791900E-03	1.00791878E-03	-2.227527E-07
3.20E-02	1.00862700E-03	1.00862701E-03	8.681237E-09
3.30E-02	1.00997100E-03	1.00997067E-03	-3.280223E-07

3.40E-02	1.01194800E-03	1.01194811E-03	1.126136E-07
3.50E-02	1.01455800E-03	1.01455768E-03	-3.199604E-07
3.60E-02	1.01779800E-03	1.01779766E-03	-3.377797E-07

As the table demonstrates, the level of agreement between the EXCEL numerical integration and the code results for the internal energy is better than ~ 5 parts in 10^7, which is about as good as can be expected, given the limitations on the GRIZ output. This establishes that the internal energies being returned by the code are reasonable.

There is also no simple closed form solution for the internal energy due to the full expression for Equation-of-State Form 8. A numerical integration was performed in EXCEL to compare against the code results. The following table gives the result of that comparison using the minimized value for $K(\varepsilon_v)$.

Table 53. Reference and Code Internal Energies for EOS Form 8

Time	Code (GRIZ)	*Reference Energy*	(*Reference* - GRIZ)/GRIZ
0.00E+00	1.00000000E-03	1.00000000E-03	0.000000E+00
1.00E-03	1.00143500E-03	1.00143476E-03	-2.421068E-07
2.00E-03	1.00572200E-03	1.00572215E-03	1.454104E-07
3.00E-03	1.00312200E-03	1.00312191E-03	-9.250571E-08
4.00E-03	1.00103000E-03	1.00103007E-03	6.838586E-08
5.00E-03	9.99449100E-04	9.99449013E-04	-8.746980E-08
6.00E-03	1.00103000E-03	1.00103007E-03	6.838616E-08
7.00E-03	1.00312200E-03	1.00312191E-03	-9.213569E-08
8.00E-03	1.00572200E-03	1.00572215E-03	1.457803E-07
9.00E-03	1.00893000E-03	1.00893002E-03	2.190173E-08
1.00E-02	1.01284600E-03	1.01284586E-03	-1.339746E-07
1.10E-02	1.01746900E-03	1.01746947E-03	4.578674E-07
1.20E-02	1.01277500E-03	1.01277473E-03	-2.660893E-07
1.30E-02	1.00864700E-03	1.00864713E-03	1.316941E-07
1.40E-02	1.00508900E-03	1.00508880E-03	-2.012210E-07
1.50E-02	1.00210200E-03	1.00210183E-03	-1.669439E-07
1.60E-02	9.99688300E-04	9.99688327E-04	2.750281E-08
1.70E-02	9.97850300E-04	9.97850354E-04	5.431351E-08
1.80E-02	9.99688300E-04	9.99688327E-04	2.750367E-08
1.90E-02	1.00210200E-03	1.00210183E-03	-1.669422E-07
2.00E-02	1.00508900E-03	1.00508880E-03	-2.012185E-07
2.10E-02	1.00864700E-03	1.00864713E-03	1.316975E-07
2.20E-02	1.01277500E-03	1.01277473E-03	-2.660851E-07
2.30E-02	1.01746900E-03	1.01746947E-03	4.578724E-07
2.40E-02	1.02280100E-03	1.02280134E-03	3.278069E-07

2.50E-02	1.02884300E-03	1.02884269E-03	-3.011130E-07
2.60E-02	1.03559500E-03	1.03559545E-03	4.364424E-07
2.70E-02	1.02880000E-03	1.02879978E-03	-2.186300E-07
2.80E-02	1.02263200E-03	1.02263250E-03	4.924374E-07
2.90E-02	1.01709500E-03	1.01709541E-03	4.065513E-07
3.00E-02	1.01219000E-03	1.01219025E-03	2.502566E-07
3.10E-02	1.00791900E-03	1.00791874E-03	-2.541549E-07
3.20E-02	1.01219000E-03	1.01219025E-03	2.502584E-07
3.30E-02	1.01709500E-03	1.01709541E-03	4.065547E-07
3.40E-02	1.02263200E-03	1.02263250E-03	4.924425E-07
3.50E-02	1.02880000E-03	1.02879978E-03	-2.186233E-07
3.60E-02	1.03559500E-03	1.03559545E-03	4.364507E-07

As the table demonstrates, the level of agreement between the EXCEL numerical integration and the code results for the internal energy is better than 5 parts in 10^7, essentially the same level of agreement as exhibited by the second term of this EOS model. The internal energy is therefore being calculated with reasonable accuracy by the code and this can always be improved by using a smaller time step in the code.

This establishes the implementation of Equation-of-State Form 8 in DYNA3D. The equation-of-state is performing as expected, in that the pressure in the cubes increases as they are compressed and decreases as they are expanded. The behavior of each of the terms in the equation-of-state has been examined and found to be performing as expected and with good accuracy. The behavior of the equation-of-state as a whole has been examined and is performing as expected and with good accuracy.

Author's Note: Two things were revealed in the testing of Equation-of-State Form 8. The first is much like the issue discovered in the testing of EOS Form 9, in that if the pressure returned by the code is dominated by the contribution of the second term, which depends on the internal energy, the accuracy of the code may suffer somewhat due to the dependence on the numerical integration to find the internal energy. This can be compensated for by using smaller time steps and is easily observed in a simple test such as this. Determining if such a situation exists in a real world calculation may be somewhat more difficult.

The second item of note is that testing of this equation-of-state revealed several bugs in the code for this EOS model. The most important of these involved an initialization error that affected the calculation of the pressure at the start of the simulation and an incorrect calculation of the pressure along the unloading/reloading lines. As of code version 14.2.0 revision 1.3320, these issues have been corrected.

Equation-of-State Form 10

Equation-of-State Form 10 is not used in this version of the code.

Equation-of-State Form 11

Equation-of-State Form 11 is a Pore Collapse model that uses two curves: the virgin loading curve and the completely crushed curve, as shown in the figure below (taken from the DYNA3D manual). The loading curves are entered into the model by defining the pressures as a

Figure 20. Illustration of EOS Form 11 from the DYNA3D manual

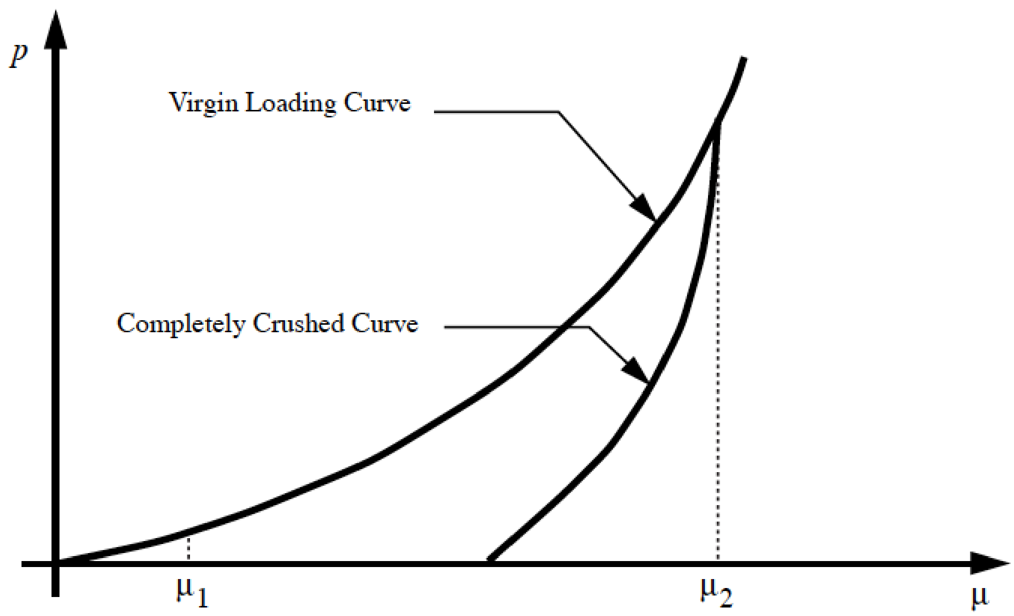


Figure 43
Pressure vs. excess compression for the Pore Collapse equation-of-state. The partially crushed curve lies between the Virgin Loading Curve and the Completely Crushed Curve.

function of the excess compression, μ (related to the density by $\mu = \rho/\rho_0 - 1$). Note that μ is positive in compression and negative in tension.

The model requires the definition of two critical points: the excess compression required for pore collapse to begin (μ_1) and the excess compression required for the material to be completely crushed (μ_2). Unloading occurs along the virgin loading curve until the excess compression exceeds μ_1. Once the excess compression exceeds μ_1, unloading occurs along a partially crushed path between the virgin and completely crushed curves defined by:

$$p_{pc}(\mu) = p_{cc}\left(\frac{(1+\mu_B)(1+\mu)}{1+\mu_{\max}} - 1\right)$$

where

$$\mu_B = p_{cc}^{-1}(p_{\max})$$

is the excess compression corresponding to a pressure of p_{max} on the completely crushed curve.

Prior to discussing the calculations using EOS Form 11, a few code issues need to be addressed and these are not necessarily readily apparent to the user. First, in order to eliminate issues with the work performed by the bulk viscosity, the two input coefficients for the bulk viscosity on the material card were set to 1.0e-20 in each of the 3 cubes. Failing to do so results in the work performed on the cube being dominated by contributions from the bulk viscosity. Finally, the code version used for this test was version 14.2.0 revision 1.3320.

The implementation of the model in DYNA3D uses a monotonic cubic spline to model the virgin loading and completely crushed curves. Previous testing of this equation-of-state model[3] revealed that cubic spline routines available for use in EXCEL returned results that differed from each other by as much as several per cent when applied to the same data sets. This makes characterization of the code results difficult if one is to rely on the values returned by these routines. Therefore, the decision was made to test this EOS model using two sets of input curves. The first set of curves would define linear relationships between the pressure and the excess compression for both the virgin loading and completely crushed curves. This would allow the pressure to be calculated exactly from the excess compression without relying on an interpolation to check the code result. The second set of curves were provided by Jerry Lin for the initial testing of this EOS model and resemble the curves that appear in the figure on the previous page. This testing requires the use of a cubic spline routine to compare to the code results. In addition, the pressure in this EOS model is defined to be independent of the internal energy and so each set of input curves was tested twice using different initial values for the internal energy to verify this independence.

The first set of curves to be tested uses 10 points to define a linear relationship between the excess compression and the pressure for both the virgin loading curve and the completely crushed curve. The defining points are given in the following table:

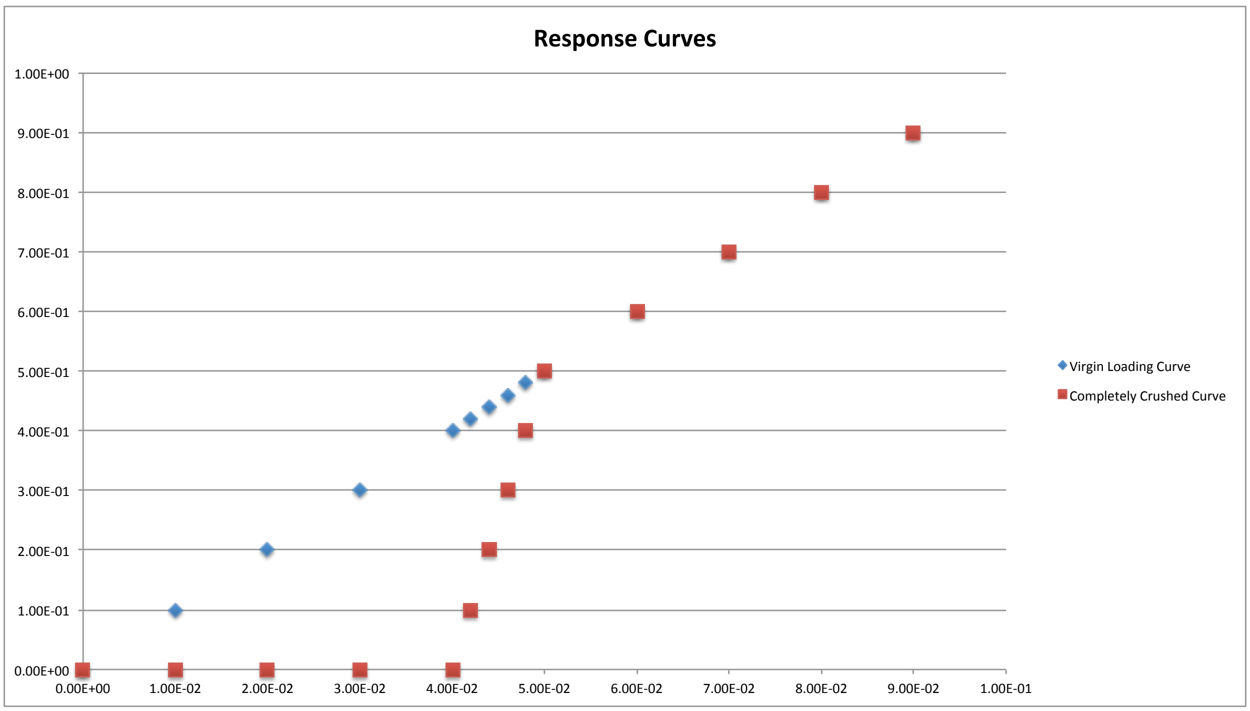
Table 54. Linear response curves used for testing EOS Form 11

Virgin Loading Curve		Completely Crushed Curve	
μ	*p*	μ	*p*
0.000000E+00	0.000000E+00	4.000000E-02	0.000000E+00
1.000000E-02	1.000000E-01	4.200000E-02	1.000000E-01
2.000000E-02	2.000000E-01	4.400000E-02	2.000000E-01
3.000000E-02	3.000000E-01	4.600000E-02	3.000000E-01
4.000000E-02	4.000000E-01	4.800000E-02	4.000000E-01
5.000000E-02	5.000000E-01	5.000000E-02	5.000000E-01
6.000000E-02	6.000000E-01	6.000000E-02	6.000000E-01
7.000000E-02	7.000000E-01	7.000000E-02	7.000000E-01
8.000000E-02	8.000000E-01	8.000000E-02	8.000000E-01
9.000000E-02	9.000000E-01	9.000000E-02	9.000000E-01

For these linear curves, $\mu_1 = 0.01$ and $\mu_2 = 0.05$. These response curves will be tested using Cubes 1 and 2, with Cube 1 having an initial internal energy of 1×10^{-6} and Cube 2 an initial internal energy of 1×10^{-3}. These linear response curves can be calculated exactly in the spreadsheet model.

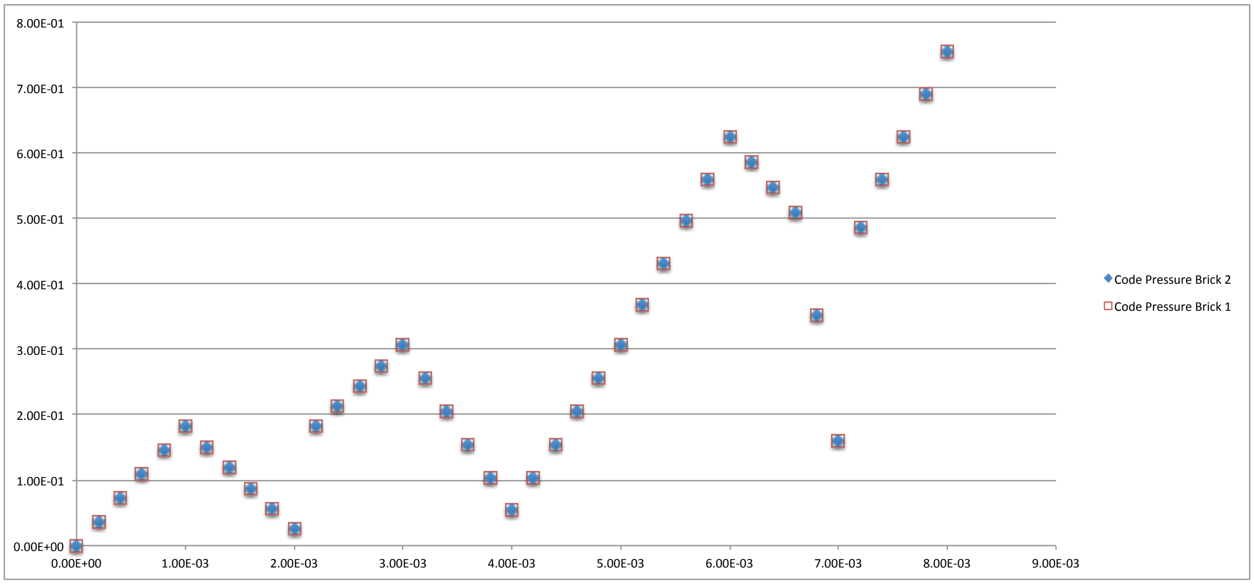
The following plot illustrates that these response curves yield a result which resembles the earlier figure from the DYNA3D manual. However, the use of these curves actually represents an overtest in terms of physical reality, in that actual curves would not display such a pronounced kink when the two curves merge. This will illuminate an issue with the cubic spline routines used in the code, which will be discussed below.

Figure 21. Linear response curves used for testing Cubes 1 and 2



Given the definition of the pressure in this equation-of-state model, one would expect Cubes 1 and 2 to return the same pressures as a function of time, which is the result obtained. The pressures for these 2 cubes are shown in the following plot as a function of time. Note that the cubes are loaded 4 times and unloaded 3 times, with two of the load/unload cycles occurring below $\mu=\mu_2$. As the plot demonstrates, at least at the level of the graph norm, the two cubes are returning the same pressure.

Figure 22. Cubes 1 and 2 pressures from testing EOS Form 11 with linear response curves



The following table makes this point more forcefully, and also reveals the issue with the cubic spline routines mentioned earlier.

Table 55. Code pressures returned for Cubes 1 and 2 from testing EOS Form 11

Time	*Theoretical Pressure*	C1 Pressure	(*Th* - C1)/C1	C2 Pressure	(*Th* -C2)/C2
0.00E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00
2.00E-04	3.608657E-02	3.608657E-02	1.539815E-12	3.608657E-02	3.095783E-13
4.00E-04	7.234699E-02	7.234699E-02	1.443081E-12	7.234699E-02	1.166665E-12
6.00E-04	1.087823E-01	1.087823E-01	1.083741E-12	1.087823E-01	1.478965E-12
8.00E-04	1.453935E-01	1.453935E-01	1.103209E-12	1.453935E-01	1.103209E-12
1.00E-03	1.821818E-01	1.821818E-01	1.195651E-12	1.821818E-01	1.365827E-12
1.20E-03	1.506962E-01	1.506962E-01	-7.343351E-13	1.506962E-01	-9.533279E-13
1.40E-03	1.192359E-01	1.192359E-01	1.007932E-13	1.192359E-01	-2.322899E-12
1.60E-03	8.780086E-02	8.780086E-02	1.771692E-12	8.780086E-02	-1.009528E-12
1.80E-03	5.639113E-02	5.639113E-02	-2.163208E-12	5.639113E-02	-3.934750E-12
2.00E-03	2.500666E-02	2.500666E-02	-7.988981E-12	2.500666E-02	1.780324E-12
2.20E-03	1.821818E-01	1.821818E-01	7.964909E-13	1.821818E-01	1.049089E-12
2.40E-03	2.129747E-01	2.129747E-01	8.994919E-13	2.129747E-01	8.478838E-13
2.60E-03	2.438918E-01	2.438918E-01	9.396698E-13	2.438918E-01	9.027977E-13
2.80E-03	2.749339E-01	2.749339E-01	9.647129E-13	2.749339E-01	5.681670E-13
3.00E-03	3.061015E-01	3.061015E-01	7.121568E-13	3.061015E-01	2.645879E-13
3.20E-03	2.554132E-01	2.554132E-01	-4.779276E-13	2.554132E-01	-1.562447E-12
3.40E-03	2.047904E-01	2.047904E-01	-1.191865E-12	2.047904E-01	-1.191865E-12
3.60E-03	1.542329E-01	1.542329E-01	-1.727964E-12	1.542329E-01	-1.364987E-12

3.80E-03	1.037408E-01	1.037408E-01	-2.775404E-12	1.037408E-01	-5.127414E-12
4.00E-03	5.331371E-02	5.331371E-02	-5.412117E-12	5.331371E-02	-9.576204E-12
4.20E-03	1.037408E-01	1.037408E-01	-3.951409E-12	1.037408E-01	-2.457290E-12
4.40E-03	1.542329E-01	1.542329E-01	-3.381426E-12	1.542329E-01	-2.590327E-12
4.60E-03	2.047904E-01	2.047904E-01	-1.841333E-12	2.047904E-01	-3.467441E-12
4.80E-03	2.554132E-01	2.554132E-01	-2.087103E-12	2.554132E-01	-4.561502E-12
5.00E-03	3.061015E-01	3.061015E-01	7.272088E-14	3.061015E-01	-8.681168E-13
5.20E-03	3.688160E-01	3.688160E-01	1.464480E-13	3.688160E-01	-5.937690E-13
5.40E-03	4.320403E-01	4.307048E-01	3.100694E-03	4.307048E-01	3.100694E-03
5.60E-03	4.957797E-01	4.957797E-01	1.359284E-13	4.957797E-01	-5.095636E-13
5.80E-03	5.600394E-01	5.600394E-01	5.669669E-14	5.600394E-01	-4.950057E-13
6.00E-03	6.248247E-01	6.248247E-01	1.648922E-13	6.248247E-01	-3.376025E-13
6.20E-03	5.858901E-01	5.858901E-01	1.743339E-13	5.858901E-01	-3.598479E-13
6.40E-03	5.471455E-01	5.471455E-01	2.075788E-13	5.471455E-01	-5.015980E-13
6.60E-03	5.085898E-01	5.085898E-01	3.147805E-13	5.085898E-01	-5.760789E-13
6.80E-03	3.511088E-01	3.511088E-01	1.961260E-12	3.511088E-01	-5.059435E-12
7.00E-03	1.602014E-01	1.602014E-01	3.188052E-12	1.602014E-01	-1.080691E-11
7.20E-03	4.788983E-01	4.868939E-01	-1.642173E-02	4.868939E-01	-1.642173E-02
7.40E-03	5.600394E-01	5.600394E-01	2.343199E-13	5.600394E-01	-4.513929E-13
7.60E-03	6.248247E-01	6.248247E-01	3.285405E-13	6.248247E-01	-3.020654E-13
7.80E-03	6.901411E-01	6.901411E-01	3.156250E-13	6.901411E-01	-2.176558E-13
8.00E-03	7.559939E-01	7.559939E-01	3.354193E-13	7.559939E-01	-2.665438E-13

As the table illustrates, the theoretical model and the code are in excellent agreement and the differences in the pressures returned by Cubes 1 and 2 are very small, as expected, since the internal energy does not play a role in determining the pressure in the equation-of-state model.

However, there are two time points where the theoretical model and the code do not agree well. The second of these is at a time of $7.2\text{x}10^{-3}$ and the discrepancy at this time as actually expected, as this point is near μ_2, which means the cubic spline in the code is drawing a smooth curve around the kink in the response curve, so it is not surprising that a disagreement is obtained at this point. The other issue occurs at a time of $5.4\text{x}10^{-3}$ and uncovering the cause of this discrepancy illustrates an issue with the cubic splines and how they are used in the code.

To improve the speed of the code, three cubic spline fits are actually employed by the code. There is a fit for the virgin loading curve, the completely crushed curve and the inverse of the completely crushed curve, which is required for loading and unloading at points between μ_1 and μ_2. The code uses the partially crushed curve defined by the earlier equation for loading and unloading for all $\mu_1<\mu<\mu_2$ and it turns out that the fits to the completely crushed curve and its inverse are not always mathematical inverses of each other, i.e.,

$$\mu = p_{cc}^{-1}\left(p_{cc}\left(\mu\right)\right)$$

does not hold for all values of μ between all of the input data pairs. This can cause the code to return a loading that does not agree exactly with the expected value and is the reason for the discrepancy between the analytical model and the code result at a time of $5.4x10^{-3}$.

Having established that the implementation of this equation-of-state model can indeed match the results of a simplified response curve, the following, more realistic response curves provided by Jerry Lin were used to test the EOS model.

Table 56. Generalized response curves used for testing EOS Form 11

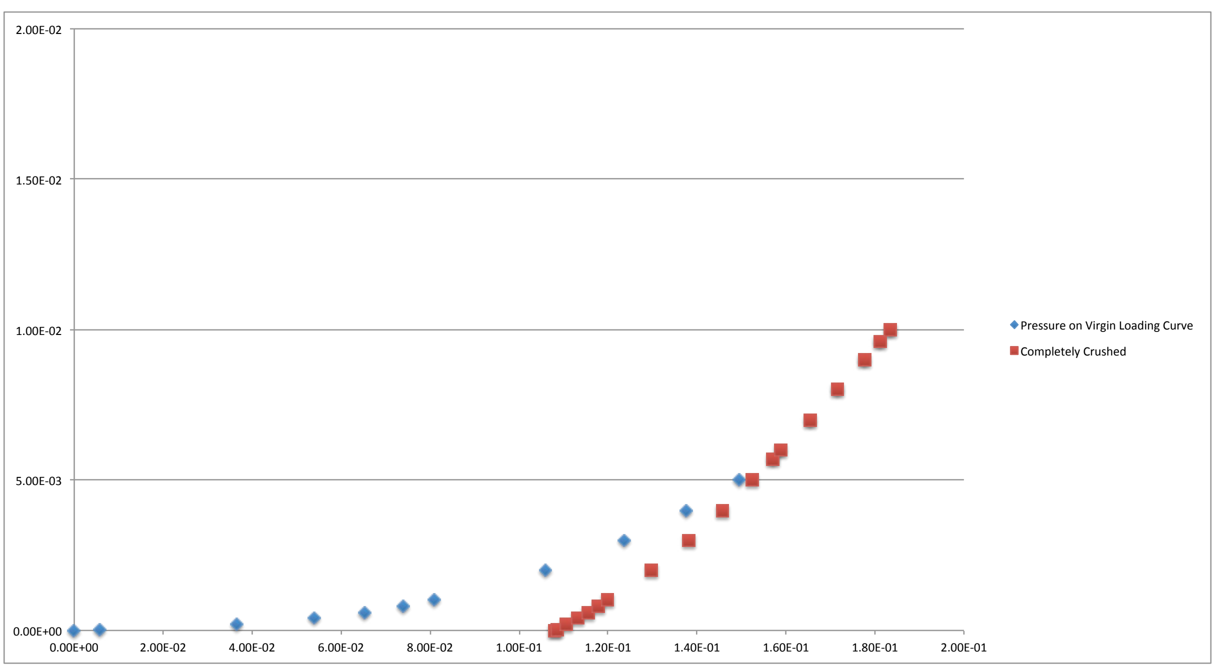
Virgin Loading Curve		Completely Crushed Curve	
μ	*p*	μ	*p*
0.00000000E+00	0.00000000E+00	1.08030000E-01	0.00000000E+00
5.63830000E-03	4.30000000E-05	1.08600000E-01	4.30000000E-05
3.63890000E-02	2.00000000E-04	1.10630000E-01	2.00000000E-04
5.40830000E-02	4.00000000E-04	1.13110000E-01	4.00000000E-04
6.53400000E-02	6.00000000E-04	1.15470000E-01	6.00000000E-04
7.39140000E-02	8.00000000E-04	1.17730000E-01	8.00000000E-04
8.09860000E-02	1.00000000E-03	1.19910000E-01	1.00000000E-03
1.06040000E-01	2.00000000E-03	1.29690000E-01	2.00000000E-03
1.23510000E-01	3.00000000E-03	1.38130000E-01	3.00000000E-03
1.37480000E-01	4.00000000E-03	1.45630000E-01	4.00000000E-03
1.49370000E-01	5.00000000E-03	1.52440000E-01	5.00000000E-03
1.56970000E-01	5.71370000E-03	1.56970000E-01	5.71370000E-03
1.58720000E-01	6.00000000E-03	1.58720000E-01	6.00000000E-03
1.65330000E-01	7.00000000E-03	1.65330000E-01	7.00000000E-03
1.71620000E-01	8.00000000E-03	1.71620000E-01	8.00000000E-03
1.77640000E-01	9.00000000E-03	1.77640000E-01	9.00000000E-03
1.81140000E-01	9.60000000E-03	1.81140000E-01	9.60000000E-03
1.83430000E-01	1.00000000E-02	1.83430000E-01	1.00000000E-02
2.09720000E-01	1.50000000E-02	2.09720000E-01	1.50000000E-02
2.32960000E-01	2.00000000E-02	2.32960000E-01	2.00000000E-02
2.50000000E-01	2.40000000E-02	2.50000000E-01	2.40000000E-02
2.71130000E-01	3.00000000E-02	2.71130000E-01	3.00000000E-02
2.86000000E-01	3.50000000E-02	2.86000000E-01	3.50000000E-02
3.00350000E-01	4.00000000E-02	3.00350000E-01	4.00000000E-02
3.27680000E-01	5.00000000E-02	3.27680000E-01	5.00000000E-02
3.78540000E-01	7.00000000E-02	3.78540000E-01	7.00000000E-02
4.48380000E-01	1.00000000E-01	4.48380000E-01	1.00000000E-01
5.56280000E-01	1.50000000E-01	5.56280000E-01	1.50000000E-01
6.68470000E-01	2.00000000E-01	6.68470000E-01	2.00000000E-01

7.72960000E-01	2.50000000E-01	7.72960000E-01	2.50000000E-01
8.48410000E-01	3.00000000E-01	8.48410000E-01	3.00000000E-01
8.97070000E-01	3.50000000E-01	8.97070000E-01	3.50000000E-01
9.39820000E-01	4.00000000E-01	9.39820000E-01	4.00000000E-01
1.01220000E+00	5.00000000E-01	1.01220000E+00	5.00000000E-01
1.12250000E+00	7.00000000E-01	1.12250000E+00	7.00000000E-01
1.20480000E+00	9.00000000E-01	1.20480000E+00	9.00000000E-01
1.23910000E+00	1.00000000E+00	1.23910000E+00	1.00000000E+00
1.36860000E+00	1.50000000E+00	1.45720000E+00	2.00000000E+00
1.45720000E+00	2.00000000E+00		

For these generalized curves, $\mu_1 = 0.0056383$ and $\mu_2 = 0.15697$. These response curves will be tested using Cubes 3 and 4, with Cube 3 having an initial internal energy of $1x10^{-6}$ and Cube 4 an initial internal energy of $1x10^{-3}$. These generalized response curves cannot be calculated exactly in the spreadsheet model, requiring instead the use of a cubic spline to model them. Based on the earlier testing of this EOS model[3], this is expected to result in a poorer match between the spreadsheet model and the code results.

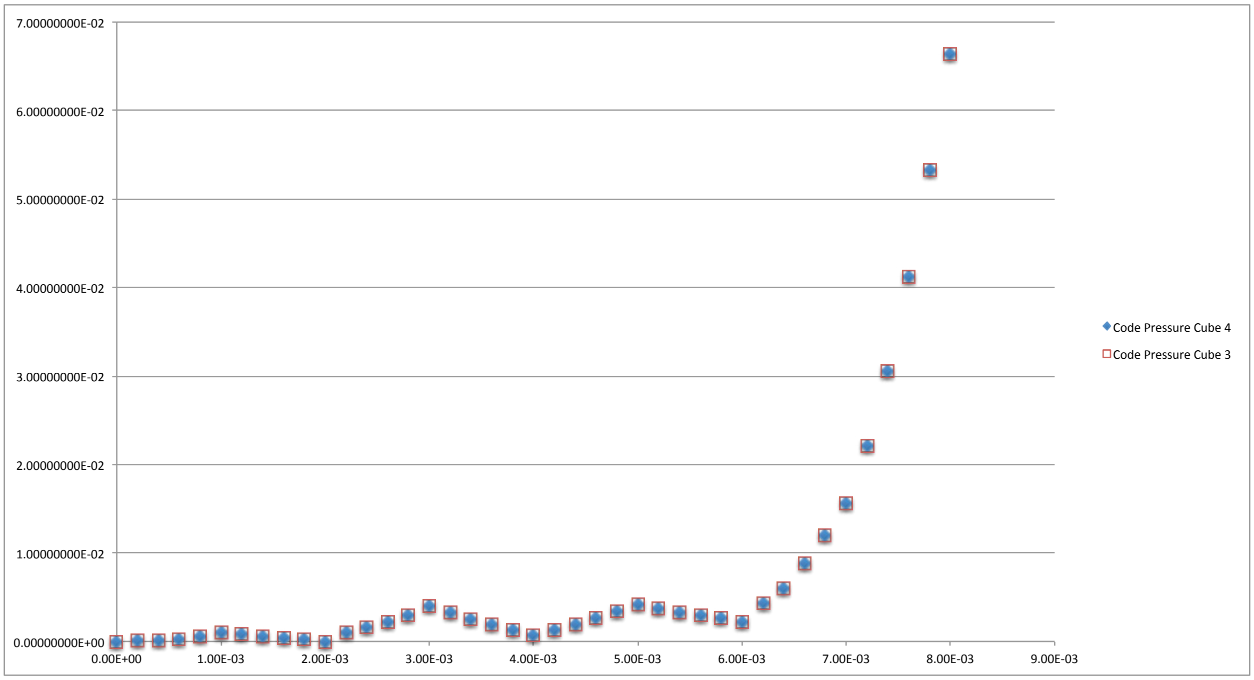
The following plot illustrates that these generalized response curves yield a result which greatly resembles the earlier figure from the DYNA3D manual. Note that the plot is displaying only the bottom part of the curves in order to accentuate the difference between the two curves. Note also that these curves join much more smoothly than the two linear curves used in the earlier tests for this EOS model and the cubic splines should not have as large an effect near the junction point as was observed in the earlier tests. The testing of the EOS model will focus on this part of the curves.

Figure 23. Generalized response curves used for testing Cubes 3 and 4



Given the definition of the pressure in this equation-of-state model, one would expect Cubes 3 and 4 to return the same pressures as a function of time, which is the result obtained. The pressures for these 2 cubes are shown in the following plot as a function of time. Note that the cubes are loaded 4 times and unloaded 3 times, with three of the load/unload cycles occurring below $\mu=\mu_2$. As the plot demonstrates, at least at the level of the graph norm, the two cubes are returning the same pressure.

Figure 24. Cubes 3 and 4 pressures from testing EOS Form 11 with generalized response curves



The following table makes this point more forcefully, and also demonstrates the reduced agreement between the reference model and the code results that was expected due to the use of cubic spline routines in both the reference model and the code.

Table 57. Code pressures returned for Cubes 3 and 4 from testing EOS Form 11

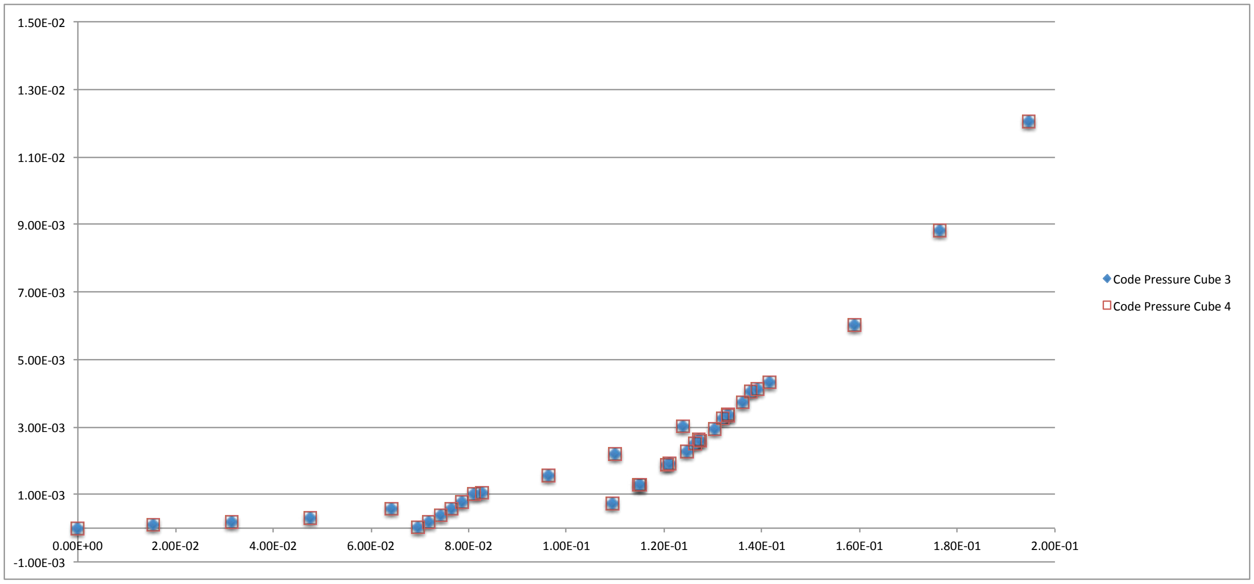
Time	*Reference Pressure*	C3 Pressure	(*Ref* - C3)/C3	C4 Pressure	(*Ref*-C4)/C4
0.00E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00
2.00E-04	9.645977E-05	9.474809E-05	1.806554E-02	9.474809E-05	1.806554E-02
4.00E-04	1.672482E-04	1.677360E-04	-2.908515E-03	1.677360E-04	-2.908515E-03
6.00E-04	3.109244E-04	3.132531E-04	-7.433834E-03	3.132531E-04	-7.433834E-03
8.00E-04	5.748602E-04	5.751803E-04	-5.564665E-04	5.751803E-04	-5.564665E-04
1.00E-03	9.999946E-04	9.999943E-04	2.925097E-07	9.999943E-04	2.925085E-07
1.20E-03	7.831329E-04	7.831286E-04	5.507328E-06	7.831286E-04	5.507325E-06
1.40E-03	5.750693E-04	5.750983E-04	-5.050622E-05	5.750983E-04	-5.050623E-05
1.60E-03	3.767314E-04	3.767335E-04	-5.594239E-06	3.767335E-04	-5.594251E-06
1.80E-03	1.882123E-04	1.881993E-04	6.902560E-05	1.881993E-04	6.902558E-05

2.00E-03	8.231522E-06	8.230771E-06	9.126185E-05	8.230771E-06	9.126147E-05
2.20E-03	1.057329E-03	1.059971E-03	-2.492685E-03	1.059971E-03	-2.492685E-03
2.40E-03	1.549730E-03	1.562714E-03	-8.308592E-03	1.562714E-03	-8.308592E-03
2.60E-03	2.198989E-03	2.192369E-03	3.019260E-03	2.192369E-03	3.019260E-03
2.80E-03	3.014766E-03	3.014835E-03	-2.297077E-05	3.014835E-03	-2.297077E-05
3.00E-03	4.030104E-03	4.027933E-03	5.390382E-04	4.027933E-03	5.390382E-04
3.20E-03	3.215352E-03	3.240665E-03	-7.810815E-03	3.240665E-03	-7.810815E-03
3.40E-03	2.499214E-03	2.523526E-03	-9.634170E-03	2.523526E-03	-9.634170E-03
3.60E-03	1.847859E-03	1.869343E-03	-1.149277E-02	1.869343E-03	-1.149277E-02
3.80E-03	1.258571E-03	1.279072E-03	-1.602833E-02	1.279072E-03	-1.602833E-02
4.00E-03	7.297018E-04	7.470227E-04	-2.318661E-02	7.470227E-04	-2.318661E-02
4.20E-03	1.280905E-03	1.301610E-03	-1.590705E-02	1.301610E-03	-1.590705E-02
4.40E-03	1.897540E-03	1.919052E-03	-1.121000E-02	1.919052E-03	-1.121000E-02
4.60E-03	2.581446E-03	2.606043E-03	-9.438089E-03	2.606043E-03	-9.438089E-03
4.80E-03	3.335888E-03	3.361754E-03	-7.694298E-03	3.361754E-03	-7.694298E-03
5.00E-03	4.128556E-03	4.118987E-03	2.323112E-03	4.118987E-03	2.323112E-03
5.20E-03	3.755325E-03	3.712124E-03	1.163770E-02	3.712124E-03	1.163770E-02
5.40E-03	3.363498E-03	3.321409E-03	1.267231E-02	3.321409E-03	1.267231E-02
5.60E-03	2.989107E-03	2.949365E-03	1.347491E-02	2.949365E-03	1.347491E-02
5.80E-03	2.631686E-03	2.594397E-03	1.437267E-02	2.594397E-03	1.437267E-02
6.00E-03	2.290757E-03	2.254829E-03	1.593411E-02	2.254829E-03	1.593411E-02
6.20E-03	4.349821E-03	4.324582E-03	5.836294E-03	4.324582E-03	5.836294E-03
6.40E-03	6.021134E-03	6.020208E-03	1.537848E-04	6.020208E-03	1.537848E-04
6.60E-03	8.810522E-03	8.810483E-03	4.400702E-06	8.810483E-03	4.400700E-06
6.80E-03	1.202203E-02	1.204345E-02	-1.778218E-03	1.204345E-02	-1.778218E-03
7.00E-03	1.566475E-02	1.565860E-02	3.926142E-04	1.565860E-02	3.926142E-04
7.20E-03	2.213134E-02	2.212437E-02	3.150547E-04	2.212437E-02	3.150547E-04
7.40E-03	3.047556E-02	3.046505E-02	3.451182E-04	3.046505E-02	3.451182E-04
7.60E-03	4.126745E-02	4.127381E-02	-1.540618E-04	4.127381E-02	-1.540618E-04
7.80E-03	5.325636E-02	5.326140E-02	-9.449795E-05	5.326140E-02	-9.449795E-05
8.00E-03	6.639880E-02	6.639596E-02	4.287370E-05	6.639596E-02	4.287370E-05

As the table illustrates, the reference model and the code exhibit markedly poorer agreement than that exhibited in the testing using the linearized response curves, a result that was expected based on the requirement to use cubic splines in both the reference model and the code. Note that the agreement between the reference model and the code results exhibits marked improvement in the vicinity of the entered data pairs in the response curves, as would be expected from the behavior of cubic splines.

As expected, the differences in the pressures returned by Cubes 3 and 4 are smaller than the number of significant digits displayed in the table, since, by definition, the internal energy does not play a role in determining the pressure in this equation-of-state model. In addition, as the following plot demonstrates, these cubes are loading and unloading in the manner expected from this EOS model.

Figure 25. Cubes 3 and 4 pressures as a function of excess compression



As the plot demonstrates, for $\mu_1<\mu<\mu_2$, the cubes unload and reload along a line that lies between the virgin loading curve and the completely crushed curve. In addition, both cubes exhibit the same behavior, as expected.

The code results for the internal energy can also be examined for the equation-of-state model. Given the use of cubic splines in the code to determine the behavior of this EOS model, there is no closed form solution for the internal energy returned by this model. Given the use of linear response curves in Cubes 1 and 2 and the excellent agreement obtained for the pressure between the analytic model and the code, one would expect to obtain good agreement for the internal energies in Cubes 1 and 2. The requirement to use cubic splines in both the reference model and the code for Cubes 3 and 4 degrades the agreement obtained for the pressures and one would expect that to also affect the results obtained for the internal energy.

The following table gives the results for the internal energy for Cube 1, which had an initial internal energy of $1.0\text{x}10^{-6}$. The code results for the internal energy were extracted using GRIZ, which limits the accuracy to 7 significant figures.

Table 58. Internal energies for Cube 1 from testing EOS Form 11

Time	Code (GRIZ)	*Reference Energy*	(*Reference* - GRIZ)/GRIZ
0.00E+00	1.00000000E-06	1.00000000E-06	0.000000E+00
2.00E-04	6.58000200E-05	6.58000156E-05	-6.618777E-08
4.00E-04	2.60200300E-04	2.60200249E-04	-1.942089E-07
6.00E-04	5.84201300E-04	5.84201264E-04	-6.233230E-08
8.00E-04	1.03780400E-03	1.03780400E-03	-2.915011E-09

1.00E-03	1.62101000E-03	1.62100977E-03	-1.435633E-07
1.20E-03	1.52232300E-03	1.52232317E-03	1.099541E-07
1.40E-03	1.44226600E-03	1.44226597E-03	-2.061316E-08
1.60E-03	1.38083800E-03	1.38083817E-03	1.227213E-07
1.80E-03	1.33804000E-03	1.33803976E-03	-1.793816E-07
2.00E-03	1.31387100E-03	1.31387074E-03	-1.991245E-07
2.20E-03	1.62101000E-03	1.62100977E-03	-1.434241E-07
2.40E-03	2.20601800E-03	2.20601811E-03	4.968109E-08
2.60E-03	2.88103100E-03	2.88103092E-03	-2.824079E-08
2.80E-03	3.64605000E-03	3.64604957E-03	-1.192449E-07
3.00E-03	4.50107500E-03	4.50107561E-03	1.345998E-07
3.20E-03	4.23683500E-03	4.23683443E-03	-1.344698E-07
3.40E-03	4.02013000E-03	4.02013026E-03	6.526612E-08
3.60E-03	3.85096300E-03	3.85096306E-03	1.478035E-08
3.80E-03	3.72933300E-03	3.72933278E-03	-5.936694E-08
4.00E-03	3.65523900E-03	3.65523940E-03	1.099970E-07
4.20E-03	3.72933300E-03	3.72933278E-03	-5.936694E-08
4.40E-03	3.85096300E-03	3.85096306E-03	1.478035E-08
4.60E-03	4.02013000E-03	4.02013026E-03	6.526610E-08
4.80E-03	4.23683500E-03	4.23683443E-03	-1.344699E-07
5.00E-03	4.50107500E-03	4.50107561E-03	1.345998E-07
5.20E-03	6.48115700E-03	6.48115703E-03	4.513066E-09
5.40E-03	8.81996100E-03	8.82129139E-03	1.508381E-04
5.60E-03	1.15134500E-02	1.15214979E-02	6.989997E-04
5.80E-03	1.45737500E-02	1.45817988E-02	5.522829E-04
6.00E-03	1.79941700E-02	1.80022195E-02	4.473409E-04
6.20E-03	1.58987000E-02	1.59067512E-02	5.064072E-04
6.40E-03	1.39328800E-02	1.39409299E-02	5.777643E-04
6.60E-03	1.20967000E-02	1.21047498E-02	6.654514E-04
6.80E-03	1.05424100E-02	1.05596761E-02	1.637772E-03
7.00E-03	9.64913500E-03	9.66640222E-03	1.789509E-03
7.20E-03	1.15148600E-02	1.15247308E-02	8.572206E-04
7.40E-03	1.45737400E-02	1.45817989E-02	5.529706E-04
7.60E-03	1.79941700E-02	1.80022195E-02	4.473419E-04
7.80E-03	2.17747400E-02	2.17827884E-02	3.696228E-04
8.00E-03	2.59154800E-02	2.59235371E-02	3.108988E-04

As the table demonstrates, the agreement between the reference model and the code is as good as can be expected, given the 7 digit output from GRIZ, until $t = 5.4 \times 10^{-3}$. This is the first time point when the reference model and the code disagree noticeably for the pressure due to the manner in which the cubic splines are employed by the code. This feeds through into the numerical integration performed by the code to determine the internal energy and the reference model and code never re-establish good agreement for the internal energy after that.

The following table gives the results for the internal energy for Cube 2, which had an initial internal energy of 1.0×10^{-3}. The code results for the internal energy were extracted using GRIZ, which limits the accuracy to 7 significant figures.

Table 59. Internal energies for Cube 2 from testing EOS Form 11

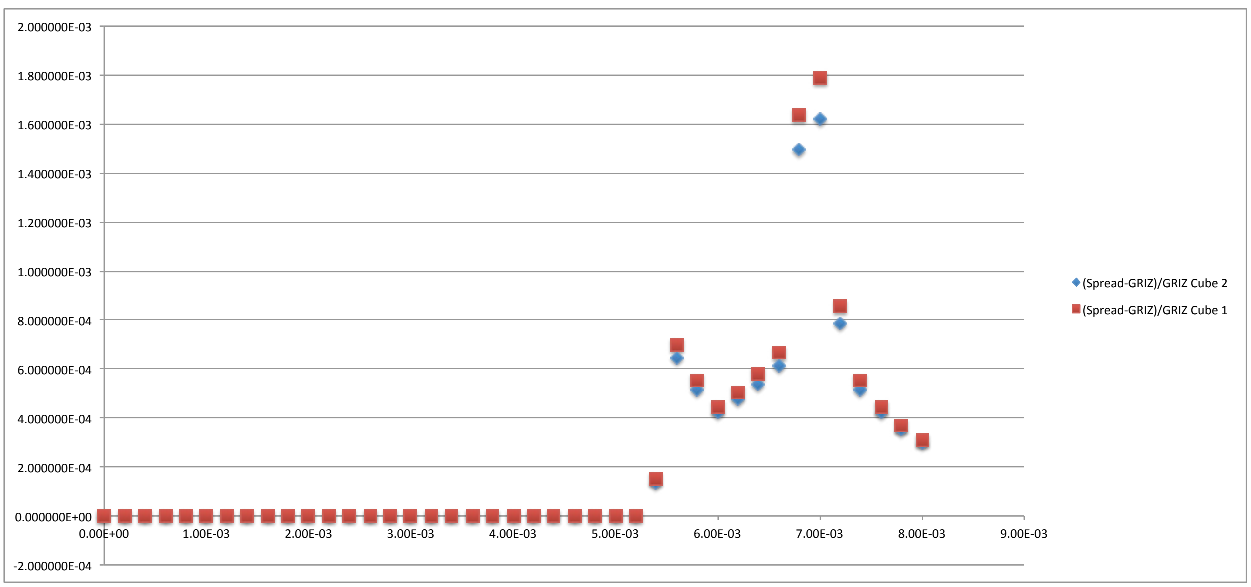
Time	Code (GRIZ)	*Reference Energy*	(*Reference* - GRIZ)/GRIZ
0.00E+00	1.00000000E-03	1.00000000E-03	0.000000E+00
2.00E-04	1.06480000E-03	1.06480002E-03	1.469276E-08
4.00E-04	1.25920000E-03	1.25920025E-03	1.981153E-07
6.00E-04	1.58320100E-03	1.58320126E-03	1.664889E-07
8.00E-04	2.03680400E-03	2.03680400E-03	-1.485270E-09
1.00E-03	2.62001000E-03	2.62000977E-03	-8.882312E-08
1.20E-03	2.52132300E-03	2.52132317E-03	6.638805E-08
1.40E-03	2.44126600E-03	2.44126597E-03	-1.217796E-08
1.60E-03	2.37983800E-03	2.37983817E-03	7.120576E-08
1.80E-03	2.33704000E-03	2.33703976E-03	-1.027024E-07
2.00E-03	2.31287100E-03	2.31287074E-03	-1.131165E-07
2.20E-03	2.62001000E-03	2.62000977E-03	-8.873703E-08
2.40E-03	3.20501800E-03	3.20501811E-03	3.419556E-08
2.60E-03	3.88003100E-03	3.88003092E-03	-2.096957E-08
2.80E-03	4.64505000E-03	4.64504957E-03	-9.359921E-08
3.00E-03	5.50007500E-03	5.50007561E-03	1.101519E-07
3.20E-03	5.23583500E-03	5.23583443E-03	-1.088129E-07
3.40E-03	5.01913000E-03	5.01913026E-03	5.227565E-08
3.60E-03	4.84996300E-03	4.84996306E-03	1.173588E-08
3.80E-03	4.72833300E-03	4.72833278E-03	-4.682392E-08
4.00E-03	4.65423900E-03	4.65423940E-03	8.638694E-08
4.20E-03	4.72833300E-03	4.72833278E-03	-4.682392E-08
4.40E-03	4.84996300E-03	4.84996306E-03	1.173587E-08
4.60E-03	5.01913000E-03	5.01913026E-03	5.227563E-08
4.80E-03	5.23583500E-03	5.23583443E-03	-1.088130E-07
5.00E-03	5.50007500E-03	5.50007561E-03	1.101519E-07
5.20E-03	7.48015700E-03	7.48015703E-03	3.910329E-09
5.40E-03	9.81896100E-03	9.82029139E-03	1.354916E-04
5.60E-03	1.25124500E-02	1.25204979E-02	6.431913E-04
5.80E-03	1.55727500E-02	1.55807988E-02	5.168536E-04

6.00E-03	1.89931700E-02	1.90012195E-02	4.238117E-04
6.20E-03	1.68977000E-02	1.69057512E-02	4.764682E-04
6.40E-03	1.49318800E-02	1.49399299E-02	5.391096E-04
6.60E-03	1.30957000E-02	1.31037498E-02	6.146877E-04
6.80E-03	1.15414100E-02	1.15586761E-02	1.496010E-03
7.00E-03	1.06481400E-02	1.06654022E-02	1.621148E-03
7.20E-03	1.25138600E-02	1.25237308E-02	7.887874E-04
7.40E-03	1.55727500E-02	1.55807989E-02	5.168548E-04
7.60E-03	1.89931700E-02	1.90012195E-02	4.238127E-04
7.80E-03	2.27737400E-02	2.27817884E-02	3.534088E-04
8.00E-03	2.69144800E-02	2.69225371E-02	2.993590E-04

As the table demonstrates, the agreement between the reference model and the code is as good as can be expected, given the 7 digit output from GRIZ, until t = $5.4\text{x}10^{-3}$. This is the first time point when the reference model and the code disagree noticeably for the pressure due to the manner in which the cubic splines are employed by the code. This feeds through into the numerical integration performed by the code to determine the internal energy and the reference model and code never re-establish good agreement for the internal energy after that.

An interesting behavior is revealed by the following plot, which shows the normalized difference between the spreadsheet numerical integration (reference model) and the code result for both Cubes 1 and 2.

Figure 26. Normalized differences for internal energy for Cubes 1 and 2



Despite a difference of three orders of magnitude in the initial value of the internal energy for Cubes 1 and 2, the normalized difference between the reference model and the code result for the internal energy returned by these cubes bear a striking resemblance to each other. This is in fact not a surprise, as the internal energy developed in Cube 1 becomes on the order of the initial value of the internal energy in Cube 2 by a time of 8x10^{-4}, which is very early in the calculation.

The following table gives the results for the internal energy for Cube 3, which had an initial internal energy of 1.0x10^{-6}, and used the generalized response curve. The code results for the internal energy were extracted using GRIZ, which limits the accuracy to 7 significant figures.

Table 60. Internal energies for Cube 3 from testing EOS Form 11

Time	Code (GRIZ)	*Reference Energy*	(*Reference* - GRIZ)/GRIZ
0.00E+00	1.00000000E-06	1.00000000E-06	0.00000000E+00
2.00E-04	1.80596600E-06	1.81834290E-06	6.85333928E-03
4.00E-04	3.76389500E-06	3.78468534E-06	5.52362251E-03
6.00E-04	7.21363400E-06	7.22450966E-06	1.50765277E-03
8.00E-04	1.36197600E-05	1.36257020E-05	4.36281390E-04
1.00E-03	2.49320600E-05	2.49449455E-05	5.16823285E-04
1.20E-03	2.31866400E-05	2.31992987E-05	5.45947248E-04
1.40E-03	2.18555100E-05	2.18681132E-05	5.76659425E-04
1.60E-03	2.09219300E-05	2.09345716E-05	6.04228454E-04
1.80E-03	2.03674900E-05	2.03801699E-05	6.22555405E-04
2.00E-03	2.01753100E-05	2.01880737E-05	6.32641486E-04
2.20E-03	2.65476100E-05	2.65584147E-05	4.06993806E-04
2.40E-03	4.12512100E-05	4.11533325E-05	-2.37271947E-03
2.60E-03	6.21536500E-05	6.19990312E-05	-2.48768711E-03
2.80E-03	9.09356100E-05	9.08311699E-05	-1.14850653E-03
3.00E-03	1.29561600E-04	1.29379950E-04	-1.40203197E-03
3.20E-03	1.13292300E-04	1.13231911E-04	-5.33034463E-04
3.40E-03	1.00351900E-04	1.00403496E-04	5.14152566E-04
3.60E-03	9.04622300E-05	9.06165804E-05	1.70624143E-03
3.80E-03	8.33530400E-05	8.36055806E-05	3.02977104E-03
4.00E-03	7.87731600E-05	7.91099118E-05	4.27495558E-03
4.20E-03	8.35865900E-05	8.38354097E-05	2.97678973E-03
4.40E-03	9.11455900E-05	9.12921790E-05	1.60829511E-03
4.60E-03	1.01735000E-04	1.01773427E-04	3.77713985E-04
4.80E-03	1.15657800E-04	1.15579024E-04	-6.81110061E-04
5.00E-03	1.33197500E-04	1.33020950E-04	-1.32547455E-03
5.20E-03	1.24404000E-04	1.24127655E-04	-2.22134977E-03
5.40E-03	1.16493200E-04	1.16120975E-04	-3.19525282E-03
5.60E-03	1.09429200E-04	1.08964184E-04	-4.24946861E-03
5.80E-03	1.03173000E-04	1.02621365E-04	-5.34669971E-03
6.00E-03	9.76918100E-05	9.70574704E-05	-6.49327270E-03
6.20E-03	1.41428900E-04	1.41287212E-04	-1.00182933E-03

6.40E-03	2.07937900E-04	2.07809627E-04	-6.16882897E-04
6.60E-03	3.03561000E-04	3.03453104E-04	-3.55433783E-04
6.80E-03	4.36807700E-04	4.36588506E-04	-5.01808113E-04
7.00E-03	6.12227800E-04	6.11870197E-04	-5.84101645E-04
7.20E-03	9.78664600E-04	9.78420002E-04	-2.49930118E-04
7.40E-03	1.47821100E-03	1.47769636E-03	-3.48152163E-04
7.60E-03	2.15277200E-03	2.15237042E-03	-1.86542489E-04
7.80E-03	3.02791800E-03	3.02745324E-03	-1.53491620E-04
8.00E-03	4.11831000E-03	4.11781346E-03	-1.20570041E-04

As the table demonstrates, the agreement between the reference model and the code is not as good as that exhibited by the results from Cubes 1 and 2. Given the use of cubic splines in the reference model, as well as the code, to determine the behavior of the response curve, this was to be expected. In addition, there is no point in time during the simulation after which the agreement between the spreadsheet model and the code has clearly degraded, as was observed in the results from Cubes 1 and 2.

The following table gives the results for the internal energy for Cube 4, which had an initial internal energy of 1.0×10^{-3}, and used the generalized response curve. The code results for the internal energy were extracted using GRIZ, which limits the accuracy to 7 significant figures.

Table 61. Internal energies for Cube 4 from testing EOS Form 11

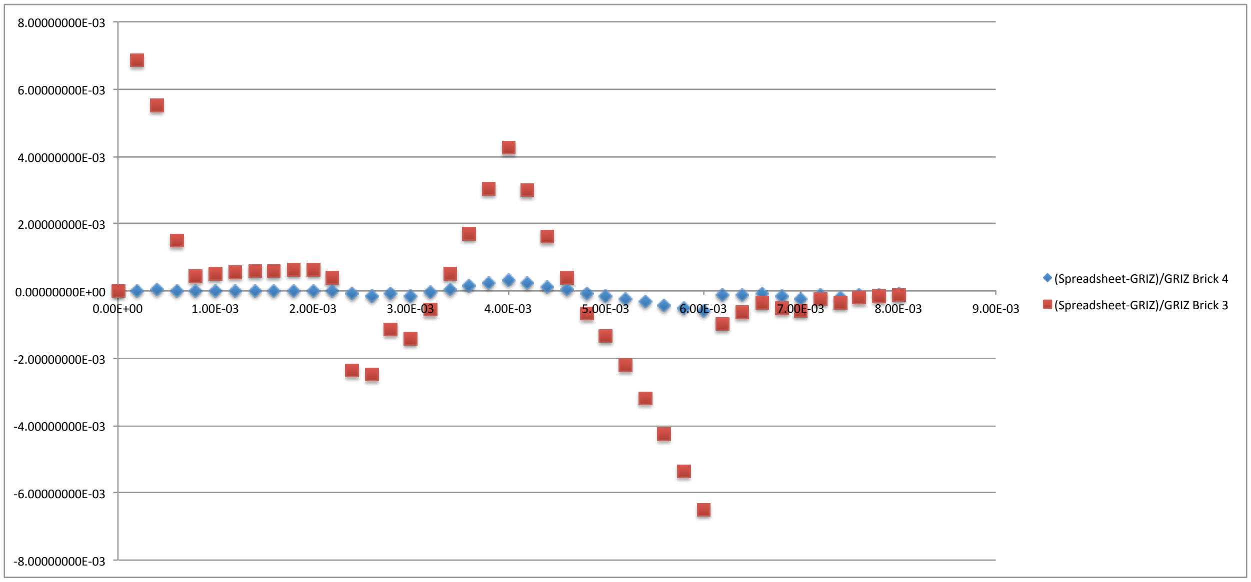
Time	Code (GRIZ)	*Reference Energy*	(*Reference* - GRIZ)/GRIZ
0.00E+00	1.00000000E-03	1.00000000E-03	0.00000000E+00
2.00E-04	1.00080600E-03	1.00081834E-03	1.23329574E-05
4.00E-04	1.00276400E-03	1.00278469E-03	2.06283185E-05
6.00E-04	1.00621400E-03	1.00622451E-03	1.04447516E-05
8.00E-04	1.01262000E-03	1.01262570E-03	5.63098480E-06
1.00E-03	1.02393200E-03	1.02394495E-03	1.26428993E-05
1.20E-03	1.02218700E-03	1.02219930E-03	1.20317291E-05
1.40E-03	1.02085600E-03	1.02086811E-03	1.18657093E-05
1.60E-03	1.01992200E-03	1.01993457E-03	1.23260604E-05
1.80E-03	1.01936700E-03	1.01938017E-03	1.29196705E-05
2.00E-03	1.01917500E-03	1.01918807E-03	1.28277605E-05
2.20E-03	1.02554800E-03	1.02555841E-03	1.01552610E-05
2.40E-03	1.04025100E-03	1.04015333E-03	-9.38884504E-05
2.60E-03	1.06115400E-03	1.06099903E-03	-1.46038029E-04
2.80E-03	1.08993600E-03	1.08983117E-03	-9.61800945E-05
3.00E-03	1.12856200E-03	1.12837995E-03	-1.61311041E-04
3.20E-03	1.11229200E-03	1.11223198E-03	-5.39618477E-05
3.40E-03	1.09935200E-03	1.09940356E-03	4.69035901E-05

3.60E-03	1.08946200E-03	1.08961665E-03	1.41948754E-04
3.80E-03	1.08235300E-03	1.08260565E-03	2.33424766E-04
4.00E-03	1.07777300E-03	1.07810998E-03	3.12662433E-04
4.20E-03	1.08258700E-03	1.08283548E-03	2.29521573E-04
4.40E-03	1.09014600E-03	1.09029225E-03	1.34153017E-04
4.60E-03	1.10073500E-03	1.10077349E-03	3.49712701E-05
4.80E-03	1.11465800E-03	1.11457909E-03	-7.07915096E-05
5.00E-03	1.13219700E-03	1.13202102E-03	-1.55434546E-04
5.20E-03	1.12340400E-03	1.12312768E-03	-2.45965273E-04
5.40E-03	1.11549300E-03	1.11512100E-03	-3.33483761E-04
5.60E-03	1.10842900E-03	1.10796421E-03	-4.19322777E-04
5.80E-03	1.10217300E-03	1.10162139E-03	-5.00473723E-04
6.00E-03	1.09669200E-03	1.09605750E-03	-5.78560926E-04
6.20E-03	1.14042900E-03	1.14028724E-03	-1.24305147E-04
6.40E-03	1.20693800E-03	1.20680965E-03	-1.06340930E-04
6.60E-03	1.30256100E-03	1.30245313E-03	-8.28133269E-05
6.80E-03	1.43580800E-03	1.43558853E-03	-1.52852765E-04
7.00E-03	1.61122800E-03	1.61087022E-03	-2.22052274E-04
7.20E-03	1.97766500E-03	1.97742003E-03	-1.23868974E-04
7.40E-03	2.47721100E-03	2.47669638E-03	-2.07740048E-04
7.60E-03	3.15177200E-03	3.15137044E-03	-1.27406748E-04
7.80E-03	4.02691800E-03	4.02645327E-03	-1.15406773E-04
8.00E-03	5.11731000E-03	5.11681348E-03	-9.70272232E-05

As the table demonstrates, the agreement between the reference model and the code is not as good as that exhibited by the results from Cubes 1 and 2. Given the use of cubic splines in the reference model, as well as the code, to determine the behavior of the response curve, this was to be expected. In addition, there is no point in time during the simulation after which the agreement between the spreadsheet model and the code has clearly degraded, as was observed in the results from Cubes 1 and 2. Finally, the normalized difference between the reference model and the code results is, in the early part of the simulation, generally about an order of magnitude better than the results from Cube 3.

This last point is made more clear by the following plot, which displays the normalized differences for the internal energy from Cubes 3 and 4. Given that the initial value of the internal energy in Cube 4 is three orders of magnitude larger than that of Cube 3, it is expected that the normalized difference from Cube 4 would be considerably smaller than that of Cube 3 until the internal energy developed in Cube 3 becomes on the order of the initial value used for Cube 4, which occurs at $t \sim 7.4\text{x}10^{-3}$.

Figure 27. Normalized differences for internal energy for Cubes 3 and 4



This establishes the implementation of Equation-of-State Form 11 in DYNA3D. The equation-of-state is performing as expected, in that the pressure in the cubes increases as they are compressed and decreases as they are expanded. The behavior of the equation-of-state as a whole has been examined using both linearized response curves, which may represent an over test of the model, and generalized response curves, which are more physically realistic but harder to predict. Equation-of-State Form 11 is performing as expected and with good accuracy.

Equation-of-State Form 12

Equation-of-State Form 12 is a modified version of Equation-of-State Form 8 for use only with material model 45. The input entries and formatting used for Equation-of-State Form 12 are identical to those used for Equation-of-State Form 8.

Therefore, Equation-of-State Form 12 is a tabulated equation-of-state that is linear in the internal energy. The form of the equation for the pressure, *p*, is

$$p\left(\varepsilon_v,\tilde{\varepsilon}_v\right)=C\left(\tilde{\varepsilon}_v\right)+\gamma T\left(\tilde{\varepsilon}_v\right)E+K\left(\tilde{\varepsilon}_v\right)\times\left(\tilde{\varepsilon}_v-\varepsilon_v\right)$$

where E is the internal energy and ε_v is the volumetric strain, defined by $\varepsilon_v=\ln(V)$, where V is the relative volume. $C(\varepsilon_v)$, $T(\varepsilon_v)$ and $K(\varepsilon_v)$ represent function evaluations from the tabulated data and the input $C(\varepsilon_v)$ therefore have the units of pressure. The minimum volumetric strain, $\tilde{\varepsilon}_v$, is given by the following expression:

$$\tilde{\varepsilon}_v\left(t\right)=\min\left[\varepsilon_v(\tau)\right],0\le\tau\le t$$

Note that the pressure is positive in compression and the volumetric strain is positive in tension. Also, the code expects the material to become stiffer with increasing compression and will issue a warning if the unloading bulk moduli do not fulfill this requirement.

It is important to note that in this equation-of-state model unloading occurs along a line using the interpolated value of the unloading bulk modulus that corresponds to the most compressive volumetric strain experienced by the system. To put this bluntly, the system unloads at the point at which the compression is relieved and unloads along a path that is probably different than the loading line and may not be linear if the contribution from the second term in the equation is important because the internal energy continues to evolve along the unloading/reloading path.

As there are really only two terms in EOS Form 12, this equation-of-state model will be tested with 3 cubes, one for each term (2 cubes) and one for the full equation-of-state model. However, due to the unloading/reloading behavior introduced by the bulk unloading moduli, the cubes do not use the same drive that has been used in all the previous tests. Instead, the cubes are compressed by moving all 8 nodes in 0.004 cm, releasing the nodes back to 0.001 cm, moving the nodes in 0.007 cm, releasing back to 0.001 cm, moving in to 0.01 cm, releasing back to 0.005 cm and then compressing back to 0.01 cm. This series of compressions and releases tests the unloading/reloading behavior introduced into this equation-of-state model.

Prior to discussing the calculations using EOS Form 12, a few code issues need to be addressed and these are not necessarily readily apparent to the user. First, in order for the term dependent on the internal energy to perform as expected, it is required to have an initial energy present in the simulation, so the initial internal energy was set to a value of 1.0e-3 in all of the cubes. In addition, in order to eliminate issues with the work performed by the bulk viscosity, the two input coefficients for the bulk viscosity on the material card were set to 1.0e-20 in each of the

3 cubes. Failing to do so results in the work performed on the cube being dominated by contributions from the bulk viscosity. Also, in order to correctly calculate the sound speed, it is necessary to use non-zero values for the $C(\varepsilon_v)$ coefficients, so these were set to very small values for the testing of the second term using Cube 2. Finally, the code version used for this test was version 15.2.0 revision 1.3377.

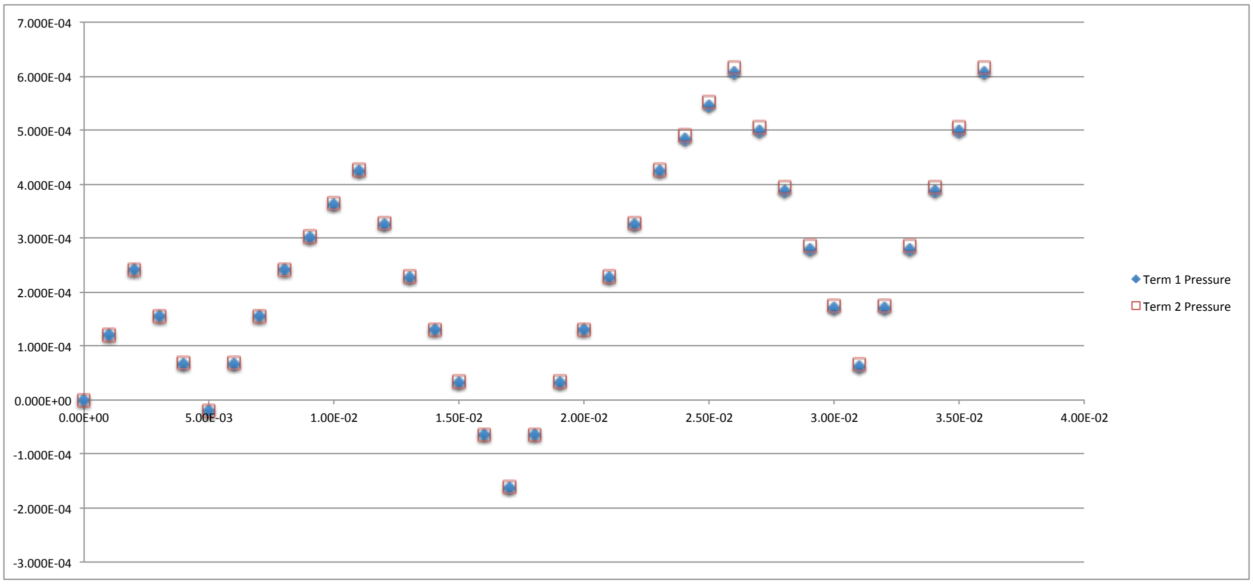
The input coefficients for Equation-of-State Form 12 chosen were the same as those used for the testing of EOS Forms 8 and 9 and are such that the contribution to the pressure from the two terms was of the same order of magnitude as a function of time during the compression and expansion of the cubes. The input coefficients were also chosen to be linear in the volumetric strain and are in fact just scaled by multiples of 10 from each other. The additional unloading bulk moduli were chosen to be linear in the relative volume. The following table lists the (truncated) values of the input coefficients for each of the cubes in the testing of EOS Form 12.

Table 62. Suite of test input coefficients for EOS Form 12

Cube									
1	ε_v	-6.19e-2	-4.08e-2	-2.02e-2	0.00	1.98e-2	3.92e-2	5.83e-2	7.70e-2
1	$C(\varepsilon_v)$	6.19e-4	4.08e-4	2.02e-4	0.00	-1.98e-4	-3.92e-4	-5.83e-4	-7.70e-4
1	$T(\varepsilon_v)$	61.9	40.8	20.2	0.00	-19.8	-39.2	-58.3	-77.0
1	γ	0.0							
1	$K(\varepsilon_v)$	0.018	0.016	0.014	0.012	0.010	0.008	0.006	0.004
2	ε_v	-6.19e-2	-4.08e-2	-2.02e-2	0.00	1.98e-2	3.92e-2	5.83e-2	7.70e-2
2	$C(\varepsilon_v)$	6.19e-10	4.08e-10	2.02e-10	0.00	-1.98e-10	-3.92e-10	-5.83e-10	-7.70e-10
2	$T(\varepsilon_v)$	61.9	40.8	20.2	0.00	-19.8	-39.2	-58.3	-77.0
2	γ	0.01							
2	$K(\varepsilon_v)$	0.018	0.016	0.014	0.012	0.010	0.008	0.006	0.004
3	ε_v	-6.19e-2	-4.08e-2	-2.02e-2	0.00	1.98e-2	3.92e-2	5.83e-2	7.70e-2
3	$C(\varepsilon_v)$	6.19e-4	4.08e-4	2.02e-4	0.00	-1.98e-4	-3.92e-4	-5.83e-4	-7.70e-4
3	$T(\varepsilon_v)$	61.9	40.8	20.2	0.00	-19.8	-39.2	-58.3	-77.0
3	γ	0.01							
3	$K(\varepsilon_v)$	0.018	0.016	0.014	0.012	0.010	0.008	0.006	0.004

The two terms in the equation-of-state were tested (almost) independently, given the requirement on the $C(\varepsilon_v)$ coefficients, then the full equation-of-state model was tested. The following plot displays the pressures from the first two terms, as returned by the code, as a function of time for this simulation.

Figure 28. Code pressures for the two terms of EOS Form 12 as a function of time



As the plot demonstrates, not only are both terms contributing pressures on the order of $6x10^{-4}$ at the peak of the compression, but the contributions of the two terms are nearly identical.

The following observations may be made from the plot. Both terms contribute an increase in the pressure as the cubes are compressed and both exhibit a decrease in pressure as the cubes are expanded, as expected. In addition, given the choice of input coefficients, the pressure of both cubes should be zero at the beginning of the simulation and this behavior is also observed. Finally, although not obvious from the plot, the slope of the unloading/reloading lines differ from the slope of the monotonic path, which is expected given the choice of input coefficients. Therefore, at least qualitatively, the code output is behaving as expected.

Using the normalized difference defined by equation 1, the agreement between the pressures for the second term as calculated using the reference expression and the results returned by the code is demonstrated in the following table as a function of time, using the expected value for the bulk unloading modulus.

Table 63. Reference and Code Pressures for the second term of EOS Form 12

Time	*Reference Pressure*	*Code Pressure*	*(Reference - Code)/Code*
0.00E+00	0.00000000E+00	0.00000000E+00	0.0000000000E+00
1.00E-03	1.20327020E-04	1.20326954E-04	5.5165968782E-07
2.00E-03	2.41654811E-04	2.41654556E-04	1.0560400266E-06
3.00E-03	1.54479117E-04	1.54498319E-04	-1.2428370418E-04
4.00E-03	6.76014836E-05	6.76397286E-05	-5.6542275342E-04
5.00E-03	-1.89782171E-05	-1.89209665E-05	3.0257775732E-03
6.00E-03	6.76014835E-05	6.76396618E-05	-5.6443717434E-04
7.00E-03	1.54479117E-04	1.54498165E-04	-1.2329029940E-04
8.00E-03	2.41654812E-04	2.41654683E-04	5.3282005686E-07
9.00E-03	3.02856625E-04	3.02856435E-04	6.2538061024E-07

1.00E-02	3.64504043E-04	3.64503763E-04	7.6994413897E-07
1.10E-02	4.26662669E-04	4.26662290E-04	8.8843537444E-07
1.20E-02	3.27605963E-04	3.27614589E-04	-2.6330795027E-05
1.30E-02	2.28989226E-04	2.29006114E-04	-7.3744224565E-05
1.40E-02	1.30812541E-04	1.30837676E-04	-1.9211113496E-04
1.50E-02	3.30759851E-05	3.31093528E-05	-1.0078029773E-03
1.60E-02	-6.42203653E-05	-6.41787843E-05	6.4789400277E-04
1.70E-02	-1.61076437E-04	-1.61026658E-04	3.0913682005E-04
1.80E-02	-6.42203656E-05	-6.41786784E-05	6.4954971629E-04
1.90E-02	3.30759839E-05	3.31092989E-05	-1.0062148624E-03
2.00E-02	1.30812538E-04	1.30837465E-04	-1.9051407712E-04
2.10E-02	2.28989221E-04	2.29005744E-04	-7.2151479788E-05
2.20E-02	3.27605955E-04	3.27614051E-04	-2.4712328103E-05
2.30E-02	4.26662658E-04	4.26662288E-04	8.6785207049E-07
2.40E-02	4.89398502E-04	4.89398028E-04	9.7014850584E-07
2.50E-02	5.52778113E-04	5.52777717E-04	7.1650450587E-07
2.60E-02	6.16868668E-04	6.16867951E-04	1.1614321975E-06
2.70E-02	5.05542241E-04	5.05550085E-04	-1.5515119336E-05
2.80E-02	3.94820409E-04	3.94835353E-04	-3.7848220107E-05
2.90E-02	2.84703298E-04	2.84725339E-04	-7.7413835043E-05
3.00E-02	1.75191019E-04	1.75220144E-04	-1.6622256211E-04
3.10E-02	6.62836756E-05	6.63198740E-05	-5.4581536632E-04
3.20E-02	1.75191018E-04	1.75219759E-04	-1.6402970454E-04
3.30E-02	2.84703295E-04	2.84724714E-04	-7.5227342288E-05
3.40E-02	3.94820403E-04	3.94834477E-04	-3.5645092011E-05
3.50E-02	5.05542230E-04	5.05548936E-04	-1.3264057397E-05
3.60E-02	6.16868651E-04	6.16867944E-04	1.1464656177E-06

As the table demonstrates, the agreement between the reference expression and the code results is very good along the monotonic portion of the loading line, where the agreement is better than about 4 parts in 10^6. However, the agreement along the unloading/reloading lines is dramatically poorer, with the agreement being as poor as 1 part in 10^3. This appears to be due to the code using a slightly different value for the bulk unloading modulus than was used in the reference model, since if the differences along the unloading/reloading lines are minimized in the reference model, the agreement improves dramatically, as demonstrated in the following table.

Table 64. Reference and Code Pressures for the second term of EOS Form 12 using min K(ε_v)

Time	*Reference Pressure*	*Code Pressure*	*(Reference - Code)/Code*
0.00E+00	0.00000000E+00	0.00000000E+00	0.0000000000E+00
1.00E-03	1.20327020E-04	1.20326954E-04	5.5165968782E-07

2.00E-03	2.41654811E-04	2.41654556E-04	1.0560400266E-06
3.00E-03	1.54498236E-04	1.54498319E-04	-5.3259227009E-07
4.00E-03	6.76396838E-05	6.76397286E-05	-6.6225899356E-07
5.00E-03	-1.89209742E-05	-1.89209665E-05	4.1003799156E-07
6.00E-03	6.76396837E-05	6.76396618E-05	3.2387776179E-07
7.00E-03	1.54498236E-04	1.54498165E-04	4.6093553743E-07
8.00E-03	2.41654812E-04	2.41654683E-04	5.3282005686E-07
9.00E-03	3.02856625E-04	3.02856435E-04	6.2538061024E-07
1.00E-02	3.64504043E-04	3.64503763E-04	7.6994413897E-07
1.10E-02	4.26662669E-04	4.26662290E-04	8.8843537444E-07
1.20E-02	3.27614331E-04	3.27614589E-04	-7.8906619122E-07
1.30E-02	2.29005945E-04	2.29006114E-04	-7.3847005042E-07
1.40E-02	1.30837594E-04	1.30837676E-04	-6.3087877714E-07
1.50E-02	3.31093552E-05	3.31093528E-05	7.2771293959E-08
1.60E-02	-6.41786946E-05	-6.41787843E-05	-1.3965384413E-06
1.70E-02	-1.61026483E-04	-1.61026658E-04	-1.0887717475E-06
1.80E-02	-6.41786949E-05	-6.41786784E-05	2.5810385343E-07
1.90E-02	3.31093540E-05	3.31092989E-05	1.6625258343E-06
2.00E-02	1.30837591E-04	1.30837465E-04	9.6648897232E-07
2.10E-02	2.29005940E-04	2.29005744E-04	8.5439257739E-07
2.20E-02	3.27614323E-04	3.27614051E-04	8.2944266878E-07
2.30E-02	4.26662658E-04	4.26662288E-04	8.6785207049E-07
2.40E-02	4.89398502E-04	4.89398028E-04	9.7014850584E-07
2.50E-02	5.52778113E-04	5.52777717E-04	7.1650450587E-07
2.60E-02	6.16868668E-04	6.16867951E-04	1.1614321975E-06
2.70E-02	5.05549505E-04	5.05550085E-04	-1.1479558303E-06
2.80E-02	3.94834921E-04	3.94835353E-04	-1.0940048037E-06
2.90E-02	2.84725043E-04	2.84725339E-04	-1.0395698054E-06
3.00E-02	1.75219984E-04	1.75220144E-04	-9.1705199078E-07
3.10E-02	6.63198451E-05	6.63198740E-05	-4.3702065217E-07
3.20E-02	1.75219983E-04	1.75219759E-04	1.2761687729E-06
3.30E-02	2.84725040E-04	2.84724714E-04	1.1470906924E-06
3.40E-02	3.94834915E-04	3.94834477E-04	1.1092048453E-06
3.50E-02	5.05549494E-04	5.05548936E-04	1.1031387627E-06
3.60E-02	6.16868651E-04	6.16867944E-04	1.1464656177E-06

As this table demonstrates, the agreement along the unloading/reloading portions of the curves has, in general, improved by about an order of magnitude. This improvement, while somewhat less than that observed in the testing of EOS Form 8, is achieved in the same manner by changing the value used for the bulk unloading modulus along the unloading/reloading curves by the amounts given in the following table.

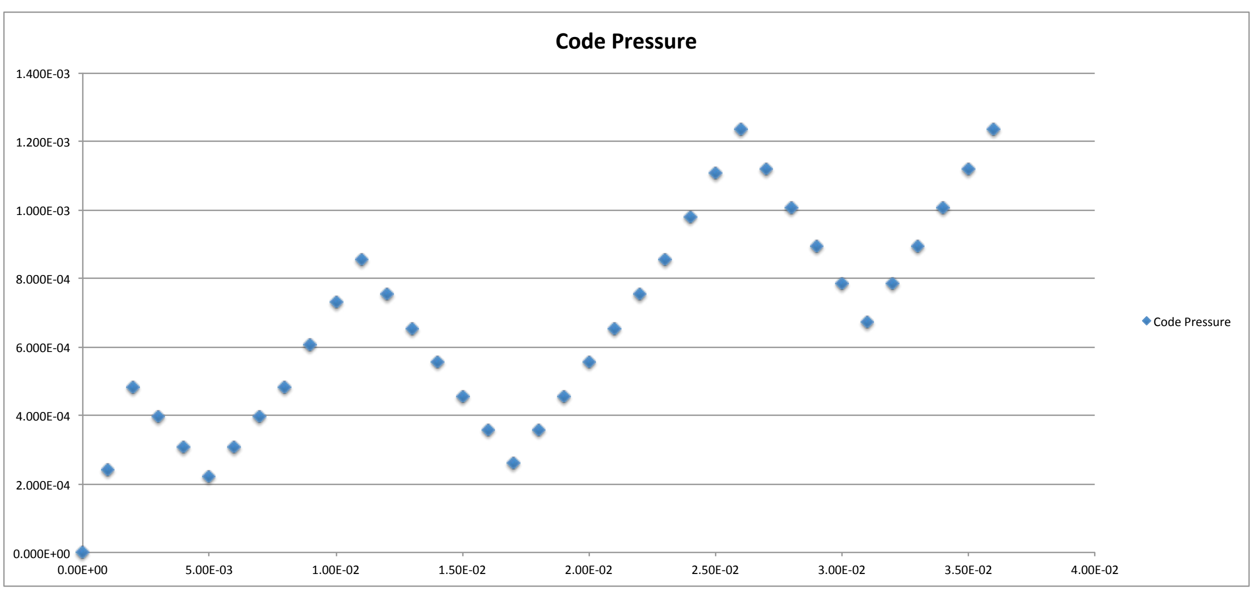
Table 65. Expected and minimizing values of $K(\varepsilon_v)$ for the second term of EOS Form 12

Expected $K(\varepsilon_v)$	Minimizing $K(\varepsilon_v)$	(Min - Expected)/Expected
0.014381	0.014377687	-2.20032E-04
0.016141	0.016140098	-8.52778E-05
0.017881	0.017879612	-6.64150E-05

As the table demonstrates, a small change in the value of the bulk unloading modulus (less than 3 parts in 10^4) results in a considerable improvement in the agreement between the reference pressures and the code results. This implies that even though the input to the code was chosen such that the unloading points corresponded to input values of $K(\varepsilon_v)$, the interpolation routine returned values for the bulk unloading modulus that differed slightly from the input values. A difference this small in the returned value from an interpolation routine is not surprising. It is worth noting that as in the testing of EOS Forms 8 and 9, the agreement between the reference expression and the code results for the first term is significantly better than that exhibited by the second term (approximately 5 orders of magnitude better), which is most likely due to the numerical integration of the internal energy, as will be demonstrated below. Note that since the pressure due to the first term is not dependent on the internal energy, it is unaffected by the code's determination of the internal energy. It is also worth noting that the improvement in the agreement between the reference model and the code results is nearly the same in the testing of EOS Form 12 as that observed in the testing of EOS Forms 8 and 9.

Now that the behavior of the pressure resulting from each of the individual terms in the expression for Equation-of-State Form 12 has been investigated, the behavior of the full expression can be examined. The following plot displays the pressure returned by the code as a function of time for EOS Form 12.

Figure 29. Code pressures for EOS Form 12 as a function of time



Note that the pressure is behaving as one would expect, in that the pressure increases as the cube is compressed and decreases as the compression is released. In addition, the initial pressure is zero, as expected from the choice of input coefficients.

The following table compares the pressure returned by the code as a function of time for the full expression for Equation-of-State Form 12 to that predicted by the reference expression.

Table 66. Reference and Code Pressures for Equation-of-State Form 12

Time	*Reference Pressure*	*Code Pressure*	*(Reference - Code)/Code*
0.00E+00	0.00000000E+00	0.000000000E+00	0.0000000000E+00
1.00E-03	2.40653800E-04	2.406536672E-04	5.5209347528E-07
2.00E-03	4.83309140E-04	4.833086291E-04	1.0564150708E-06
3.00E-03	3.95789183E-04	3.958085045E-04	-4.8816338765E-05
4.00E-03	3.08566392E-04	3.086047569E-04	-1.2431614003E-04
5.00E-03	2.21640643E-04	2.216980123E-04	-2.5877448399E-04
6.00E-03	3.08566392E-04	3.086044520E-04	-1.2332808477E-04
7.00E-03	3.95789183E-04	3.958081106E-04	-4.7821068434E-05
8.00E-03	4.83309140E-04	4.833088822E-04	5.3294141551E-07
9.00E-03	6.05712643E-04	6.057122641E-04	6.2536941474E-07
1.00E-02	7.29007356E-04	7.290067950E-04	7.6989159052E-07
1.10E-02	8.53324483E-04	8.533237251E-04	8.8834936468E-07
1.20E-02	7.53214264E-04	7.532232344E-04	-1.1910019423E-05
1.30E-02	6.53542357E-04	6.535595840E-04	-2.6359147517E-05
1.40E-02	5.54308861E-04	5.543343329E-04	-4.5951133343E-05
1.50E-02	4.55513870E-04	4.555475808E-04	-7.3999635316E-05
1.60E-02	3.57157479E-04	3.571994059E-04	-1.1737760775E-04
1.70E-02	2.59239775E-04	2.592898969E-04	-1.9330249369E-04
1.80E-02	3.57157479E-04	3.571988179E-04	-1.1573167302E-04
1.90E-02	4.55513870E-04	4.555468292E-04	-7.2349997803E-05
2.00E-02	5.54308861E-04	5.543334298E-04	-4.4322006088E-05
2.10E-02	6.53542357E-04	6.535585230E-04	-2.4735674298E-05
2.20E-02	7.53214264E-04	7.532219911E-04	-1.0259405225E-05
2.30E-02	8.53324483E-04	8.533237132E-04	9.0220283562E-07
2.40E-02	9.78796059E-04	9.787950667E-04	1.0139321503E-06
2.50E-02	1.10555517E-03	1.105554318E-03	7.7154801360E-07
2.60E-02	1.23373617E-03	1.233734657E-03	1.2295921558E-06
2.70E-02	1.12025471E-03	1.120263196E-03	-7.5720586183E-06
2.80E-02	1.00737662E-03	1.007392196E-03	-1.5457695727E-05
2.90E-02	8.95102082E-04	8.951247552E-04	-2.5329711888E-05
3.00E-02	7.83431247E-04	7.834610059E-04	-3.7984137082E-05

3.10E-02	6.72364269E-04	6.724011179E-04	-5.4801549461E-05
3.20E-02	7.83431247E-04	7.834592830E-04	-3.5785165315E-05
3.30E-02	8.95102082E-04	8.951227856E-04	-2.3129343949E-05
3.40E-02	1.00737662E-03	1.007389955E-03	-1.3232919400E-05
3.50E-02	1.12025471E-03	1.120260641E-03	-5.2918074369E-06
3.60E-02	1.23373617E-03	1.233734630E-03	1.2512061875E-06

As might have been expected, given the analysis of the second term for this EOS model, the agreement between the theoretical expression and the code results is very good along the monotonic portion of the loading line, where the agreement is better than about 1 part in 10^6, which is similar to that observed in the testing of EOS Form 8. However, the agreement along the unloading/reloading lines is dramatically poorer, with the agreement being as poor as ~ 3 parts in 10^4. This appears to be due to the code using a slightly different value for the bulk unloading modulus than was used in the reference model, since if the differences along the unloading/reloading lines are minimized in the reference model, the agreement improves dramatically, as demonstrated in the following table.

Table 67. Reference and Code Pressures for EOS Form 12 using min K(ε_v)

Time	*Reference Pressure*	*Code Pressure*	*(Reference - Code)/Code*
0.00E+00	0.00000000E+00	0.000000000E+00	0.0000000000E+00
1.00E-03	2.40653800E-04	2.406536672E-04	5.5209347528E-07
2.00E-03	4.83309140E-04	4.833086291E-04	1.0564150708E-06
3.00E-03	3.95808323E-04	3.958085045E-04	-4.5749905300E-07
4.00E-03	3.08604636E-04	3.086047569E-04	-3.9320912365E-07
5.00E-03	2.21697950E-04	2.216980123E-04	-2.8207980461E-07
6.00E-03	3.08604636E-04	3.086044520E-04	5.9496859499E-07
7.00E-03	3.95808323E-04	3.958081106E-04	5.3781939879E-07
8.00E-03	4.83309140E-04	4.833088822E-04	5.3294141551E-07
9.00E-03	6.05712643E-04	6.057122641E-04	6.2536941474E-07
1.00E-02	7.29007356E-04	7.290067950E-04	7.6989159052E-07
1.10E-02	8.53324483E-04	8.533237251E-04	8.8834936468E-07
1.20E-02	7.53222632E-04	7.532232344E-04	-7.9996137089E-07
1.30E-02	6.53559077E-04	6.535595840E-04	-7.7649941616E-07
1.40E-02	5.54333915E-04	5.543343329E-04	-7.5393051873E-07
1.50E-02	4.55547243E-04	4.555475808E-04	-7.4241160982E-07
1.60E-02	3.57199152E-04	3.571994059E-04	-7.1105985819E-07
1.70E-02	2.59289733E-04	2.592898969E-04	-6.3150779575E-07
1.80E-02	3.57199152E-04	3.571988179E-04	9.3506692582E-07
1.90E-02	4.55547243E-04	4.555468292E-04	9.0734675990E-07
2.00E-02	5.54333915E-04	5.543334298E-04	8.7527037146E-07

2.10E-02	6.53559077E-04	6.535585230E-04	8.4701533636E-07
2.20E-02	7.53222632E-04	7.532219911E-04	8.5067116574E-07
2.30E-02	8.53324483E-04	8.533237132E-04	9.0220283562E-07
2.40E-02	9.78796059E-04	9.787950667E-04	1.0139321503E-06
2.50E-02	1.10555517E-03	1.105554318E-03	7.7154801360E-07
2.60E-02	1.23373617E-03	1.233734657E-03	1.2295921558E-06
2.70E-02	1.12026199E-03	1.120263196E-03	-1.0739929891E-06
2.80E-02	1.00739117E-03	1.007392196E-03	-1.0201442935E-06
2.90E-02	8.95123876E-04	8.951247552E-04	-9.8197860284E-07
3.00E-02	7.83460276E-04	7.834610059E-04	-9.3117621903E-07
3.10E-02	6.72400519E-04	6.724011179E-04	-8.8996502543E-07
3.20E-02	7.83460276E-04	7.834592830E-04	1.2678770298E-06
3.30E-02	8.95123876E-04	8.951227856E-04	1.2184429118E-06
3.40E-02	1.00739117E-03	1.007389955E-03	1.2046641544E-06
3.50E-02	1.12026199E-03	1.120260641E-03	1.2062730098E-06
3.60E-02	1.23373617E-03	1.233734630E-03	1.2512061875E-06

As this table demonstrates, the agreement along the unloading/reloading portions of the curves has improved dramatically, with the agreement now being better by orders of magnitude, just as observed in the testing of EOS Form 8. This improvement is achieved by changing the value used for the bulk unloading modulus along the unloading/reloading curves by the amounts given in the following table.

Table 68. Expected and minimizing values of $K(\varepsilon_v)$ for EOS Form 12

Expected $K(\varepsilon_v)$	Minimizing $K(\varepsilon_v)$	(Min - Expected)/Expected
0.014381	0.014377683	-2.202795863E-04
0.016141	0.016140098	-8.528302341E-05
0.017881	0.01787961	-6.656329659E-05

As the table demonstrates, the changes in the value of the bulk unloading modulus are very small and result in a dramatic improvement in the agreement between the reference pressures and the code results, as was observed in the previous testing. This implies that even though the input to the code was chosen such that the unloading points corresponded to input values of $K(\varepsilon_v)$, the interpolation routine returned values for the bulk unloading modulus that differed slightly from the input values. A difference this small in the returned value from an interpolation routine is not surprising. It is also worth noting that the values used for the full expression of EOS Form 12 are essentially identical to those used for the analysis of the second term of this equation-of-state model. This is not a surprise, as the non-linear behavior along the unloading/reloading curve is due to the evolution of the internal energy and this term is the same in both cubes.

The code results for the internal energy can also be examined for this equation-of-state model. As the pressure for the first term is independent of the internal energy, we shall concentrate on the behavior of the second term and the full expression for this EOS model. Given the form for the pressure along the unloading/reloading lines, there is no simple closed form solution for the internal energy along these lines and so the code results will be compared to those obtained from a simple numerical integration performed in EXCEL (*Reference Energy)*. The following table makes this comparison for the second term in EOS Form 12 using the minimized value for $K(\varepsilon_v)$.

Table 69. Reference and Code Internal Energies for the second term of EOS Form 12

Time	Code (GRIZ)	*Reference Energy*	(*Reference* - GRIZ)/GRIZ
0.00E+00	1.00000000E-03	1.00000000E-03	0.000000E+00
1.00E-03	1.00071700E-03	1.00071738E-03	3.792183E-07
2.00E-03	1.00286100E-03	1.00286108E-03	7.576553E-08
3.00E-03	1.00168900E-03	1.00168952E-03	5.180532E-07
4.00E-03	1.00103000E-03	1.00103007E-03	7.287402E-08
5.00E-03	1.00088500E-03	1.00088511E-03	1.131035E-07
6.00E-03	1.00103000E-03	1.00103007E-03	7.250348E-08
7.00E-03	1.00168900E-03	1.00168952E-03	5.176827E-07
8.00E-03	1.00286100E-03	1.00286108E-03	7.744130E-08
9.00E-03	1.00446500E-03	1.00446502E-03	1.693502E-08
1.00E-02	1.00642300E-03	1.00642294E-03	-5.954258E-08
1.10E-02	1.00873500E-03	1.00873474E-03	-2.546050E-07
1.20E-02	1.00653100E-03	1.00653077E-03	-2.253202E-07
1.30E-02	1.00489800E-03	1.00489786E-03	-1.408413E-07
1.40E-02	1.00383800E-03	1.00383808E-03	8.419717E-08
1.50E-02	1.00335400E-03	1.00335352E-03	-4.791312E-07
1.60E-02	1.00344600E-03	1.00344621E-03	2.120758E-07
1.70E-02	1.00411800E-03	1.00411820E-03	1.965543E-07
1.80E-02	1.00344600E-03	1.00344621E-03	2.113500E-07
1.90E-02	1.00335400E-03	1.00335352E-03	-4.820295E-07
2.00E-02	1.00383800E-03	1.00383808E-03	7.769001E-08
2.10E-02	1.00489800E-03	1.00489785E-03	-1.523779E-07
2.20E-02	1.00653100E-03	1.00653076E-03	-2.432864E-07
2.30E-02	1.00873500E-03	1.00873472E-03	-2.803757E-07
2.40E-02	1.01140100E-03	1.01140064E-03	-3.511651E-07
2.50E-02	1.01442100E-03	1.01442131E-03	3.092989E-07
2.60E-02	1.01779800E-03	1.01779768E-03	-3.099844E-07
2.70E-02	1.01455800E-03	1.01455769E-03	-3.020986E-07
2.80E-02	1.01194800E-03	1.01194812E-03	1.226869E-07
2.90E-02	1.00997100E-03	1.00997067E-03	-3.235538E-07

3.00E-02	1.00862700E-03	1.00862701E-03	9.759291E-09
3.10E-02	1.00791900E-03	1.00791878E-03	-2.228285E-07
3.20E-02	1.00862700E-03	1.00862701E-03	8.632773E-09
3.30E-02	1.00997100E-03	1.00997067E-03	-3.280495E-07
3.40E-02	1.01194800E-03	1.01194811E-03	1.126015E-07
3.50E-02	1.01455800E-03	1.01455768E-03	-3.199634E-07
3.60E-02	1.01779800E-03	1.01779766E-03	-3.377797E-07

As the table demonstrates, the level of agreement between the EXCEL numerical integration and the code results for the internal energy is better than ~ 5 parts in 10^7, which is about as good as can be expected, given the limitations on the GRIZ output. This establishes that the internal energies being returned by the code are reasonable for the second term in EOS Form 12.

There is also no simple closed form solution for the internal energy due to the full expression for Equation-of-State Form 12. A numerical integration was performed in EXCEL (*Reference Energy)* to compare against the code results. The following table gives the result of that comparison using the minimized value for $K(\varepsilon_v)$.

Table 70. Reference and Code Internal Energies for EOS Form 12

Time	Code (GRIZ)	*Reference Energy*	(*Reference* - GRIZ)/GRIZ
0.00E+00	1.00000000E-03	1.00000000E-03	0.000000E+00
1.00E-03	1.00143500E-03	1.00143476E-03	-2.421068E-07
2.00E-03	1.00572200E-03	1.00572215E-03	1.454104E-07
3.00E-03	1.00312200E-03	1.00312191E-03	-9.254975E-08
4.00E-03	1.00103000E-03	1.00103007E-03	6.820907E-08
5.00E-03	9.99449100E-04	9.99449012E-04	-8.786879E-08
6.00E-03	1.00103000E-03	1.00103007E-03	6.820937E-08
7.00E-03	1.00312200E-03	1.00312191E-03	-9.217973E-08
8.00E-03	1.00572200E-03	1.00572215E-03	1.457803E-07
9.00E-03	1.00893000E-03	1.00893002E-03	2.190173E-08
1.00E-02	1.01284600E-03	1.01284586E-03	-1.339746E-07
1.10E-02	1.01746900E-03	1.01746947E-03	4.578674E-07
1.20E-02	1.01277500E-03	1.01277473E-03	-2.661050E-07
1.30E-02	1.00864700E-03	1.00864713E-03	1.316312E-07
1.40E-02	1.00508900E-03	1.00508880E-03	-2.013634E-07
1.50E-02	1.00210200E-03	1.00210183E-03	-1.671981E-07
1.60E-02	9.99688300E-04	9.99688327E-04	2.710428E-08
1.70E-02	9.97850300E-04	9.97850354E-04	5.373789E-08
1.80E-02	9.99688300E-04	9.99688327E-04	2.710514E-08
1.90E-02	1.00210200E-03	1.00210183E-03	-1.671964E-07
2.00E-02	1.00508900E-03	1.00508880E-03	-2.013609E-07

2.10E-02	1.00864700E-03	1.00864713E-03	1.316345E-07
2.20E-02	1.01277500E-03	1.01277473E-03	-2.661008E-07
2.30E-02	1.01746900E-03	1.01746947E-03	4.578724E-07
2.40E-02	1.02280100E-03	1.02280134E-03	3.278069E-07
2.50E-02	1.02884300E-03	1.02884269E-03	-3.011130E-07
2.60E-02	1.03559500E-03	1.03559545E-03	4.364424E-07
2.70E-02	1.02880000E-03	1.02879978E-03	-2.186758E-07
2.80E-02	1.02263200E-03	1.02263250E-03	4.922528E-07
2.90E-02	1.01709500E-03	1.01709541E-03	4.061334E-07
3.00E-02	1.01219000E-03	1.01219025E-03	2.495096E-07
3.10E-02	1.00791900E-03	1.00791874E-03	-2.553281E-07
3.20E-02	1.01219000E-03	1.01219025E-03	2.495113E-07
3.30E-02	1.01709500E-03	1.01709541E-03	4.061369E-07
3.40E-02	1.02263200E-03	1.02263250E-03	4.922579E-07
3.50E-02	1.02880000E-03	1.02879978E-03	-2.186691E-07
3.60E-02	1.03559500E-03	1.03559545E-03	4.364507E-07

As the table demonstrates, the level of agreement between the EXCEL numerical integration and the code results for the internal energy is better than ~ 5 parts in 10^7, which is similar to that exhibited by the second term of this EOS model.

This establishes the implementation of Equation-of-State Form 12 in DYNA3D. The equation-of-state is performing as expected, in that the pressure in the cubes increases as they are compressed and decreases as they are expanded. The behavior of each of the terms in the equation-of-state has been examined and found to be performing as expected and with reasonable accuracy. The behavior of the equation-of-state as a whole has been examined and is performing as expected and with reasonable accuracy.

It is interesting to note that the results achieved in this testing are essentially the same as those obtained in the testing of EOS Form 8, which is essentially the same equation-of-state. Therefore, the change in the material model has had little, if any, impact on the EOS results.

Equation-of-State Form 13

Equation-of-State Form 13 is used to calculate the shock initiation and detonation wave propagation of solid high explosives. It serves as an alternative to the programmed burn options available in the code. This equation-of-state must be used only with Material Type 9 or 10.

This equation-of-state uses a JWL equation to describe both the unreacted explosive (designated by a subscript 'e') and the reaction products (denoted by a subscript 'p'). The pressure in the unreacted explosive is given by

$$p_e = R_{1e} e^{-R_{5e} V_e} + R_{2e} e^{-R_{6e} V_e} + R_{3e} \frac{T_e}{V_e}$$

where p is the pressure, V is the relative volume and T is the temperature. R_{3e} is a constant related to the specific heat c_{ve} and the JWL parameter ω by

$$R_{3e} = \omega_e c_{ve}.$$

The pressure in the reaction products is given by a similar JWL equation

$$p_p = R_{1p} e^{-R_{5p} V_p} + R_{2p} e^{-R_{6p} V_p} + R_{3p} \frac{T_p}{V_p}$$

where p is the pressure, V is the relative volume and T is the temperature. R_{3p} is a constant related to the specific heat c_{vp} and the JWL parameter ω by

$$R_{3p} = \omega_p c_{vp}.$$

As the unreacted explosive is converted to reaction products, these two JWL equations are used to calculate the pressure of the mixture. The mixture is defined by the reacted fraction, F, where $F = 0$ indicates no reactions have occurred (all unreacted explosive) and $F = 1$ indicates complete reaction (all reaction products). The temperatures and pressures of the reactants and products are assumed to be in equilibrium ($T_e = T_p$ and $p_e = p_p$) and the relative volumes are additive

$$V = (1-F)V_e + V_p.$$

Author's Note: This equation is taken from the manual version dated June, 2013. If the definitions given in the paper by Cochran and Chan[7] *are followed, this equation for the volumes is*

[7]Cochran and Chan, Shock Initiation and Detonation Models in 1 and 2 Dimension, UCID-18024, 1979.

incorrect. It should read $V=(1-F)V_e + FV_p$*, and is being corrected in the code manual.*

The reacted fraction, F, is defined by three terms: an ignition term which models the conversion of a small amount of explosive into reaction products after being compressed by the shock wave, a slow growth term which models the spread of this initial reaction and a rapid completion term that dominates at high pressure and temperature. This leads to the following form for the reaction rate

$$\frac{\partial F}{\partial t} = \dot{F}_1 + \dot{F}_2 + \dot{F}_3$$

where the ignition term is given by

$$\dot{F}_1 = F_q (1-F)^{F_r} \left[\frac{1}{V_e} - 1 - C_{crit} \right]^{\eta},$$

the growth term is given by

$$\dot{F}_2 = G_1 (1-F)^{s_1} F^{a_1} p^m,$$

the completion term is given by

$$\dot{F}_3 = G_2 (1-F)^{s_2} F^{a_2} p^n,$$

and F_q, F_r, C_{crit}, η, G_1, s_1, a_1, m, G_2, s_2, a_2, and n are given constants. The ignition term is set to zero when $F \geq F_{max,ig}$, the growth term is set to zero when $F \geq F_{max,gr}$, and the completion term is set to zero when $F \leq F_{min,gr}$, where these three limits are also input parameters.

Testing of this equation-of-state model will be performed using 12 cubes. The JWL equation for the unreacted explosive will be tested using the first four cubes, with the growth parameters set to zero. The first three cubes will test the three individual terms and the fourth cube will test the entire expression. The JWL equation for the reaction products will be tested using cubes 5 through 8 with the growth parameters made large enough to convert all of the unreacted explosive to reaction products essentially instantaneously. The first three cubes will test the three individual terms and the fourth cube will test the entire expression. The final four cubes will be used to test a modification of the equation-of-state model for a representative material. The first three cubes will test each of the growth terms individually and the fourth cube will test the three terms combined. The input coefficients for the growth terms for this representative material will be modified from the known values to achieve a reasonable amount of growth for this testing considering the loading curve in use.

Prior to discussing the calculations using EOS Form 13, a few code issues need to be addressed and these are not necessarily readily apparent to the user. First, in order to eliminate issues with the work performed by the bulk viscosity, the two input coefficients for the bulk viscosity on the material card were set to 1.0e-20 in each of the 9 cubes. Failing to do so results in the work performed on the cube being dominated by contributions from the bulk viscosity. In addition, in order to test the individual terms, it is necessary to use positive R_i input coefficients in order to eliminate attempting to take the square root of a negative number to find the sound speed. Finally, the code version used for this test was version 14.2.0 revision 1.3342.

The first four cubes test the JWL equation for the unreacted explosive by setting each of the three terms in the reaction rate equation to zero. This is achieved by setting F_q, G_1 and G_2 to zero, so the reaction rate is identically zero. The following table lists the values of the input coefficients used in Cubes 1-4 for the testing of EOS Form 13.

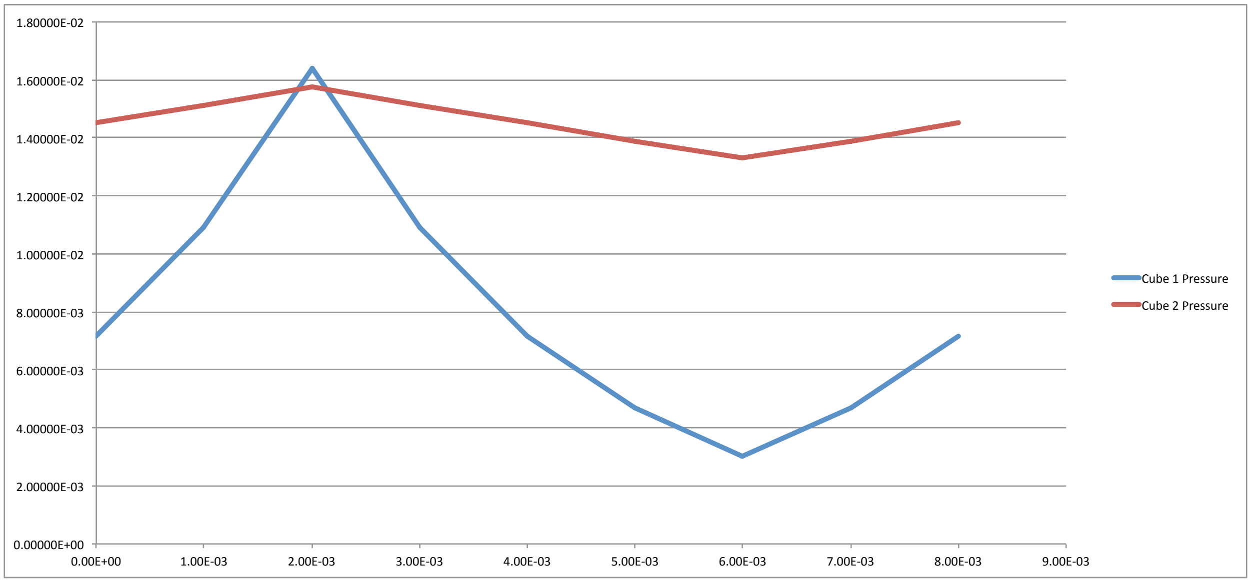
Table 71. Input coefficients for Cubes 1-4 for the reactant JWL in EOS Form 13

	Cube 1	Cube 2	Cube 3	Cube 4
R_{1p}	0	0	0	0
R_{2p}	0	0	0	0
R_{5p}	4.6	4.6	4.6	4.6
R_{6p}	1.3	1.3	1.3	1.3
F_r	0.667	0.667	0.667	0.667
R_{3p}	0	0	0	0
R_{1e}	9522.0	0	0	9522.0
R_{2e}	0	0.05944	0	-0.05944
R_{3e}	0	0	2.4656e-5	2.4656e-5
R_{5e}	14.1	14.1	14.1	14.1
R_{6e}	1.41	1.41	1.41	1.41
$F_{max,ig}$	0.3	0.3	0.3	0.3
F_q	0	0	0	0
G_1	0	0	0	0
m	1.0	1.0	1.0	1.0
a_1	0.111	0.111	0.111	0.111
s_1	0.667	0.667	0.667	0.667
c_{vp}	1.0e-5	1.0e-5	1.0e-5	1.0e-5
c_{ve}	2.7813e-5	2.7813e-5	2.7813e-5	2.7813e-5
η	20	20	20	20
C_{crit}	0	0	0	0
Q_r	0.102	0.102	0.102	0.102
T_0	298.0	298.0	298.0	298.0
G_2	0	0	0	0
a_2	1	1	1	1
s_2	0.333	0.333	0.333	0.333
n	2	2	2	2
$F_{max,gr}$	0.5	0.5	0.5	0.5

$F_{min,gr}$	0	0	0	0

The results from Cubes 1 and 2 are displayed in the following plot, which displays the pressure returned by the code as a function of time for these two cubes.

Figure 30. Code pressures for Cubes 1 and 2 for EOS Form 13 as a function of time



The following observations may be made from the plot. Both cubes exhibit an increase in the pressure as the cubes are compressed and both exhibit a decrease in pressure as the cubes are expanded, as expected. In addition, given the choice of input coefficients, the pressure of both cubes is not expected to be zero at the beginning of the simulation and this behavior is also observed. Finally, the pressure at the end of the simulation is the same as at the beginning, as expected. Therefore, at least qualitatively, the code output is behaving as expected.

Using the normalized difference defined by equation 1, the agreement between the pressure calculated using the reference expression and the code pressure for Cube 1, which tests the first term in the reactant JWL, is given in the following table.

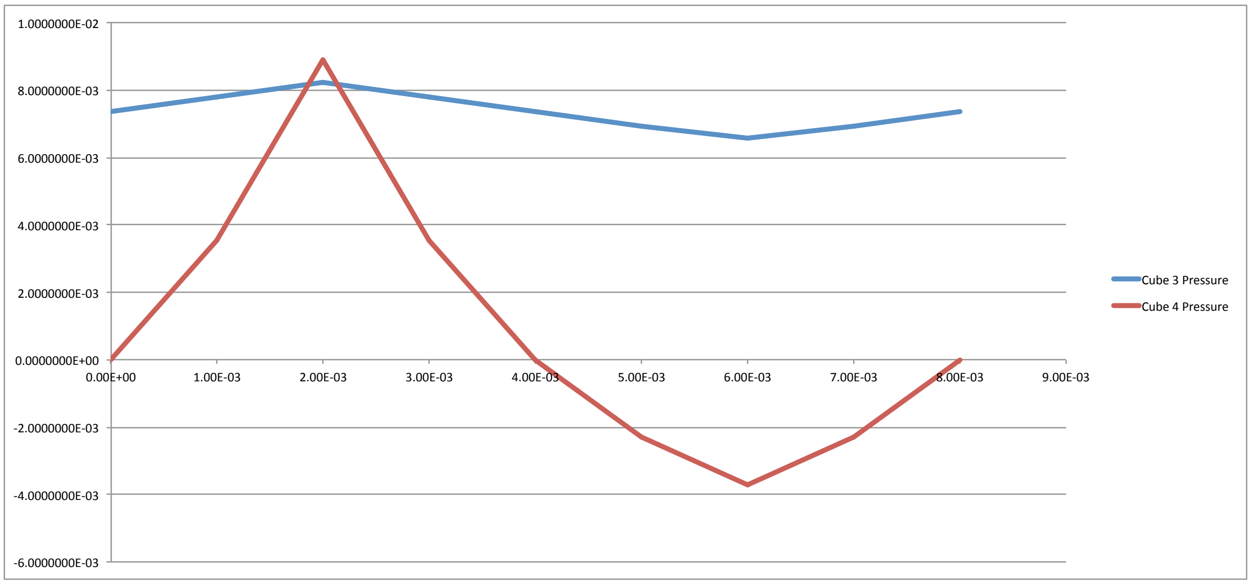
Table 72. Reference and Code Pressures for Cube 1 for the reactant JWL in EOS Form 13

Time	*Reference Pressure*	*Code Pressure*	*(Reference - Code)/Code*
0.00E+00	7.16434E-03	7.16434E-03	6.05333E-16
1.00E-03	1.08906E-02	1.08906E-02	-1.35983E-12
2.00E-03	1.64102E-02	1.64102E-02	-2.67404E-12
3.00E-03	1.08906E-02	1.08906E-02	-1.35983E-12
4.00E-03	7.16434E-03	7.16434E-03	6.05333E-16
5.00E-03	4.67333E-03	4.67333E-03	1.41946E-12
6.00E-03	3.02250E-03	3.02250E-03	2.90814E-12
7.00E-03	4.67333E-03	4.67333E-03	1.41946E-12
8.00E-03	7.16434E-03	7.16434E-03	-6.41653E-15

As the table demonstrates, the agreement between the reference expression and the code results is excellent, with the agreement being better than about 3 parts in 10^{12}. The agreement for Cube 2, which tests the second term in the JWL, is actually about an order of magnitude better than that exhibited by Cube 1.

Cube 3 tests the performance of the third term in the reactant JWL, while Cube 4 tests the full reactant JWL expression. The following plot displays the pressures returned by these cubes as a function of time for this simulation.

Figure 31. Code pressures for Cubes 3 and 4 for EOS Form 13 as a function of time



The following observations may be made from the plot. Both cubes exhibit an increase in the pressure as the cubes are compressed and both exhibit a decrease in pressure as the cubes are expanded, as expected. In addition, given the choice of input coefficients, the pressure of both cubes is not expected to be zero at the beginning of the simulation and this behavior is also observed. Finally, the pressure at the end of the simulation is the same as at the beginning, as expected. Therefore, at least qualitatively, the code output is behaving as expected.

It is interesting to note that the pressure returned by Cube 3 has essentially the same shape as a function of time as that returned by Cube 2, although the magnitude of the pressures is dramatically different. The same can be said of the pressures returned by Cubes 1 and 4. It is not clear if this reveals anything important about the behavior of this equation-of-state.

Using the normalized difference defined by equation 1, the agreement between the pressure calculated using the reference expression and the code pressure for Cube 3, which tests the third term in the reactant JWL, is given in the following table.

Table 73. Reference and Code Pressures for Cube 3 for the reactant JWL in EOS Form 13

Time	*Reference Pressure*	*Code Pressure*	*(Reference - Code)/Code*
0.00E+00	7.3474880E-03	7.3474880E-03	0.000000000E+00
1.00E-03	7.7775238E-03	7.7775246E-03	-1.093422813E-07
2.00E-03	8.2370097E-03	8.2370105E-03	-9.098005328E-08

3.00E-03	7.7775238E-03	7.7775246E-03	-1.093422774E-07
4.00E-03	7.3474880E-03	7.3474880E-03	2.715121137E-15
5.00E-03	6.9451599E-03	6.9451587E-03	1.638888395E-07
6.00E-03	6.5685022E-03	6.5685033E-03	-1.671139442E-07
7.00E-03	6.9451599E-03	6.9451587E-03	1.638888410E-07
8.00E-03	7.3474880E-03	7.3474880E-03	-1.298536196E-15

As the table demonstrates, the agreement between the reference expression and the code results is not as good as that obtained in the testing of Cubes 1 and 2, with the level of agreement being approximately 5 orders of magnitude lower. The agreement for Cube 4, which tests the full JWL expression for the reactants, is about the same. This reduction in the agreement is most likely due to the evaluation of the temperature, which now appears in the JWL for these two cubes. The temperature will be related to the internal energy, which we will see later is not well determined for these two cubes.

Cubes 5-8 test the JWL equation for the explosive products by setting each of the three terms in the reaction rate to such large values that the conversion from reactant to products is essentially instantaneous. This is achieved by setting F_q, G_1 and G_2 to values that ensure this result. Cube 5 tests the first term in the product JWL, Cube 6 the second term, Cube 7 the third term and Cube 8 the full expression. The following table lists the values of the input coefficients used in Cubes 5-8 for the testing of EOS Form 13. Note that the values for the reactant JWL are set for each cube to ensure the initial pressure is properly defined.

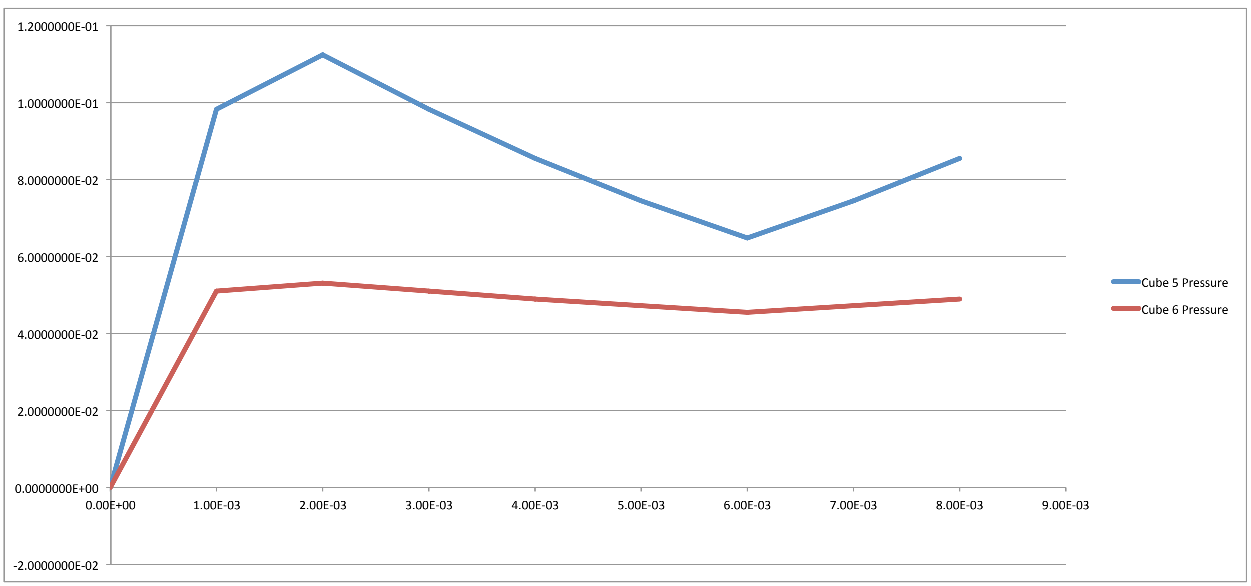
Table 74. Input coefficients for Cubes 5-8 for the product JWL in EOS Form 13

	Cube 5	Cube 6	Cube 7	Cube 8
R_{1p}	8.524	0	0	8.524
R_{2p}	0	0.1802	0	0.1802
R_{5p}	4.6	4.6	4.6	4.6
R_{6p}	1.3	1.3	1.3	1.3
F_r	0.667	0.667	0.667	0.667
R_{3p}	0	0	3.8e-6	3.8e-6
R_{1e}	9522.0	9522.0	9522.0	9522.0
R_{2e}	-0.05944	-0.05944	-0.05944	-0.05944
R_{3e}	2.4656e-5	2.4656e-5	2.4656e-5	2.4656e-5
R_{5e}	14.1	14.1	14.1	14.1
R_{6e}	1.41	1.41	1.41	1.41
$F_{max,ig}$	0.3	0.3	0.3	0.3
F_q	7.43e25	7.43e25	7.43e25	7.43e25
G_1	3.1e16	3.1e16	3.1e16	3.1e16
m	1.0	1.0	1.0	1.0
a_1	0.111	0.111	0.111	0.111

s_1	0.667	0.667	0.667	0.667
c_{vp}	1.0e-5	1.0e-5	1.0e-5	1.0e-5
c_{ve}	2.7813e-5	2.7813e-5	2.7813e-5	2.7813e-5
η	20	20	20	20
C_{crit}	0	0	0	0
Q_r	0.102	0.102	0.102	0.102
T_0	298.0	298.0	298.0	298.0
G_2	4.0e16	4.0e16	4.0e16	4.0e16
a_2	1.0	1.0	1.0	1.0
s_2	0.333	0.333	0.333	0.333
n	2	2	2	2
$F_{max,gr}$	0.5	0.5	0.5	0.5
$F_{min,gr}$	0	0	0	0

The results from Cubes 5 and 6 are displayed in the following plot, which shows the pressure returned by the code as a function of time for these two cubes.

Figure 32. Code pressures for Cubes 5 and 6 for EOS Form 13 as a function of time



The following observations may be made from the plot. Both cubes exhibit an increase in the pressure as the cubes are compressed and both exhibit a decrease in pressure as the cubes are expanded, as expected. In addition, given the choice of input coefficients, the pressure of both cubes is not expected to be zero at the beginning of the simulation and this behavior is also observed. Finally, the pressure at the end of the simulation is not the same as at the beginning, which is to be expected given that the reactants are being converted to products and this should lead to an increase in the pressure. Therefore, at least qualitatively, the code output is behaving as expected.

Using the normalized difference defined by equation 1, the agreement between the pressure calculated using the reference expression and the code pressure for Cube 5, which tests the first term in the product JWL, is given in the following table.

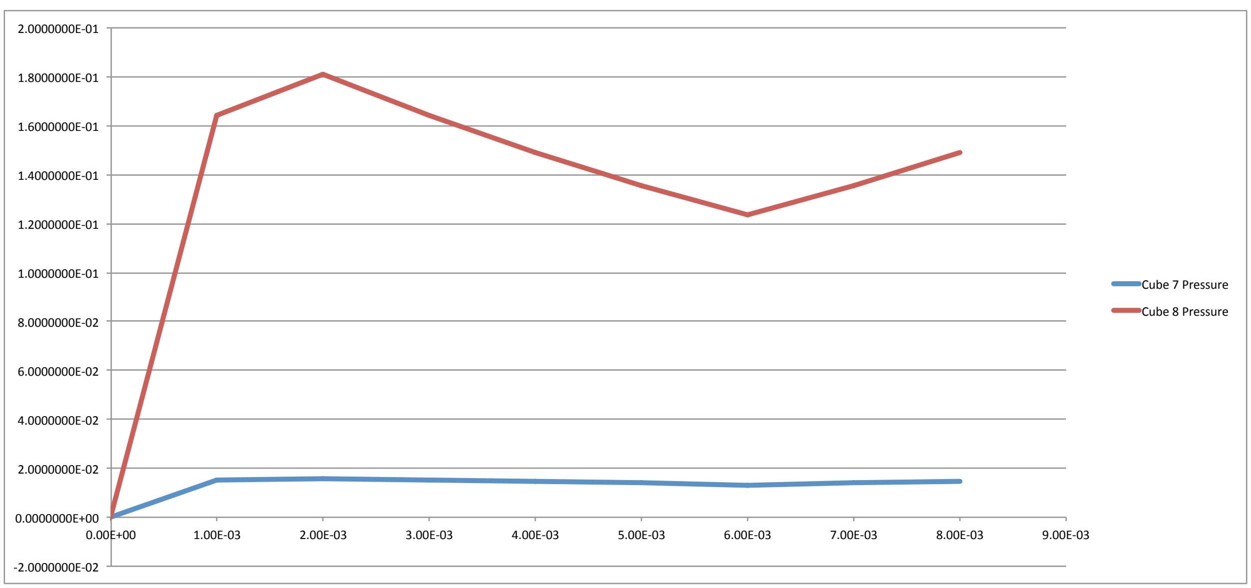
Table 75. Reference and Code Pressures for Cube 5 for the product JWL in EOS Form 13

Time	*Reference Pressure*	*Code Pressure*	*(Reference - Code)/Code*
0.00E+00	-5.214550E-08	-5.2145502E-08	0.000000000E+00
1.00E-03	9.822547E-02	9.8225474E-02	1.411719891E-12
2.00E-03	1.122833E-01	1.122833E-01	2.760273340E-12
3.00E-03	9.822547E-02	9.822547E-02	1.411719891E-12
4.00E-03	8.568185E-02	8.568185E-02	9.718129207E-16
5.00E-03	7.453407E-02	7.453407E-02	-1.462739051E-12
6.00E-03	6.465621E-02	6.465621E-02	-2.985852389E-12
7.00E-03	7.453407E-02	7.453407E-02	-1.462739051E-12
8.00E-03	8.568185E-02	8.568185E-02	-3.725282863E-15

As the table demonstrates, the agreement between the reference expression and the code results is excellent, with the agreement being better than about 3 parts in 10^{12}. The agreement for Cube 6, which tests the second term in the product JWL, is actually about an order of magnitude better than that exhibited by Cube 5.

Cube 7 tests the performance of the third term in the product JWL, while Cube 8 tests the full product JWL expression. The following plot displays the pressures returned by these cubes as a function of time for this simulation.

Figure 33. Code pressures for Cubes 7 and 8 for EOS Form 13 as a function of time



The following observations may be made from the plot. Both cubes exhibit an increase in the pressure as the cubes are compressed and both exhibit a decrease in pressure as the cubes are expanded, as expected. In addition, given the choice of input coefficients, the pressure of both cubes is not expected to be zero at the beginning of the simulation and this behavior is also observed. Finally, the pressure at the end of the simulation is not the same as at the beginning, which is to be expected given that the reactants are being converted to products and this should lead to an increase in the pressure. Therefore, at least qualitatively, the code output is behaving as expected.

Using the normalized difference defined by equation 1, the agreement between the pressure calculated using the reference expression and the code pressure for Cube 7, which tests the third term in the product JWL, is given in the following table.

Table 76. Reference and Code Pressures for Cube 7 for the product JWL in EOS Form 13

Time	*Reference Pressure*	*Code Pressure*	*(Reference - Code)/Code*
0.00E+00	-5.214550E-08	-5.2145502E-08	0.000000000E+00
1.00E-03	1.507082E-02	1.5070818E-02	-1.093989003E-07
2.00E-03	1.571709E-02	1.571709E-02	2.207679042E-08
3.00E-03	1.507082E-02	1.507082E-02	-1.093989070E-07
4.00E-03	1.445661E-02	1.445661E-02	1.000561393E-07
5.00E-03	1.387318E-02	1.387318E-02	-8.709966649E-09
6.00E-03	1.331870E-02	1.331870E-02	-2.863228938E-08
7.00E-03	1.387318E-02	1.387318E-02	-8.709973901E-09
8.00E-03	1.445661E-02	1.445661E-02	1.000561393E-07

As the table demonstrates, the agreement between the reference expression and the code results is not as good as that obtained in the testing of Cubes 5 and 6, with the level of agreement being approximately 5 orders of magnitude lower. The agreement for Cube 8, which tests the full JWL expression for the products, is actually better by about 2 orders of magnitude, which may be a result of the increased pressure for this cube. This reduction in the agreement, compared to the results for Cubes 5 and 6, is most likely due to the evaluation of the temperature, which now appears in the JWL for Cubes 7 and 8. The temperature will be related to the internal energy, which we will see later is not well determined for these two cubes.

Now that the behavior of the two individual JWL expressions has been investigated, the behavior of the full equation-of-state can be examined. This examination is performed using four cubes, one for each of the three growth terms in the reaction rate and the final one for the expression as a whole. The growth terms were set to achieve a reasonable amount of growth during the simulation, as shown in the following table.

Table 77. Input coefficients for Cubes 9-12 for EOS Form 13

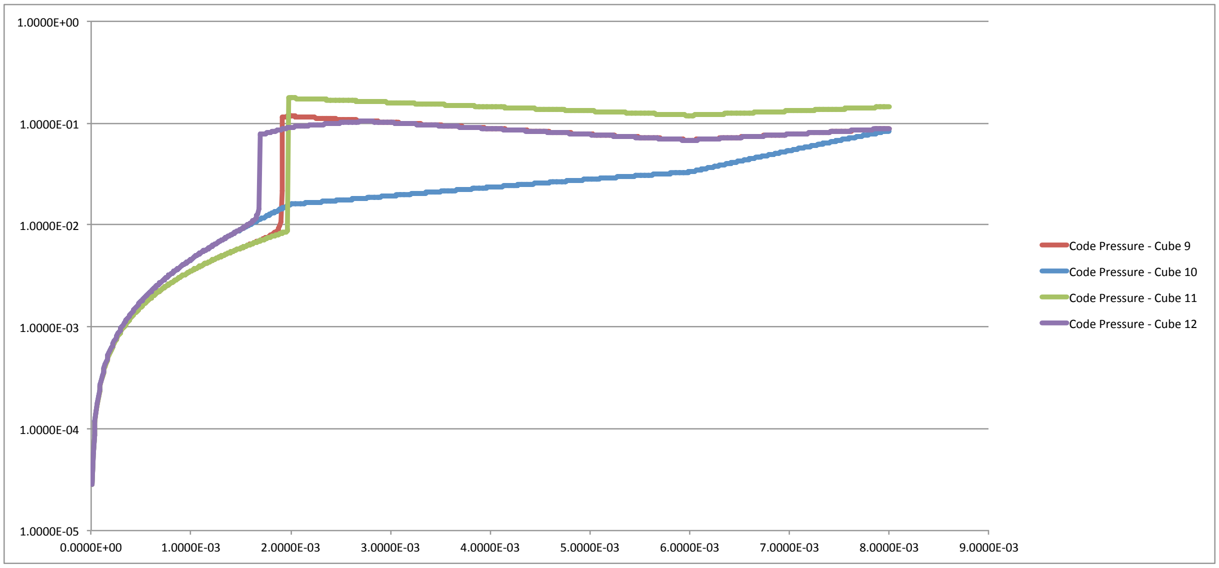
	Cube 9	Cube 10	Cube 11	Cube 12
R_{1p}	8.524	8.524	8.524	8.524
R_{2p}	0.1802	0.1802	0.1802	0.1802
R_{5p}	4.6	4.6	4.6	4.6
R_{6p}	1.3	1.3	1.3	1.3
F_r	0.667	0.667	0.667	0.667

R_{3p}	3.8e-6	3.8e-6	3.8e-6	3.8e-6
R_{1e}	9522.0	9522.0	9522.0	9522.0
R_{2e}	-0.05944	-0.05944	-0.05944	-0.05944
R_{3e}	2.4656e-5	2.4656e-5	2.4656e-5	2.4656e-5
R_{5e}	14.1	14.1	14.1	14.1
R_{6e}	1.41	1.41	1.41	1.41
$F_{max,ig}$	0.5	0.3	0.3	0.3
F_q	7.43e25	0	0	7.43e24
G_1	0	3100	0	3100
m	1.0	1.0	1.0	1.0
a_1	0.111	0.111	0.111	0.111
s_1	0.667	0.667	0.667	0.667
c_{vp}	1.0e-5	1.0e-5	1.0e-5	1.0e-5
c_{ve}	2.7813e-5	2.7813e-5	2.7813e-5	2.7813e-5
η	20	20	20	20
C_{crit}	0	0	0	0
Q_r	0.102	0.102	0.102	0.102
T_0	298.0	298.0	298.0	298.0
G_2	0	0	1.0e10	400
a_2	1.0	1.0	1.0	1.0
s_2	0.333	0.333	0.333	0.333
n	2	2	2	2
$F_{max,gr}$	0.5	0.5	0.5	0.5
$F_{min,gr}$	0	0	0	0

As the table illustrates, the growth terms were modified by changing the values of F_q, G_1 and G_2 from cube to cube to achieve a reasonable amount of growth during the simulation. The amount of growth achieved for each cube will be demonstrated later.

The following plot displays the code pressures for each of these four cubes as a function of time for this simulation.

Figure 34. Code pressures for Cubes 9-12 for EOS Form 13 as a function of time

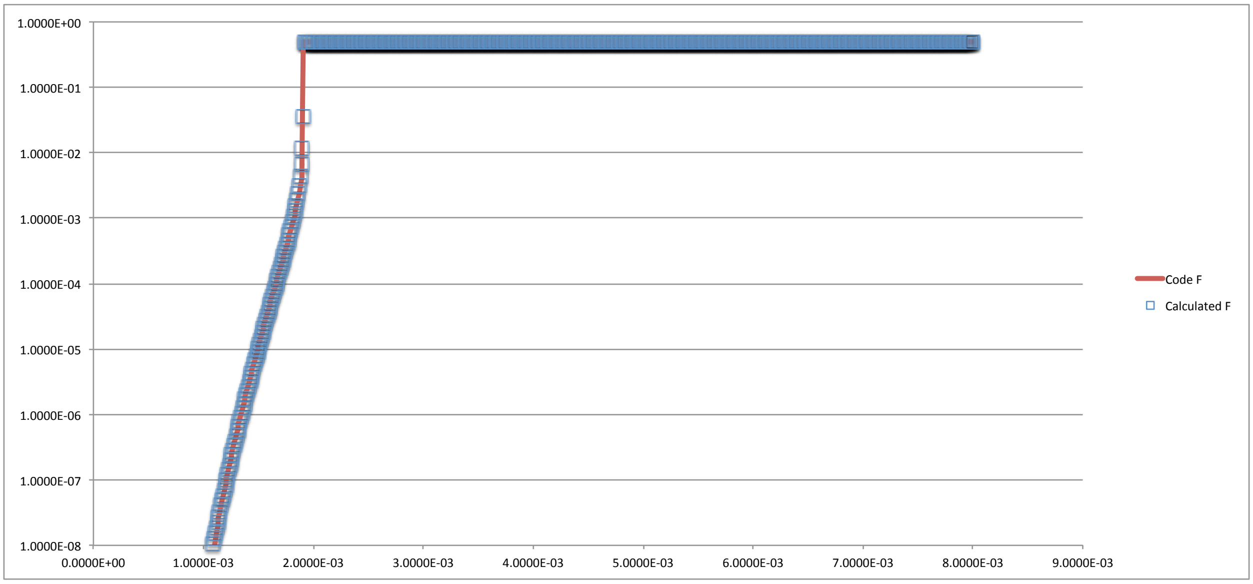


The following observations may be made from the plot. All of the cubes exhibit an increase in the pressure as the cubes are compressed and all exhibit a decrease in pressure as the cubes are expanded, as expected. In addition, Cubes 9, 11 and 12 exhibit a rapid increase in pressure during the simulation at a time when there is a rapid conversion of reactant to product. This does not occur in Cube 10 because the growth term in that cube doesn't saturate as it does in the others. Also, given the choice of input coefficients, the pressure of the cubes is not expected to be zero at the beginning of the simulation and this behavior is also observed. Finally, the pressure at the end of the simulation is not the same as at the beginning, which is to be expected given that the reactants are being converted to products and this should lead to an increase in the pressure. Therefore, at least qualitatively, the code output is behaving as expected.

Unfortunately, building a predictive spreadsheet model for this equation-of-state model does not seem to be possible. Therefore, to investigate the behavior of this EOS model, the equations governing the evolution of the reacted fraction, *F*, were entered into a spreadsheet model and this predictive model for *F* will be shown to be consistent with the code output. Solving the resulting equations is beyond the capability of a simple spreadsheet model and, therefore, the evolution of *F* was combined with the code value of β, the real volume fraction occupied by the reactants, to determine the volume fractions of the reactants and products. Using these volume fractions and the relationships for the relative volumes given in Cochran and Chan[7], the evolution of the pressure can be determined from the respective JWL equations and will be shown to be consistent with the code output. Use of the code output to determine the volume fractions means this model is not predictive but rather confirmatory.

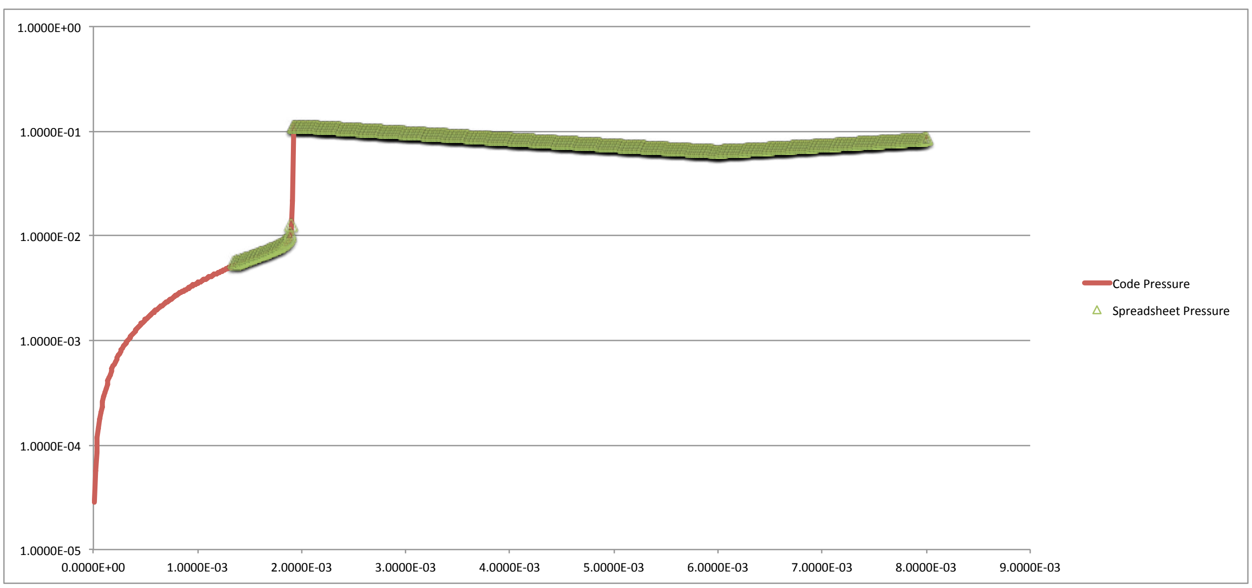
Cube 9 tests the ignition term, given by the expression for F_1, in the evolution of the reacted fraction, *F*. The following figure plots the reference result for *F* as a function of time for Cube 9, as well as the code result.

Figure 35. Time evolution of *F* for Cube 9 in EOS Form 13



As the plot clearly demonstrates, the reference model matches the code result for the evolution of *F* as a function of time, including the saturation of *F* at a value of 0.5. Using this result for *F*, the code results for β and the temperature, and the expressions for the relative volumes given in Cochran and Chan[7], the JWL equations for the reactants and products can be used to determine the pressure for this equation-of-state model. The figure below compares the reference result to that of the code for Cube 9.

Figure 36. Time evolution of the pressure **for Cube 9 in EOS Form 13**

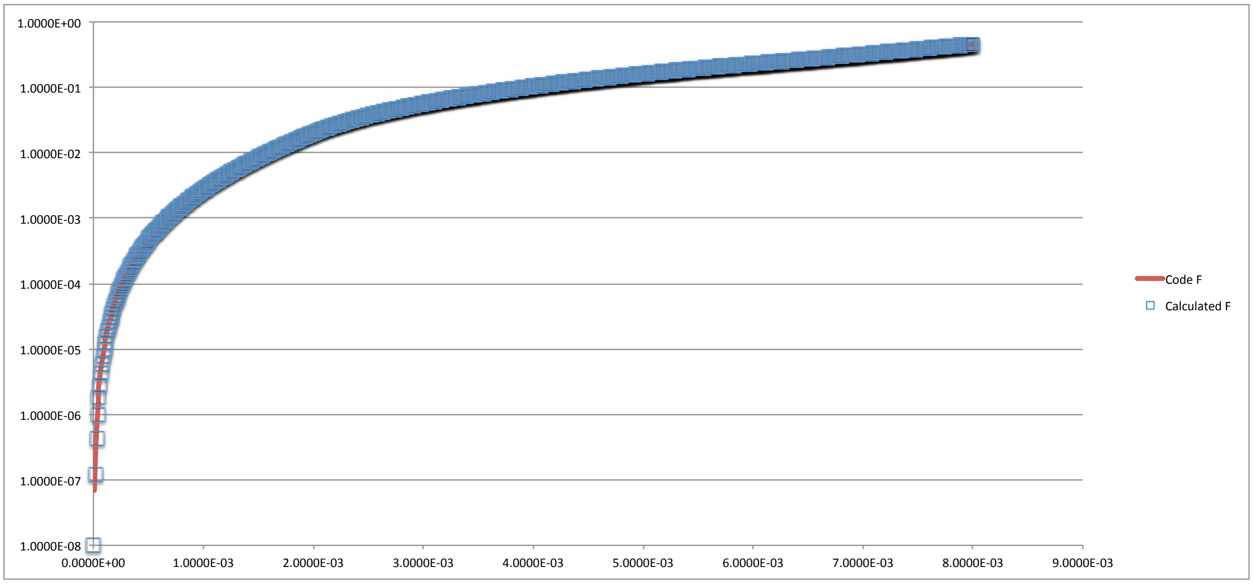


As the figure clearly demonstrates, the pressure resulting from the reference model for the products is consistent with the code result for the pressure. The level of agreement is typically better than a few per cent, which is not as good as the results observed for the other EOS models nor is it as good as that observed for the individual terms in this EOS model.

Prior to the rapid increase in pressure, the reactant JWL in the reference model also agrees well with the code result. This is not true after the rapid increase in pressure, when the reactant JWL in the reference model predicts a pressure that is 30 - 50% lower than the code result. The reason for this discrepancy has not yet been discovered. This discrepancy is also not observed in the results for the other cubes, as shall be demonstrated below.

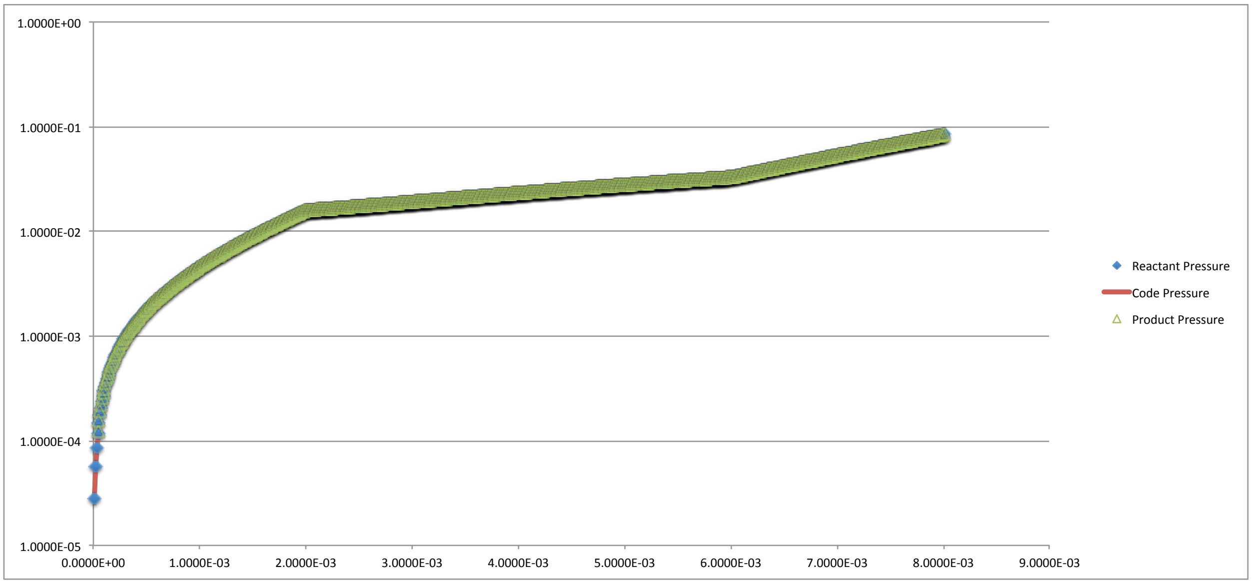
Cube 10 tests the growth term, given by the expression for F_2, in the evolution of the reacted fraction, F. The following figure plots the reference result for F as a function of time for Cube 10, as well as the code result.

Figure 37. Time evolution of *F* for Cube 10 in EOS Form 13



As the plot clearly demonstrates, the reference model matches the code result for the evolution of F as a function of time. Note that, unlike Cube 9, the parameters chosen for Cube 10 do not result in the value of F saturating during the simulation. Using this result for F, the code results for β and the temperature, and the expressions for the relative volumes given in Cochran and Chan[7], the JWL equations for the reactants and products can be used to determine the pressure for this equation-of-state model. The figure below compares the reference result to that of the code for Cube 10.

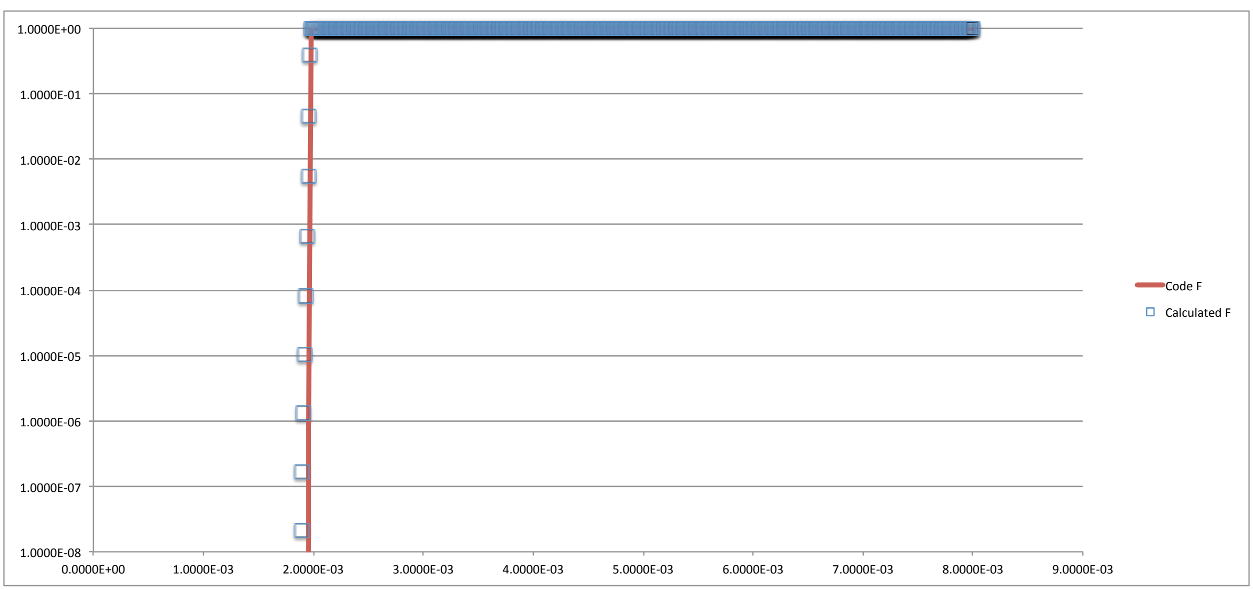
Figure 38. Time evolution of the pressure **for Cube 10 in EOS Form 13**



As the figure clearly demonstrates, both the reactant and the product pressures resulting from the reference model are consistent with the code result for the pressure. The level of agreement is typically a few tenths of a per cent or better, which is not as good as the results observed for the other EOS models. Note that the discrepancy between the reactant pressure and the code pressure does not occur in this test, as it did in Cube 9. As we shall observe in the following, the discrepancy does not occur in the testing of the completion term nor in the testing of the full expression.

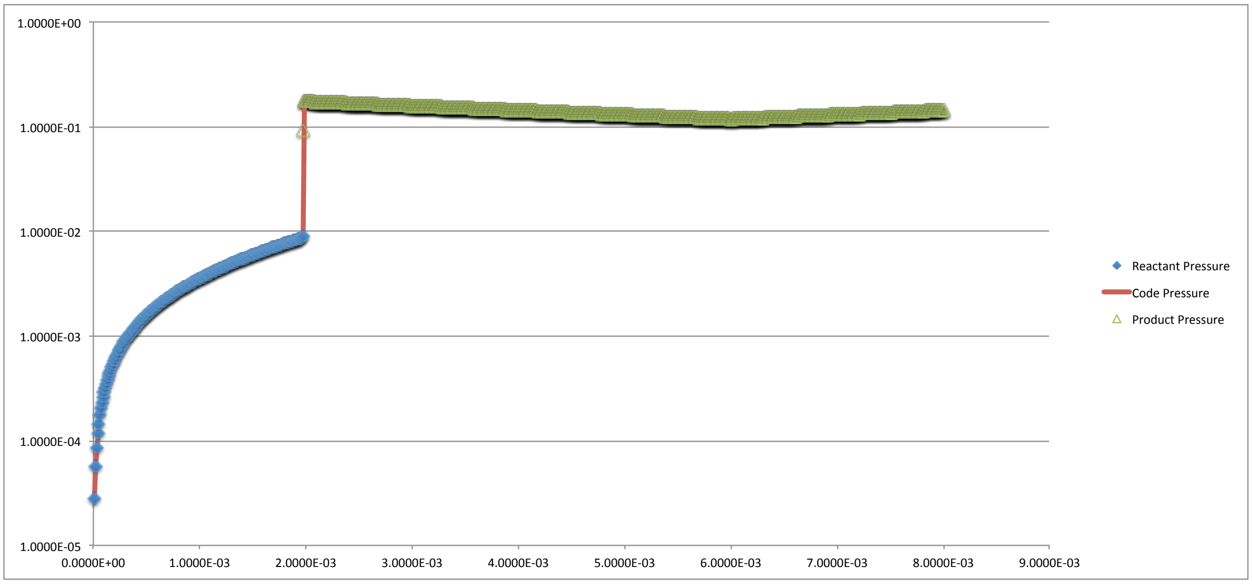
Cube 11 tests the completion term, given by the expression for F_3, in the evolution of the reacted fraction, F. The following figure plots the reference result for F as a function of time for Cube 11, as well as the code result.

Figure 39. Time evolution of *F* for Cube 11 in EOS Form 13



As the plot clearly demonstrates, the reference model matches the code result for the evolution of F as a function of time, including the saturation of F at a value of 1. Using this result for F, the code results for β and the temperature, and the expressions for the relative volumes given in Cochran and Chan[7], the JWL equations for the reactants and products can be used to determine the pressure for this equation-of-state model. The figure below compares the reference result to that of the code for Cube 11.

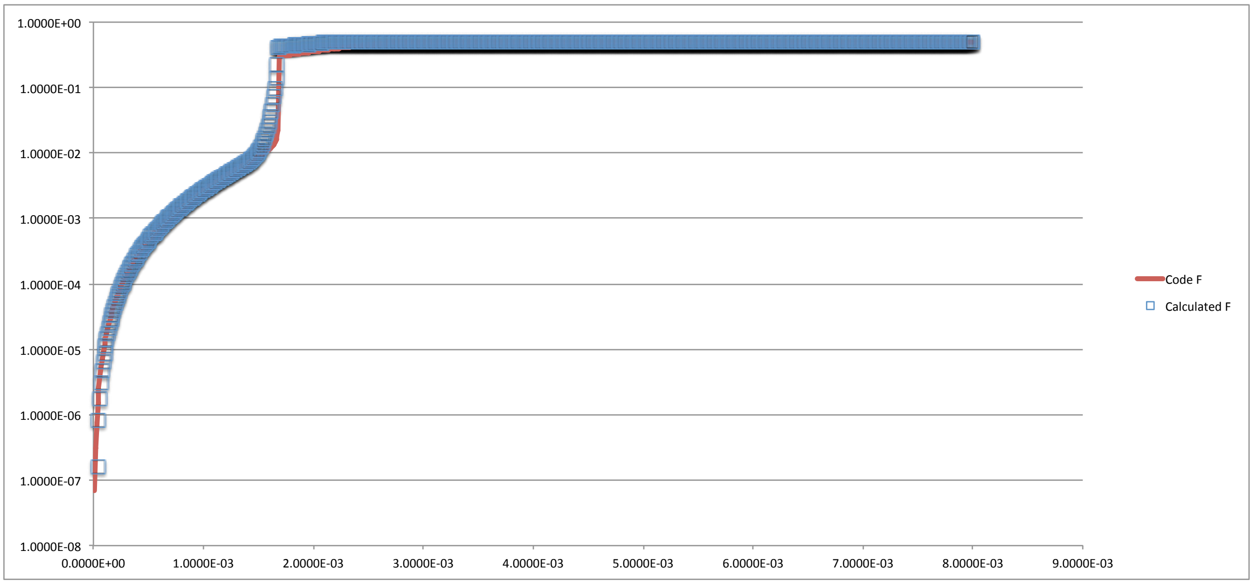
Figure 40. Time evolution of the pressure **for Cube 11 in EOS Form 13**



As the figure clearly demonstrates, both the reactant and the product pressures resulting from the reference model are consistent with the code result for the pressure. The level of agreement is typically better than 3 parts in 10^8, which is much better than observed for the other terms in this test and is similar to the results observed for the other EOS models. Note that the discrepancy between the reactant pressure and the code pressure also does not occur in this test, as it did in Cube 9, despite the rapid increase in pressure that follows the saturation of F. Also note that the reactant pressure goes to zero as F goes to 1 and there is no product pressure until F is non-zero.

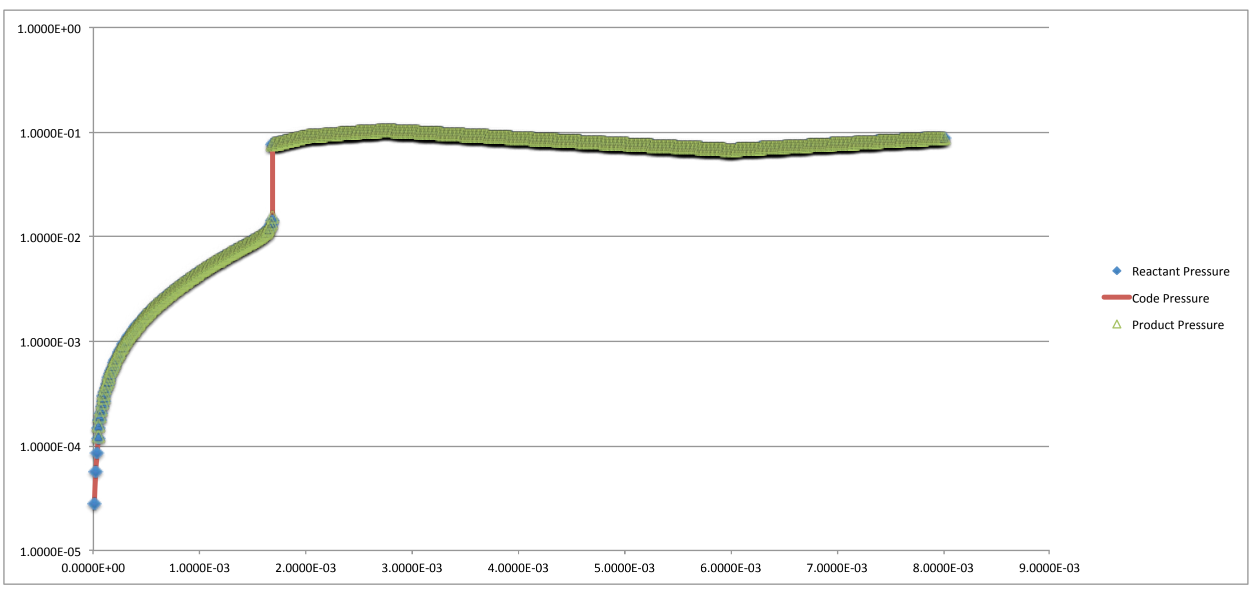
Cube 12 tests the full expression for the evolution of the reacted fraction, F. The following figure plots the reference result for F as a function of time for Cube 12, as well as the code result.

Figure 41. Time evolution of *F* for Cube 12 in EOS Form 13



As the plot clearly demonstrates, the reference model matches the code result for the evolution of *F* as a function of time quite well, including the saturation of *F* at a value of ~ 0.5, although the detailed structure near the rapid increase in the value of *F* is not matched exactly. Using this result for *F*, the code results for β and the temperature, and the expressions for the relative volumes given in Cochran and Chan[7], the JWL equations for the reactants and products can be used to determine the pressure for this equation-of-state model. The figure below compares the reference result to that of the code for Cube 12.

Figure 42. Time evolution of the pressure **for Cube 12 in EOS Form 13**



As the figure clearly demonstrates, both the reactant and the product pressures resulting from the reference model are consistent with the code result for the pressure. The level of agreement is typically better than 5 parts in 10^4, which is much better than observed for the first 2 terms in this test but not as good as the agreement observed for the third term. Note that the discrepancy between the reactant pressure and the code pressure also does not occur in this test, as it did in Cube 9, despite the rapid increase in pressure that follows the saturation of *F*.

Numerical integrations were performed in EXCEL to examine the behavior of the internal energy for this equation-of-state model. Cubes 1 and 2, which investigate the behavior of the first two exponential terms in the reactant JWL, exhibit agreement between the EXCEL numerical integration and the code results for the internal energy on the order of a few parts in 10^7 or better. Cubes 3 and 4, which now include a contribution to the pressure from the temperature, which is related to the internal energy, exhibit agreement between the EXCEL numerical integration and the code results that is on the order of a few parts in 10^5 for Cube 3 and a few parts in 10^4 for Cube 4. This reduction in agreement for Cubes 3 and 4, compared to the results of Cubes 1 and 2, is most likely due to the contribution to the pressure due to the temperature, which is not determined as accurately as it could be. Note also that changes in the temperature in this equation-of-state model occur only as a result of *PdV* work and there is no contribution to temperature changes as a result of the chemistry occurring during the burning of the HE.

These numerical integrations were repeated for Cube 5 - 8, with similar results, in that Cubes 5 and 6 exhibit agreement similar to that observed for Cubes 1 and 2, while Cubes 7 and 8 exhibit agreement similar to that observed for Cubes 3 and 4. The numerical integrations were not repeated for Cubes 9 - 12, as these cubes are expected to follow the behavior of Cubes 4 and 8.

This establishes the implementation of Equation-of-State Form 13 in DYNA3D. The equation-of-state is performing as expected, in that the pressure in the cubes increases as they are compressed and decreases as they are expanded. The behavior of each of the terms in the equation-of-state has been examined and found to be performing as expected and with acceptable accuracy. The behavior of the equation-of-state as a whole has been examined and is performing as expected and with acceptable accuracy.

Author's Note: An important issue was revealed in the testing of Equation-of-State Form 13. The testing of this equation-of-state revealed a bug in the code for this EOS model. It has been known for some time that calculations performed in DYNA3D/ParaDyn using Equation-of-State Form 13 did not return results consistent with the same calculations performed in LS-DYNA and ALE3D. The cause for this discrepancy was not discovered until the creation of this test suite. This testing revealed that the initial pressure was not being passed correctly to the relevant subroutines. As of code version 14.2.0 revision 1.3339, this issue has been corrected.

Equation-of-State Form 14

Equation-of-State Form 14 is a modified version of Equation-of-State Form 8 for use only with material model 65. The input entries and formatting used for Equation-of-State Form 14 are similar to those used for Equation-of-State Form 8. There are differences, however, and the user is encouraged to read the manual to ensure those differences are understood and accounted for in the input file.

Therefore, Equation-of-State Form 14 is a tabulated equation-of-state that is linear in the internal energy. The form of the equation for the pressure, *p*, is

$$p\left(\varepsilon_v,\tilde{\varepsilon}_v\right)=C\left(\tilde{\varepsilon}_v\right)+\gamma T\left(\tilde{\varepsilon}_v\right)E+K\left(\tilde{\varepsilon}_v\right)\times\left(\tilde{\varepsilon}_v-\varepsilon_v\right)$$

where E is the internal energy and ε_v is the volumetric strain, defined by $\varepsilon_v=\ln(V)$, where V is the relative volume. $C(\varepsilon_v)$, $T(\varepsilon_v)$ and $K(\varepsilon_v)$ represent function evaluations from the tabulated data and the input $C(\varepsilon_v)$ therefore have the units of pressure. The minimum volumetric strain, $\tilde{\varepsilon}_v$, is given by the following expression:

$$\tilde{\varepsilon}_v\left(t\right)=\min\left[\varepsilon_v(\tau)\right],0\leq\tau\leq t$$

Note that the pressure is positive in compression and the volumetric strain is positive in tension. Also, the code expects the material to become stiffer with increasing compression and will issue a warning if the unloading bulk moduli do not fulfill this requirement.

It is important to note that in this equation-of-state model unloading occurs along a line using the interpolated value of the unloading bulk modulus that corresponds to the most compressive volumetric strain experienced by the system. To put this bluntly, the system unloads at the point at which the compression is relieved and unloads along a path that is probably different than the loading line and may not be linear if the contribution from the second term in the equation is important because the internal energy continues to evolve along the unloading/reloading path.

As there are really only two terms in EOS Form 14, this equation-of-state model will be tested with 3 cubes, one for each term (2 cubes) and one for the full equation-of-state model. However, due to the unloading/reloading behavior introduced by the bulk unloading moduli, the cubes do not use the same drive that has been used in all the previous tests. Instead, the cubes are compressed by moving all 8 nodes in 0.004 cm, releasing the nodes back to 0.001 cm, moving the nodes in 0.007 cm, releasing back to 0.001 cm, moving in to 0.01 cm, releasing back to 0.005 cm and then compressing back to 0.01 cm. This series of compressions and releases tests the unloading/reloading behavior introduced into this equation-of-state model.

Prior to discussing the calculations using EOS Form 14, a few code issues need to be addressed and these are not necessarily readily apparent to the user. First, in order for the term dependent on the internal energy to perform as expected, it is required to have an initial energy present in the simulation, so the initial internal energy was set to a value of 1.0e-3 in all of the cubes. In addition, in order to eliminate issues with the work performed by the bulk viscosity, the two input coefficients for the bulk viscosity on the material card were set to 1.0e-20 in each of the 3 cubes. Failing to do so results in the work performed on the cube being dominated by contributions from the bulk viscosity. Also, in order to correctly calculate the sound speed, it is necessary to use non-zero values for the $C(\varepsilon_v)$ coefficients, so these were set to very small values for the testing of the second term using Cube 2. Finally, the code version used for this test was version 15.2.0 revision 1.3377.

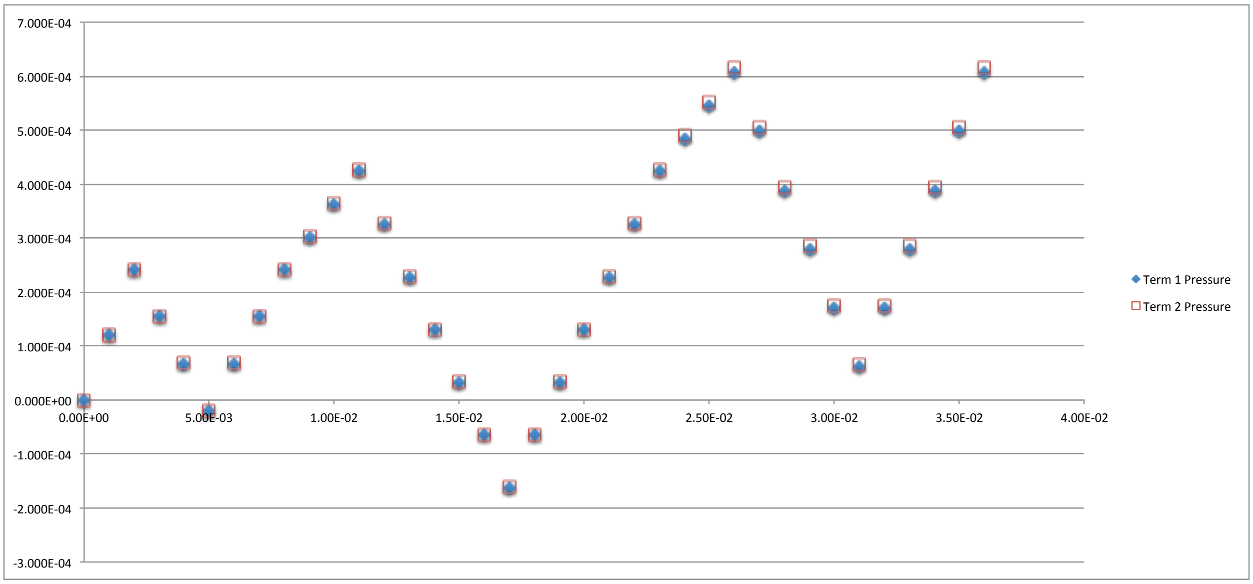
The input coefficients for Equation-of-State Form 14 chosen were the same as those used for the testing of EOS Forms 8, 9 and 12 and are such that the contribution to the pressure from the two terms was of the same order of magnitude as a function of time during the compression and expansion of the cubes. The input coefficients were also chosen to be linear in the volumetric strain and are in fact just scaled by multiples of 10 from each other. The additional unloading bulk moduli were chosen to be linear in the relative volume. The following table lists the (truncated) values of the input coefficients for each of the cubes in the testing of EOS Form 14.

Table 78. Suite of test input coefficients for EOS Form 14

Cube									
1	ε_v	-6.19e-2	-4.08e-2	-2.02e-2	0.00	1.98e-2	3.92e-2	5.83e-2	7.70e-2
1	$C(\varepsilon_v)$	6.19e-4	4.08e-4	2.02e-4	0.00	-1.98e-4	-3.92e-4	-5.83e-4	-7.70e-4
1	$T(\varepsilon_v)$	61.9	40.8	20.2	0.00	-19.8	-39.2	-58.3	-77.0
1	γ	0.0							
1	$K(\varepsilon_v)$	0.018	0.016	0.014	0.012	0.010	0.008	0.006	0.004
2	ε_v	-6.19e-2	-4.08e-2	-2.02e-2	0.00	1.98e-2	3.92e-2	5.83e-2	7.70e-2
2	$C(\varepsilon_v)$	6.19e-10	4.08e-10	2.02e-10	0.00	-1.98e-10	-3.92e-10	-5.83e-10	-7.70e-10
2	$T(\varepsilon_v)$	61.9	40.8	20.2	0.00	-19.8	-39.2	-58.3	-77.0
2	γ	0.01							
2	$K(\varepsilon_v)$	0.018	0.016	0.014	0.012	0.010	0.008	0.006	0.004
3	ε_v	-6.19e-2	-4.08e-2	-2.02e-2	0.00	1.98e-2	3.92e-2	5.83e-2	7.70e-2
3	$C(\varepsilon_v)$	6.19e-4	4.08e-4	2.02e-4	0.00	-1.98e-4	-3.92e-4	-5.83e-4	-7.70e-4
3	$T(\varepsilon_v)$	61.9	40.8	20.2	0.00	-19.8	-39.2	-58.3	-77.0
3	γ	0.01							
3	$K(\varepsilon_v)$	0.018	0.016	0.014	0.012	0.010	0.008	0.006	0.004

The two terms in the equation-of-state were tested (almost) independently, given the requirement on the $C(\varepsilon_v)$ coefficients, then the full equation-of-state model was tested. The following plot displays the pressures from the first two terms, as returned by the code, as a function of time for this simulation.

Figure 43. Code pressures for the two terms of EOS Form 14 as a function of time



As the plot demonstrates, not only are both terms contributing pressures on the order of $6x10^{-4}$ at the peak of the compression, but the contributions of the two terms are nearly identical.

The following observations may be made from the plot. Both terms contribute an increase in the pressure as the cubes are compressed and both exhibit a decrease in pressure as the cubes are expanded, as expected. In addition, given the choice of input coefficients, the pressure of both cubes should be zero at the beginning of the simulation and this behavior is also observed. Finally, although not obvious from the plot, the slope of the unloading/reloading lines differ from the slope of the monotonic path, which is expected given the choice of input coefficients. Therefore, at least qualitatively, the code output is behaving as expected.

Using the normalized difference defined by equation 1, the agreement between the pressures for the second term as calculated using the reference expression and the results returned by the code is demonstrated in the following table as a function of time, using the expected value for the bulk unloading modulus.

Table 79. Reference and Code Pressures for the second term of EOS Form 14

Time	*Reference Pressure*	*Code Pressure*	*(Reference - Code)/Code*
0.00E+00	0.00000000E+00	0.00000000E+00	0.0000000000E+00
1.00E-03	1.20327020E-04	1.20326954E-04	5.5165968782E-07
2.00E-03	2.41654811E-04	2.41654556E-04	1.0560400266E-06
3.00E-03	1.54479117E-04	1.54498319E-04	-1.2428370418E-04
4.00E-03	6.76014836E-05	6.76397286E-05	-5.6542275342E-04
5.00E-03	-1.89782171E-05	-1.89209665E-05	3.0257775732E-03
6.00E-03	6.76014835E-05	6.76396618E-05	-5.6443717434E-04
7.00E-03	1.54479117E-04	1.54498165E-04	-1.2329029940E-04
8.00E-03	2.41654812E-04	2.41654683E-04	5.3282005664E-07
9.00E-03	3.02856625E-04	3.02856435E-04	6.2538061006E-07

1.00E-02	3.64504043E-04	3.64503763E-04	7.6994413882E-07
1.10E-02	4.26662669E-04	4.26662290E-04	8.8843537431E-07
1.20E-02	3.27605963E-04	3.27614589E-04	-2.6330795028E-05
1.30E-02	2.28989226E-04	2.29006114E-04	-7.3744224565E-05
1.40E-02	1.30812541E-04	1.30837676E-04	-1.9211113496E-04
1.50E-02	3.30759851E-05	3.31093528E-05	-1.0078029773E-03
1.60E-02	-6.42203653E-05	-6.41787843E-05	6.4789400277E-04
1.70E-02	-1.61076437E-04	-1.61026658E-04	3.0913682005E-04
1.80E-02	-6.42203656E-05	-6.41786784E-05	6.4954971630E-04
1.90E-02	3.30759839E-05	3.31092989E-05	-1.0062148624E-03
2.00E-02	1.30812538E-04	1.30837465E-04	-1.9051407712E-04
2.10E-02	2.28989221E-04	2.29005744E-04	-7.2151479789E-05
2.20E-02	3.27605955E-04	3.27614051E-04	-2.4712328104E-05
2.30E-02	4.26662658E-04	4.26662288E-04	8.6785207037E-07
2.40E-02	4.89398502E-04	4.89398028E-04	9.7014850562E-07
2.50E-02	5.52778113E-04	5.52777717E-04	7.1650450567E-07
2.60E-02	6.16868668E-04	6.16867951E-04	1.1614321973E-06
2.70E-02	5.05542241E-04	5.05550085E-04	-1.5515119336E-05
2.80E-02	3.94820409E-04	3.94835353E-04	-3.7848220107E-05
2.90E-02	2.84703298E-04	2.84725339E-04	-7.7413835044E-05
3.00E-02	1.75191019E-04	1.75220144E-04	-1.6622256211E-04
3.10E-02	6.62836756E-05	6.63198740E-05	-5.4581536632E-04
3.20E-02	1.75191018E-04	1.75219759E-04	-1.6402970454E-04
3.30E-02	2.84703295E-04	2.84724714E-04	-7.5227342289E-05
3.40E-02	3.94820403E-04	3.94834477E-04	-3.5645092012E-05
3.50E-02	5.05542230E-04	5.05548936E-04	-1.3264057397E-05
3.60E-02	6.16868651E-04	6.16867944E-04	1.1464656172E-06

As the table demonstrates, the agreement between the reference expression and the code results is very good along the monotonic portion of the loading line, where the agreement is better than about 4 parts in 10^6. However, the agreement along the unloading/reloading lines is dramatically poorer, with the agreement being as poor as 3 parts in 10^3. This appears to be due to the code using a slightly different value for the bulk unloading modulus than was used in the theoretical model, since if the differences along the unloading/reloading lines are minimized in the theoretical model, the agreement improves dramatically, as demonstrated in the following table.

Table 80. Reference and Code Pressures for the second term of EOS Form 14 using min K(ε_v)

Time	*Reference Pressure*	*Code Pressure*	*(Reference - Code)/Code*
0.00E+00	0.00000000E+00	0.00000000E+00	0.0000000000E+00
1.00E-03	1.20327020E-04	1.20326954E-04	5.5165968782E-07

2.00E-03	2.41654811E-04	2.41654556E-04	1.0560400266E-06
3.00E-03	1.54498236E-04	1.54498319E-04	-5.3259226588E-07
4.00E-03	6.76396838E-05	6.76397286E-05	-6.6225897512E-07
5.00E-03	-1.89209742E-05	-1.89209665E-05	4.1003789415E-07
6.00E-03	6.76396837E-05	6.76396618E-05	3.2387777982E-07
7.00E-03	1.54498236E-04	1.54498165E-04	4.6093554112E-07
8.00E-03	2.41654812E-04	2.41654683E-04	5.3282005664E-07
9.00E-03	3.02856625E-04	3.02856435E-04	6.2538061006E-07
1.00E-02	3.64504043E-04	3.64503763E-04	7.6994413882E-07
1.10E-02	4.26662669E-04	4.26662290E-04	8.8843537431E-07
1.20E-02	3.27614331E-04	3.27614589E-04	-7.8906619122E-07
1.30E-02	2.29005945E-04	2.29006114E-04	-7.3847005042E-07
1.40E-02	1.30837594E-04	1.30837676E-04	-6.3087877631E-07
1.50E-02	3.31093552E-05	3.31093528E-05	7.2771298871E-08
1.60E-02	-6.41786946E-05	-6.41787843E-05	-1.3965384447E-06
1.70E-02	-1.61026483E-04	-1.61026658E-04	-1.0887717492E-06
1.80E-02	-6.41786949E-05	-6.41786784E-05	2.5810384921E-07
1.90E-02	3.31093540E-05	3.31092989E-05	1.6625258393E-06
2.00E-02	1.30837591E-04	1.30837465E-04	9.6648897357E-07
2.10E-02	2.29005940E-04	2.29005744E-04	8.5439257739E-07
2.20E-02	3.27614323E-04	3.27614051E-04	8.2944266861E-07
2.30E-02	4.26662658E-04	4.26662288E-04	8.6785207037E-07
2.40E-02	4.89398502E-04	4.89398028E-04	9.7014850562E-07
2.50E-02	5.52778113E-04	5.52777717E-04	7.1650450567E-07
2.60E-02	6.16868668E-04	6.16867951E-04	1.1614321973E-06
2.70E-02	5.05549505E-04	5.05550085E-04	-1.1479558295E-06
2.80E-02	3.94834921E-04	3.94835353E-04	-1.0940048008E-06
2.90E-02	2.84725043E-04	2.84725339E-04	-1.0395697991E-06
3.00E-02	1.75219984E-04	1.75220144E-04	-9.1705197809E-07
3.10E-02	6.63198451E-05	6.63198740E-05	-4.3702060803E-07
3.20E-02	1.75219983E-04	1.75219759E-04	1.2761687856E-06
3.30E-02	2.84725040E-04	2.84724714E-04	1.1470906983E-06
3.40E-02	3.94834915E-04	3.94834477E-04	1.1092048480E-06
3.50E-02	5.05549494E-04	5.05548936E-04	1.1031387636E-06
3.60E-02	6.16868651E-04	6.16867944E-04	1.1464656172E-06

As this table demonstrates, the agreement along the unloading/reloading portions of the curves has, in general, improved by about two orders of magnitude. This improvement, similar to that observed in the testing of EOS Form 8, is achieved in the same manner by changing the value used for the bulk unloading modulus along the unloading/reloading curves by the amounts given in the following table.

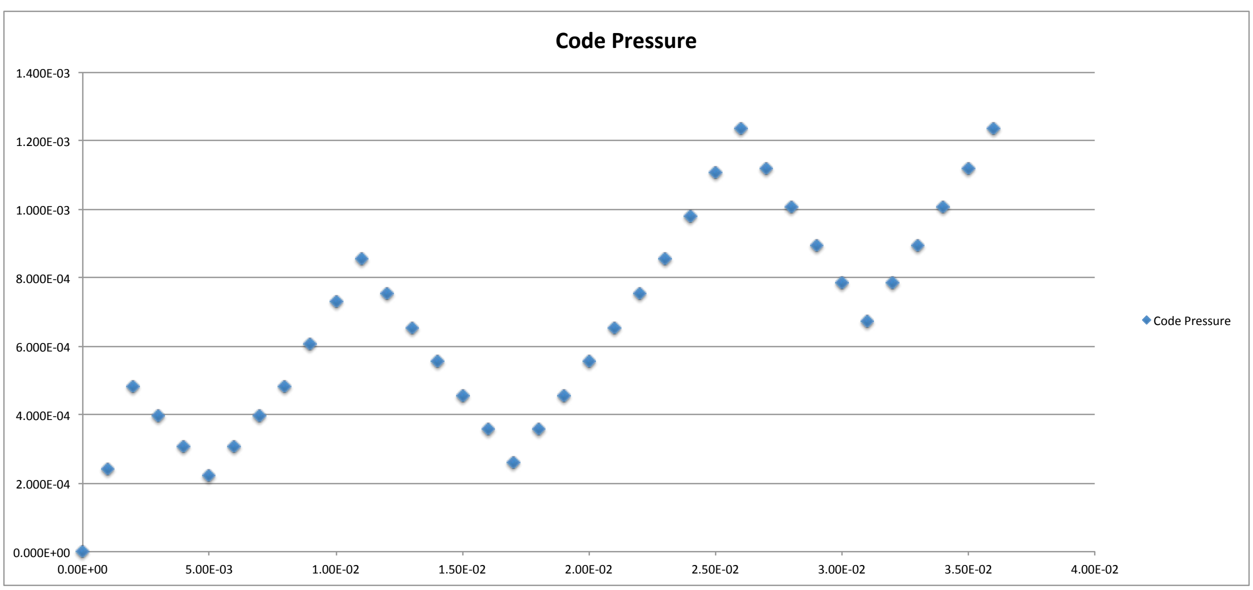
Table 81. Expected and minimizing values of $K(\varepsilon_v)$ for the second term of EOS Form 14

Expected $K(\varepsilon_v)$	Minimizing $K(\varepsilon_v)$	(Min - Expected)/Expected
0.014381	0.014377687	-2.20032E-04
0.016141	0.016140098	-8.52778E-05
0.017881	0.017879612	-6.64150E-05

As the table demonstrates, a small change in the value of the bulk unloading modulus (less than 3 parts in 10^4) results in a considerable improvement in the agreement between the reference pressures and the code results. This implies that even though the input to the code was chosen such that the unloading points corresponded to input values of $K(\varepsilon_v)$, the interpolation routine returned values for the bulk unloading modulus that differed slightly from the input values. A difference this small in the returned value from an interpolation routine is not surprising. It is worth noting that as in the testing of EOS Forms 8, 9 and 12, the agreement between the reference expression and the code results for the first term is significantly better than that exhibited by the second term (approximately 5 orders of magnitude better), which is most likely due to the numerical integration of the internal energy, as will be demonstrated below. Note that since the pressure due to the first term is not dependent on the internal energy, it is unaffected by the code's determination of the internal energy.

Now that the behavior of the pressure resulting from each of the individual terms in the expression for Equation-of-State Form 14 has been investigated, the behavior of the full expression can be examined. The following plot displays the pressure returned by the code as a function of time for EOS Form 14.

Figure 44. Code pressures for EOS Form 14 as a function of time



Note that the pressure is behaving as one would expect, in that the pressure increases as the cube is compressed and decreases as the compression is released. In addition, the initial pressure is zero, as expected from the choice of input coefficients.

The following table compares the pressure returned by the code as a function of time for the full expression for Equation-of-State Form 14 to that predicted by the reference expression.

Table 82. Reference and Code Pressures for Equation-of-State Form 14

Time	*Reference Pressure*	*Code Pressure*	*(Reference - Code)/Code*
0.00E+00	0.00000000E+00	0.000000000E+00	0.0000000000E+00
1.00E-03	2.40653800E-04	2.406536672E-04	5.5209347528E-07
2.00E-03	4.83309140E-04	4.833086291E-04	1.0564150708E-06
3.00E-03	3.95789183E-04	3.958085045E-04	-4.8816338765E-05
4.00E-03	3.08566392E-04	3.086047569E-04	-1.2431614003E-04
5.00E-03	2.21640643E-04	2.216980123E-04	-2.5877448399E-04
6.00E-03	3.08566392E-04	3.086044520E-04	-1.2332808477E-04
7.00E-03	3.95789183E-04	3.958081106E-04	-4.7821068434E-05
8.00E-03	4.83309140E-04	4.833088822E-04	5.3294141551E-07
9.00E-03	6.05712643E-04	6.057122641E-04	6.2536941474E-07
1.00E-02	7.29007356E-04	7.290067950E-04	7.6989159052E-07
1.10E-02	8.53324483E-04	8.533237251E-04	8.8834936468E-07
1.20E-02	7.53214264E-04	7.532232344E-04	-1.1910019423E-05
1.30E-02	6.53542357E-04	6.535595840E-04	-2.6359147517E-05
1.40E-02	5.54308861E-04	5.543343329E-04	-4.5951133343E-05
1.50E-02	4.55513870E-04	4.555475808E-04	-7.3999635316E-05
1.60E-02	3.57157479E-04	3.571994059E-04	-1.1737760775E-04
1.70E-02	2.59239775E-04	2.592898969E-04	-1.9330249369E-04
1.80E-02	3.57157479E-04	3.571988179E-04	-1.1573167302E-04
1.90E-02	4.55513870E-04	4.555468292E-04	-7.2349997803E-05
2.00E-02	5.54308861E-04	5.543334298E-04	-4.4322006089E-05
2.10E-02	6.53542357E-04	6.535585230E-04	-2.4735674298E-05
2.20E-02	7.53214264E-04	7.532219911E-04	-1.0259405226E-05
2.30E-02	8.53324483E-04	8.533237132E-04	9.0220283562E-07
2.40E-02	9.78796059E-04	9.787950667E-04	1.0139321501E-06
2.50E-02	1.10555517E-03	1.105554318E-03	7.7154801360E-07
2.60E-02	1.23373617E-03	1.233734657E-03	1.2295921558E-06
2.70E-02	1.12025471E-03	1.120263196E-03	-7.5720586183E-06
2.80E-02	1.00737662E-03	1.007392196E-03	-1.5457695727E-05
2.90E-02	8.95102082E-04	8.951247552E-04	-2.5329711888E-05
3.00E-02	7.83431247E-04	7.834610059E-04	-3.7984137083E-05
3.10E-02	6.72364269E-04	6.724011179E-04	-5.4801549461E-05

3.20E-02	7.83431247E-04	7.834592830E-04	-3.5785165315E-05
3.30E-02	8.95102082E-04	8.951227856E-04	-2.3129343949E-05
3.40E-02	1.00737662E-03	1.007389955E-03	-1.3232919400E-05
3.50E-02	1.12025471E-03	1.120260641E-03	-5.2918074369E-06
3.60E-02	1.23373617E-03	1.233734630E-03	1.2512061875E-06

As might have been expected, given the analysis of the second term for this EOS model, the agreement between the reference expression and the code results is very good along the monotonic portion of the loading line, where the agreement is better than about 1 part in 10^6, similar to that observed in the testing of EOS Forms 8 and 12. However, the agreement along the unloading/reloading lines is dramatically poorer, with the agreement being as poor as ~ 3 parts in 10^4. This appears to be due to the code using a slightly different value for the bulk unloading modulus than was used in the theoretical model, since if the differences along the unloading/reloading lines are minimized in the theoretical model, the agreement improves dramatically, as demonstrated in the following table.

Table 83. Reference and Code Pressures for EOS Form 14 using min K(ε_v)

Time	*Reference Pressure*	*Code Pressure*	*(Reference - Code)/Code*
0.00E+00	0.00000000E+00	0.000000000E+00	0.0000000000E+00
1.00E-03	2.40653800E-04	2.406536672E-04	5.5209347528E-07
2.00E-03	4.83309140E-04	4.833086291E-04	1.0564150708E-06
3.00E-03	3.95808323E-04	3.958085045E-04	-4.5749905451E-07
4.00E-03	3.08604636E-04	3.086047569E-04	-3.9320912751E-07
5.00E-03	2.21697950E-04	2.216980123E-04	-2.8207981268E-07
6.00E-03	3.08604636E-04	3.086044520E-04	5.9496859112E-07
7.00E-03	3.95808323E-04	3.958081106E-04	5.3781939729E-07
8.00E-03	4.83309140E-04	4.833088822E-04	5.3294141551E-07
9.00E-03	6.05712643E-04	6.057122641E-04	6.2536941474E-07
1.00E-02	7.29007356E-04	7.290067950E-04	7.6989159052E-07
1.10E-02	8.53324483E-04	8.533237251E-04	8.8834936468E-07
1.20E-02	7.53222632E-04	7.532232344E-04	-7.9996136959E-07
1.30E-02	6.53559077E-04	6.535595840E-04	-7.7649941301E-07
1.40E-02	5.54333915E-04	5.543343329E-04	-7.5393051325E-07
1.50E-02	4.55547243E-04	4.555475808E-04	-7.4241160101E-07
1.60E-02	3.57199152E-04	3.571994059E-04	-7.1105984453E-07
1.70E-02	2.59289733E-04	2.592898969E-04	-6.3150777233E-07
1.80E-02	3.57199152E-04	3.571988179E-04	9.3506693948E-07
1.90E-02	4.55547243E-04	4.555468292E-04	9.0734676846E-07
2.00E-02	5.54333915E-04	5.543334298E-04	8.7527037654E-07
2.10E-02	6.53559077E-04	6.535585230E-04	8.4701533935E-07

2.20E-02	7.53222632E-04	7.532219911E-04	8.5067116675E-07
2.30E-02	8.53324483E-04	8.533237132E-04	9.0220283562E-07
2.40E-02	9.78796059E-04	9.787950667E-04	1.0139321501E-06
2.50E-02	1.10555517E-03	1.105554318E-03	7.7154801360E-07
2.60E-02	1.23373617E-03	1.233734657E-03	1.2295921558E-06
2.70E-02	1.12026199E-03	1.120263196E-03	-1.0739929887E-06
2.80E-02	1.00739117E-03	1.007392196E-03	-1.0201442930E-06
2.90E-02	8.95123876E-04	8.951247552E-04	-9.8197860162E-07
3.00E-02	7.83460276E-04	7.834610059E-04	-9.3117621751E-07
3.10E-02	6.72400519E-04	6.724011179E-04	-8.8996502285E-07
3.20E-02	7.83460276E-04	7.834592830E-04	1.2678770315E-06
3.30E-02	8.95123876E-04	8.951227856E-04	1.2184429130E-06
3.40E-02	1.00739117E-03	1.007389955E-03	1.2046641551E-06
3.50E-02	1.12026199E-03	1.120260641E-03	1.2062730100E-06
3.60E-02	1.23373617E-03	1.233734630E-03	1.2512061875E-06

As this table demonstrates, the agreement along the unloading/reloading portions of the curves has improved dramatically, with the agreement now being better by orders of magnitude, just as observed in the testing of EOS Forms 8 and 12. This improvement is achieved by changing the value used for the bulk unloading modulus along the unloading/reloading curves by the amounts given in the following table.

Table 84. Expected and minimizing values of $K(\varepsilon_v)$ for EOS Form 14

Expected $K(\varepsilon_v)$	Minimizing $K(\varepsilon_v)$	(Min - Expected)/Expected
0.014381	0.014377683	-2.202795863E-04
0.016141	0.016140098	-8.528302342E-05
0.017881	0.01787961	-6.656329659E-05

As the table demonstrates, the results of this testing are similar to those obtained from the testing of EOS Forms 8 and 12. The changes in the value of the bulk unloading modulus are very small (less than 2 parts in 10^4) and result in a dramatic improvement in the agreement between the reference pressures and the code results, as was observed in the previous testing of EOS Forms 8 and 12. This implies that even though the input to the code was chosen such that the unloading points corresponded to input values of $K(\varepsilon_v)$, the interpolation routine returned values for the bulk unloading modulus that differed slightly from the input values. A difference this small in the returned value from an interpolation routine is not surprising. It is also worth noting that the values used for the full expression of EOS Form 14 are essentially identical to those used for the analysis of the second term of this equation-of-state model. This is not a surprise, as the non-linear behavior along the unloading/reloading curve is due to the evolution of the internal energy and this term is the same in both cubes.

The code results for the internal energy can also be examined for this equation-of-state model. As the pressure for the first term is independent of the internal energy, we shall concentrate on the behavior of the second term and the full expression for this EOS model. Given the form for the pressure along the unloading/reloading lines, there is no simple closed form solution for the internal energy along these lines and so the code results will be compared to those obtained from a simple numerical integration performed in EXCEL (*Reference Energy*). The following table makes this comparison for the second term in EOS Form 14 using the minimized value for $K(\varepsilon_v)$.

Table 85. Reference and Code Internal Energies for the second term of EOS Form 14

Time	Code (GRIZ)	*Reference Energy*	(*Reference* - GRIZ)/GRIZ
0.00E+00	1.00000000E-03	1.00000000E-03	0.000000E+00
1.00E-03	1.00071700E-03	1.00071738E-03	3.792183E-07
2.00E-03	1.00286100E-03	1.00286108E-03	7.576553E-08
3.00E-03	1.00168900E-03	1.00168952E-03	5.180532E-07
4.00E-03	1.00103000E-03	1.00103007E-03	7.287402E-08
5.00E-03	1.00088500E-03	1.00088511E-03	1.131035E-07
6.00E-03	1.00103000E-03	1.00103007E-03	7.250348E-08
7.00E-03	1.00168900E-03	1.00168952E-03	5.176827E-07
8.00E-03	1.00286100E-03	1.00286108E-03	7.744130E-08
9.00E-03	1.00446500E-03	1.00446502E-03	1.693502E-08
1.00E-02	1.00642300E-03	1.00642294E-03	-5.954258E-08
1.10E-02	1.00873500E-03	1.00873474E-03	-2.546050E-07
1.20E-02	1.00653100E-03	1.00653077E-03	-2.253202E-07
1.30E-02	1.00489800E-03	1.00489786E-03	-1.408413E-07
1.40E-02	1.00383800E-03	1.00383808E-03	8.419717E-08
1.50E-02	1.00335400E-03	1.00335352E-03	-4.791312E-07
1.60E-02	1.00344600E-03	1.00344621E-03	2.120758E-07
1.70E-02	1.00411800E-03	1.00411820E-03	1.965543E-07
1.80E-02	1.00344600E-03	1.00344621E-03	2.113500E-07
1.90E-02	1.00335400E-03	1.00335352E-03	-4.820295E-07
2.00E-02	1.00383800E-03	1.00383808E-03	7.769001E-08
2.10E-02	1.00489800E-03	1.00489785E-03	-1.523779E-07
2.20E-02	1.00653100E-03	1.00653076E-03	-2.432864E-07
2.30E-02	1.00873500E-03	1.00873472E-03	-2.803757E-07
2.40E-02	1.01140100E-03	1.01140064E-03	-3.511651E-07
2.50E-02	1.01442100E-03	1.01442131E-03	3.092989E-07
2.60E-02	1.01779800E-03	1.01779768E-03	-3.099844E-07
2.70E-02	1.01455800E-03	1.01455769E-03	-3.020986E-07
2.80E-02	1.01194800E-03	1.01194812E-03	1.226869E-07
2.90E-02	1.00997100E-03	1.00997067E-03	-3.235538E-07

3.00E-02	1.00862700E-03	1.00862701E-03	9.759291E-09
3.10E-02	1.00791900E-03	1.00791878E-03	-2.228285E-07
3.20E-02	1.00862700E-03	1.00862701E-03	8.632773E-09
3.30E-02	1.00997100E-03	1.00997067E-03	-3.280495E-07
3.40E-02	1.01194800E-03	1.01194811E-03	1.126015E-07
3.50E-02	1.01455800E-03	1.01455768E-03	-3.199634E-07
3.60E-02	1.01779800E-03	1.01779766E-03	-3.377797E-07

As the table demonstrates, the level of agreement between the EXCEL numerical integration and the code results for the internal energy is better than ~ 5 parts in 10^7, which is about as good as can be expected, given the limitations on the GRIZ output. This establishes that the internal energies being returned by the code are reasonable for the second term in EOS Form 14.

There is also no simple closed form solution for the internal energy due to the full expression for Equation-of-State Form 14. A numerical integration was performed in EXCEL (*Reference Energy*) to compare against the code results. The following table gives the result of that comparison using the minimized value for $K(\varepsilon_v)$.

Table 86. Reference and Code Internal Energies for EOS Form 14

Time	Code (GRIZ)	*Reference Energy*	(*Reference* - GRIZ)/GRIZ
0.00E+00	1.00000000E-03	1.00000000E-03	0.000000E+00
1.00E-03	1.00143500E-03	1.00143476E-03	-2.421068E-07
2.00E-03	1.00572200E-03	1.00572215E-03	1.454104E-07
3.00E-03	1.00312200E-03	1.00312191E-03	-9.254975E-08
4.00E-03	1.00103000E-03	1.00103007E-03	6.820907E-08
5.00E-03	9.99449100E-04	9.99449012E-04	-8.786879E-08
6.00E-03	1.00103000E-03	1.00103007E-03	6.820937E-08
7.00E-03	1.00312200E-03	1.00312191E-03	-9.217973E-08
8.00E-03	1.00572200E-03	1.00572215E-03	1.457803E-07
9.00E-03	1.00893000E-03	1.00893002E-03	2.190173E-08
1.00E-02	1.01284600E-03	1.01284586E-03	-1.339746E-07
1.10E-02	1.01746900E-03	1.01746947E-03	4.578674E-07
1.20E-02	1.01277500E-03	1.01277473E-03	-2.661050E-07
1.30E-02	1.00864700E-03	1.00864713E-03	1.316312E-07
1.40E-02	1.00508900E-03	1.00508880E-03	-2.013634E-07
1.50E-02	1.00210200E-03	1.00210183E-03	-1.671981E-07
1.60E-02	9.99688300E-04	9.99688327E-04	2.710428E-08
1.70E-02	9.97850300E-04	9.97850354E-04	5.373789E-08
1.80E-02	9.99688300E-04	9.99688327E-04	2.710514E-08
1.90E-02	1.00210200E-03	1.00210183E-03	-1.671964E-07
2.00E-02	1.00508900E-03	1.00508880E-03	-2.013609E-07

2.10E-02	1.00864700E-03	1.00864713E-03	1.316345E-07
2.20E-02	1.01277500E-03	1.01277473E-03	-2.661008E-07
2.30E-02	1.01746900E-03	1.01746947E-03	4.578724E-07
2.40E-02	1.02280100E-03	1.02280134E-03	3.278069E-07
2.50E-02	1.02884300E-03	1.02884269E-03	-3.011130E-07
2.60E-02	1.03559500E-03	1.03559545E-03	4.364424E-07
2.70E-02	1.02880000E-03	1.02879978E-03	-2.186758E-07
2.80E-02	1.02263200E-03	1.02263250E-03	4.922528E-07
2.90E-02	1.01709500E-03	1.01709541E-03	4.061334E-07
3.00E-02	1.01219000E-03	1.01219025E-03	2.495096E-07
3.10E-02	1.00791900E-03	1.00791874E-03	-2.553281E-07
3.20E-02	1.01219000E-03	1.01219025E-03	2.495113E-07
3.30E-02	1.01709500E-03	1.01709541E-03	4.061369E-07
3.40E-02	1.02263200E-03	1.02263250E-03	4.922579E-07
3.50E-02	1.02880000E-03	1.02879978E-03	-2.186691E-07
3.60E-02	1.03559500E-03	1.03559545E-03	4.364507E-07

As the table demonstrates, the results of this testing are similar to those obtained from EOS Form 12. The level of agreement between the EXCEL numerical integration and the code results for the internal energy is better than ~ 5 parts in 10^7, so the level of agreement is similar to that exhibited by the second term of this EOS model, as expected.

This establishes the implementation of Equation-of-State Form 14 in DYNA3D. The equation-of-state is performing as expected, in that the pressure in the cubes increases as they are compressed and decreases as they are expanded. The behavior of each of the terms in the equation-of-state has been examined and found to be performing as expected and with good accuracy. The behavior of the equation-of-state as a whole has been examined and is performing as expected and with good accuracy.

It is interesting to note that the results achieved in this testing are essentially the same as those obtained in the testing of EOS Forms 8 and 12, which is essentially the same equation-of-state. In fact, to 15 significant figures, the output obtained from EOS Forms 12 and 14 are identical, while the output obtained from EOS Form 8 differs in the last 3 or 4 digits. The simulations for EOS Forms 12 and 14 require exactly the same number of cycles, while that for EOS Form 8 requires about 2/3 as many cycles. It is believed that if the input to EOS Form 8 was modified to increase the number of cycles to a similar number, the results would be identical to those obtained from EOS Forms 12 and 14. Therefore, the change in the material model has had little, if any, impact on the EOS results.

Equation-of-State Form 15

Equation-of-State Form 15 is a modified form of Equation-of-State Form 1 intended for use only with Material Type 64, a Steinberg-Guinan model that incorporates a 3D crack model. As such, EOS Form 15 is a polynomial that is a function of the excess compression and is linear in the internal energy. The expression for EOS Form 15 is as follows:

$$p = C_0+C_1\mu+C_2\overline{\mu}^2+C_3\mu^3+(C_4+C_5\mu+C_6\overline{\mu}^2)E,$$

where p is the pressure, μ is the excess compression (related to the density by $\mu = \rho/\rho_0 - 1$), and E is the specific internal energy (energy per unit initial volume). The tension-limited excess compression, $\overline{\mu}$, is given by:

$$\overline{\mu} = \max(\mu,0).$$

As was the case with EOS Form 1, Equation-of-State Form 15 was tested using 10 cubes, one for each of the coefficients (7 cubes), one for the sum of the first four terms, one for the sum of the last three terms (As before, these two cubes are included because these are the quantities actually calculated by DYNA3D) and one for the full equation-of-state model. This testing used a drive similar to that used in the testing of EOS Form 1, so the 10 cubes were compressed hydrostatically to approximately 94% of the original volume, driven back to the original volume, hydrostatically expanded out to ~ 103% of the original volume (a change from EOS Form 1) and then released back to the original state.

Inclusion of a 3D crack (failure) model in the Steinberg-Guinan material model complicated testing of this equation-of-state model. Initial attempts to run a simulation using this combination were unsuccessful in completing a simulation in which the material did not fail. As the intent of this testing is to test the implementation of the EOS model and not the material model, it was necessary to iterate on the input to the simulation until the material model did not trigger a failure. This proved to be more difficult than anticipated. The end result was that the amount of tension the cubes were placed under was reduced, as was the strain rate, to prevent activation of the failure model.

Prior to discussing the calculations using EOS Form 15, a few code issues need to be addressed and these are not necessarily readily apparent to the user. First, because the sound speed looks like $dp/d\rho$ and μ is proportional to ρ, in order to avoid divide by zero issues in calculations using the sound speed, it is necessary that the C_1 coefficient not be zero, so an input value of 1.0e-20 was used for this coefficient when testing the other terms in the polynomial. Also, in order for the terms dependent on the internal energy to perform as expected, it is required to have an initial energy present in the simulation, so the initial internal energy was set to a value of 1.0e-3 in the cubes testing these terms (Cubes 5, 6, 7, 9 and 10). In the cubes testing the other coefficients (Cubes 1, 2, 3, 4 and 8), the initial internal energy was set to 1.0e-9. In addition, in order to eliminate issues with the work performed by the bulk viscosity, the two input coefficients for the bulk viscosity on the material card were set to 1.0e-20 in each of the 10 cubes. Failing to do so results in the work performed on the cube being dominated by contributions from the bulk viscosity. Finally, the code version used for this test was version 15.2.0 revision 1.3359.

Input coefficients for Equation-of-State Form 15 were developed for the purposes of this testing. The values were chosen so that the contribution from each term was of the same order of magnitude (with the exception of the first term, which is constant). The following values were used as input for the testing of the full implementation of EOS Form 1: C_0 = 1.0e-9, C_1 = 1.224e-4, C_2 = 1.2e-3, C_3 = 1.3e-2, C_4 = 1.1e-2, C_5 = 2.4e-4 and C_6 = 1.3. The following table gives the values of the coefficients for each of the 10 cubes in the test suite.

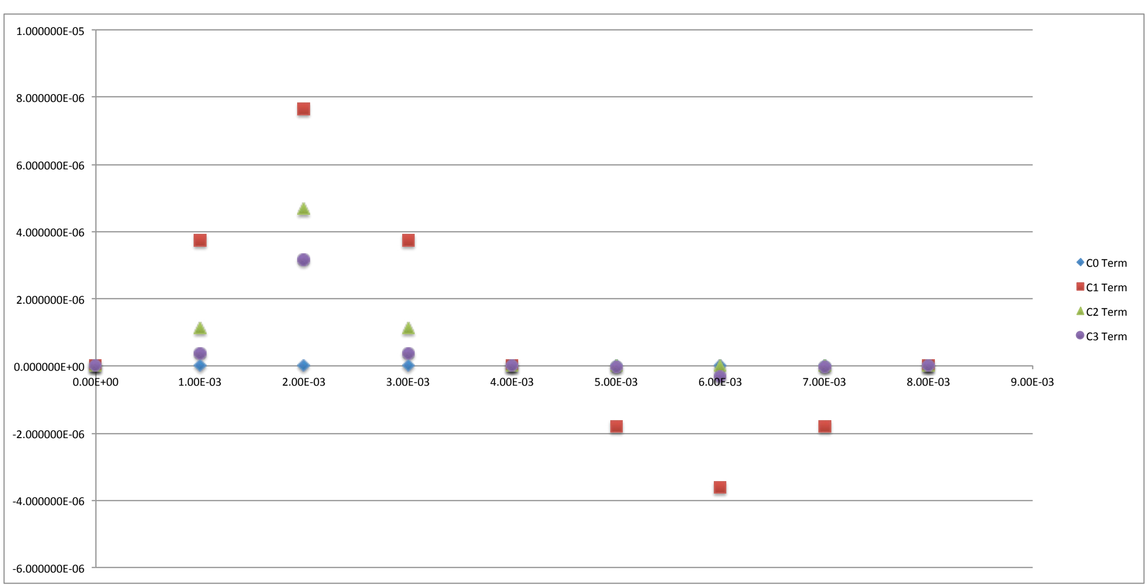
Table 87. Suite of test input coefficients for EOS Form 15

Cube	C_0	C_1	C_2	C_3	C_4	C_5	C_6
1	1.0e-9	1.0e-20	0	0	0	0	0
2	0	1.224e-4	0	0	0	0	0
3	0	1.0e-20	1.2e-3	0	0	0	0
4	0	1.0e-20	0	1.3e-2	0	0	0
5	0	1.0e-20	0	0	1.1e-2	0	0
6	0	1.0e-20	0	0	0	2.4e-4	0
7	0	1.0e-20	0	0	0	0	1.3
8	1.0e-9	1.224e-4	1.2e-3	1.3e-2	0	0	0
9	0	1.0e-20	0	0	1.1e-2	2.4e-4	1.3
10	1.0e-9	1.224e-4	1.2e-3	1.3e-2	1.1e-2	2.4e-4	1.3

As stated above, the intent of this test was to create a situation in which each term in the polynomial was making essentially an equal contribution to the final pressure (with the exception of the C_0 term, which represents a constant offset) and not to create a test that was reflective of any real material.

Each term in the polynomial was tested independently, then the sums of the first four terms and the last three terms, followed by testing of the EOS as a whole. The following plot contains the pressure from each of the first four terms in the polynomial, as returned by the code, as a function of time for this simulation.

Figure 45. Code pressures for the first four coefficients as a function of time



As the plot demonstrates, each of the terms depending on μ returns a peak pressure on the order of 10^{-6} in compression and on the order of -10^{-6} in tension. Note that the C_2 term depends on $\overline{\mu}$, not μ, and therefore makes no contribution to the pressure when the cube is in tension. Note also that the pressures in tension are lower than in compression due to the smaller displacements used to prevent failure of the material.

The following observations can be made from the code output. Coefficient 0 represents a constant pressure offset and was set to a value of 1.0e-9 in the first cube. To better than 1 part in 10^{12}, the cube remains at this pressure during the cycling of its volume. Coefficient 1 is linear in the excess compression. It should therefore return zero pressure when the compression is zero, return a positive value when the cube is compressed and should be negative when the cube is expanded, which is reflected in the code output. Coefficient 2 goes as the square of the tension-limited excess compression and should therefore only return positive pressures when the cube is compressed, which is what the code returns. Coefficient 3 is proportional to the cube of the excess compression. It should therefore return zero pressure when the compression is zero, return a positive value when the cube is compressed and should be negative when the cube is expanded, which is reflected in the code output. Therefore, the code output is behaving qualitatively as expected.

Using the normalized difference defined in the testing of EOS Form 1, the agreement between the pressures for the C_3 coefficient is demonstrated to be better than 1 part in 10^{11} in the following table.

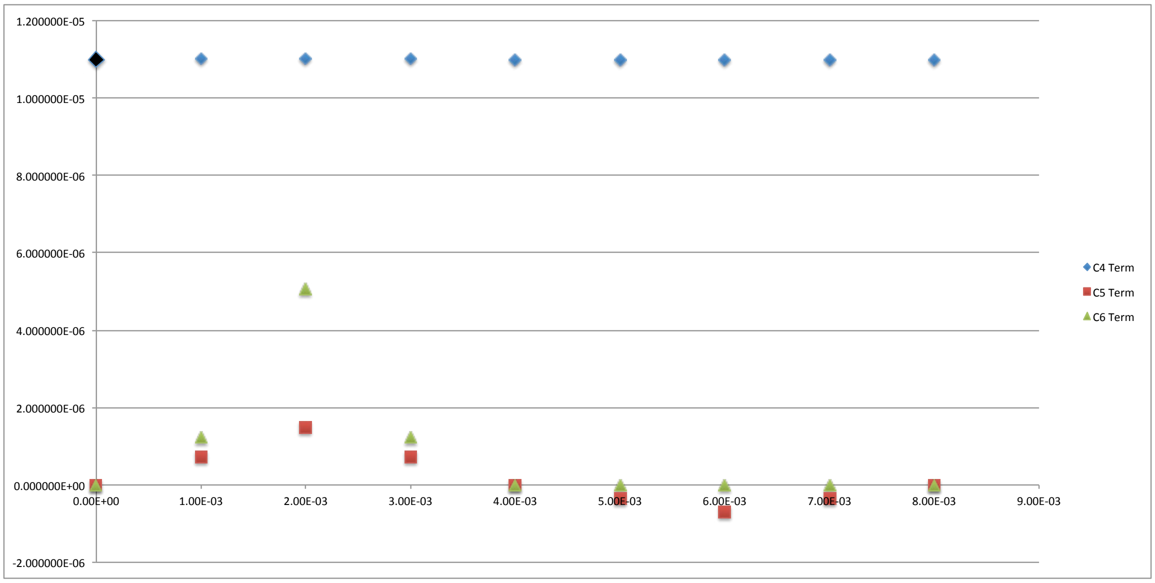
Table 88. Exact and Code Pressures for the C_3 Coefficient

Time	*Theoretical*	*Code*	*(Theoretical - Code)/Code*
0.00E+00	0.000000E+00	0.000000E+00	0.000000E+00
1.00E-03	3.728549E-07	3.728549E-07	3.765283E-12
2.00E-03	3.171158E-06	3.171158E-06	7.890289E-13
3.00E-03	3.728549E-07	3.728549E-07	-2.457323E-12
4.00E-03	0.000000E+00	0.000000E+00	0.000000E+00
5.00E-03	-4.258254E-08	-4.258254E-08	5.089752E-12
6.00E-03	-3.306906E-07	-3.306906E-07	4.020127E-12
7.00E-03	-4.258254E-08	-4.258254E-08	1.137175E-11
8.00E-03	0.000000E+00	0.000000E+00	0.000000E+00

As the table clearly demonstrates, the predictions of theoretical expression and the code results are in excellent agreement. Similar, or better, levels of agreement are exhibited between the theoretical expression and the code results for the C_0, C_1 and C_2 coefficient terms.

The next plot displays the pressure from each of the last three terms in the polynomial, as returned by the code, as a function of time for this simulation.

Figure 46. Code pressures for the last three coefficients as a function of time



As the plot demonstrates, the C_4 term, which depends only on the internal energy, makes a contribution on the order of 10^{-5}, while the C_5 term returns a peak pressure on the order of 10^{-6} in compression and on the order of -10^{-6} in tension. Note that the C_6 term depends on $\overline{\mu}$, not μ, and therefore makes no contribution to the pressure when the cube is in tension. Note also that the pressures in tension are lower than in compression due to the smaller displacements used to prevent failure of the material.

Coefficient 4 is proportional to the internal energy and should therefore return a value of 1.1e-5 when the cube is at its original volume, a value larger than this when compressed and a value smaller than this when expanded. This is again reflected in the code output, with the value at zero compression being equal to the expected value to better than 1 part in 10^{14}. Coefficient 5 is linear in both the excess compression and the internal energy. It should therefore return zero pressure when the compression is zero, return a positive value when the cube is compressed and should be negative when the cube is expanded, which is reflected in the code output. Coefficient 6 is linear in the internal energy and proportional to the square of the tension-limited excess Compression. It should therefore only return positive pressures when the cube is compressed, which is what the code returns. Therefore, the code output is behaving qualitatively as expected.

Using the normalized difference defined in the testing of EOS Form 1, the agreement between the theoretical expression and the code result can be quantified as illustrated in the following table for the C_5 coefficient.

Table 89. Exact and Code Pressures for the C_5 Coefficient

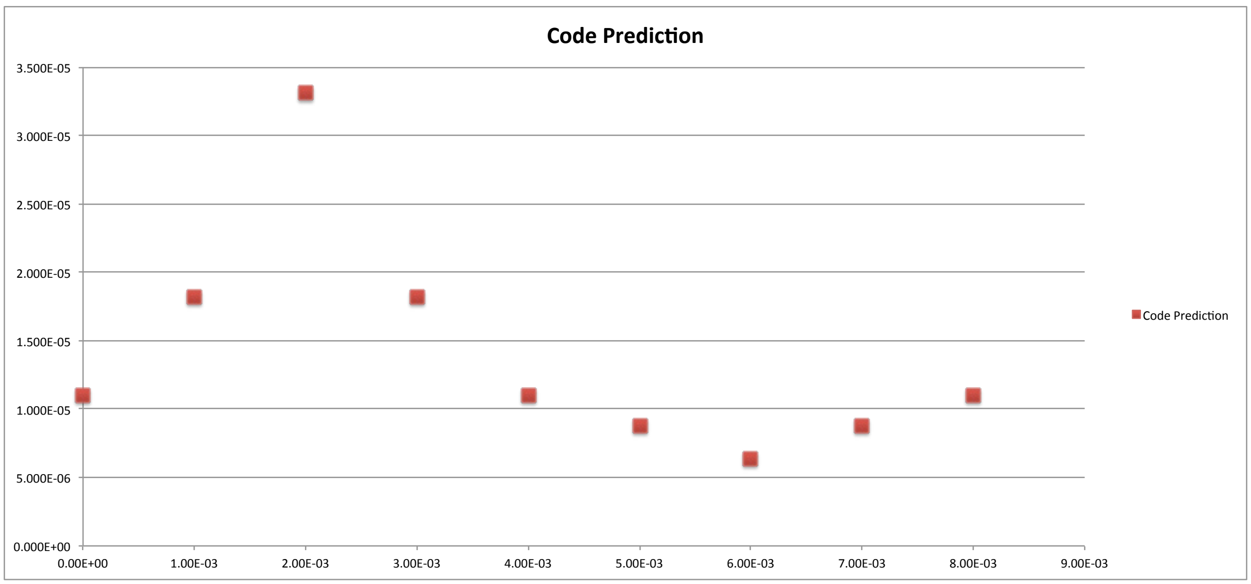
Time	*Theoretical*	*Code*	*(Theoretical - Code)/Code*
0.00E+00	0.000000E+00	0.000000E+00	0.000000E+00
1.00E-03	7.346516E-07	7.346516E-07	1.773992E-12
2.00E-03	1.499644E-06	1.499644E-06	6.875304E-13
3.00E-03	7.346516E-07	7.346516E-07	1.685069E-12
4.00E-03	0.000000E+00	0.000000E+00	0.000000E+00

5.00E-03	-3.564307E-07	-3.564307E-07	-2.009718E-12
6.00E-03	-7.058441E-07	-7.058441E-07	-6.270148E-14
7.00E-03	-3.564307E-07	-3.564307E-07	-2.674970E-13
8.00E-03	0.000000E+00	0.000000E+00	0.000000E+00

As was observed in the results from the first four coefficients, the agreement between the code results and the theoretical expression is better than 1 part in 10^{11}. Similar, or better, levels of agreement are exhibited between the theoretical expression and the code results for the C_4 and C_6 coefficient terms.

Now that the behavior of each of the individual terms in the expression for Equation-of-State Form 15 has been investigated, the behavior of the full expression can be examined. The following plot contains the pressure returned by the code for the full equation-of-state as a function of time.

Figure 47. Code pressure for EOS 15 as a function of time



Note that the pressure is behaving as one would expect, in that the pressure increases as the cube is compressed, decreases back to the starting value as the compression is released, further decreases as the cube is placed into tension and then relaxes back to the starting value as the tension is released. Also, while the pressures in compression are similar to those returned from the testing of EOS Form 1, the change in pressure exhibited by the cube while in tension is substantially reduced due to the smaller displacement required to prevent activation of the failure model.

The following table compares the pressure returned by the code as a function of time for the full equation-of-state to that predicted by the theoretical expression.

Table 90. Exact and Code Pressures for Equation-of-State Form 15

Time	*Code*	*Theoretical*	*(Theoretical - Code)/Code*
0.00E+00	1.1001000E-05	1.100100000E-05	0.000000E+00

1.00E-03	1.8203052E-05	1.820305106E-05	-6.094160E-08
2.00E-03	3.3099799E-05	3.309977696E-05	-6.594155E-07
3.00E-03	1.8203052E-05	1.820302423E-05	-1.534894E-06
4.00E-03	1.1001000E-05	1.100096614E-05	-3.077507E-06
5.00E-03	8.7826078E-06	8.782607694E-06	-1.608609E-08
6.00E-03	6.3619805E-06	6.362419780E-06	6.904992E-05
7.00E-03	8.7826078E-06	8.784738686E-06	2.426216E-04
8.00E-03	1.1001000E-05	1.100144737E-05	4.066614E-05

As demonstrated in the table, the code result agrees with the theoretical expression to better than 2 parts in 10^6 in compression and about 2.5 parts in 10^4 in tension. These results establish confidence in the pressures returned by the implementation of Equation-of-State Form 1 in DYNA3D.

It is unclear why the agreement is poorer in tension than in compression, or why the agreement is lower than that exhibited for the individual terms. It is worth noting that the level of agreement exhibited in Table 90 is similar to the results from the testing of EOS Form 1 (See Table 4).

The code results for the internal energy can also be examined for EOS Form 15. If one assumes that $C_0=C_1=C_2=C_3=0$, then a simple closed form solution for the internal energy resulting from the remaining terms can be derived[1]. The form of the solution is as follows:

$$E = \exp\{- (C_4(V-1) + C_5(\ln V - V +1) + C_6(-1/V - 2\ln V + V)) + \ln E_0\}$$

where V is the final volume of the cube and E_0 is the initial specific internal energy. This solution takes advantage of the fact that the initial volume of the cube is 1 cm^3. Note also that the C_6 term contributes to the internal energy only when the tension-limited excess compression is non-zero.

Unfortunately, DYNA3D does not write the internal energy to the high-speed edit file, so GRIZ was used to extract the internal energy from the code results. This limits the accuracy of the comparison because the GRIZ output contains only 7 significant figures. A numerical integration (similar to that performed by DYNA3D) was performed using EXCEL as a check on both the results of the closed form solution and the internal energy as extracted using GRIZ.

The internal energy resulting from each of the three terms, extracted from the code output using GRIZ, was compared to the closed form solution. The following table displays the results for the internal energy resulting from the contribution of the C_5 term as a function of time.

Table 91. Exact and Code results for the Internal Energy from the C_5 term

Time	Code (GRIZ)	*Closed Form*	(*Closed* - GRIZ)/GRIZ
0.00E+00	1.00000000E-03	1.000000E-03	0.000000E+00
1.00E-03	1.00001100E-03	1.000011E-03	-1.997580E-07
2.00E-03	1.00004300E-03	1.000043E-03	2.038514E-07
3.00E-03	1.00001100E-03	1.000011E-03	-1.997580E-07
4.00E-03	1.00000000E-03	1.000000E-03	2.168404E-16
5.00E-03	1.00000300E-03	1.000003E-03	-2.999842E-07

6.00E-03	1.00001100E-03	1.000011E-03	-1.997609E-07
7.00E-03	1.00000300E-03	1.000003E-03	-2.999842E-07
8.00E-03	1.00000000E-03	1.000000E-03	2.168404E-16

As expected, given the restrictions on the GRIZ output, agreement between the two numbers is at the level of a few parts in 10^7. This level of agreement is similar to that obtained for the C_4 and C_6 coefficients, as well.

The closed form solution for the internal energy resulting from the contribution for the three coefficients combined can also be compared to the code results, which is displayed in the following table.

Table 92. Exact and Code results for the Internal Energy from all 3 terms

Time	Code (GRIZ)	C_4 - C_6 *Closed Form*	(*Closed* - GRIZ)/GRIZ
0.00E+00	1.00000000E-03	1.00000000E-03	0.00000000E+00
1.00E-03	1.00034900E-03	1.00034945E-03	4.50177450E-07
2.00E-03	1.00078700E-03	1.00078689E-03	-1.06876630E-07
3.00E-03	1.00034900E-03	1.00034945E-03	4.50177450E-07
4.00E-03	1.00000000E-03	1.00000000E-03	2.16840434E-16
5.00E-03	9.99836800E-04	9.99836887E-04	8.69547783E-08
6.00E-03	9.99677600E-04	9.99677541E-04	-5.88393734E-08
7.00E-03	9.99836800E-04	9.99836887E-04	8.69547783E-08
8.00E-03	1.00000000E-03	1.00000000E-03	2.16840434E-16

As expected, the agreement between the two numbers is at the level of a few parts in 10^7, similar to the agreement displayed in the examination of the behavior of the individual coefficients and limited by the precision of the GRIZ output.

DYNA3D uses numerical integration for these calculations rather than a closed form solution. Therefore, a numerical integration was performed in EXCEL to check against the closed form solution, which should be exact. The following table compares the results for the internal energy from the numerical integration scheme to the closed form solution for the C_5 coefficient.

Table 93. Exact and Numerical Integration results for the Internal Energy from the C_5 term

Time	Numerical Int	*Closed Form*	(*Closed* - NI)/NI
0.00E+00	1.00000000E-03	1.00000000E-03	0.00000000E+00
1.00E-03	1.00001079E-03	1.00001080E-03	1.09090606E-08
2.00E-03	1.00004318E-03	1.00004320E-03	2.20412156E-08
3.00E-03	1.00001059E-03	1.00001080E-03	2.14983742E-07
4.00E-03	1.00000019E-03	1.00000000E-03	-1.88848754E-07
5.00E-03	1.00000270E-03	1.00000270E-03	2.68658524E-09
6.00E-03	1.00001110E-03	1.00001080E-03	-2.97324236E-07
7.00E-03	1.00000290E-03	1.00000270E-03	-1.97100923E-07

8.00E-03	1.00000030E-03	1.00000000E-03	-2.97297692E-07

As the table demonstrates, the agreement between the closed form solution and the EXCEL numerical integration is about the same as that exhibited by the closed form solution and the code results (as extracted using GRIZ). This is not surprising, as the GRIZ output is limited to 7 significant figures.

The level of agreement exhibited by the C_5 coefficient is also obtained for the C_6 coefficient, while the C_4 coefficient exhibits agreement between the numerical integration scheme and the closed form solution that is about 2 orders of magnitude better. As the contribution of the C_4 coefficient depends only on E (and not μ), this is not surprising.

The closed form solution for the internal energy resulting from the contribution for the three coefficients combined can also be compared to the results of the EXCEL numerical integration, which is displayed in the following table.

Table 94. Exact and Numerical Integration results for the Internal Energy from all 3 terms

Time	C_4 - C_6 Numerical Int	C_4 - C_6 *Closed Form*	(*Closed* - NI)/NI
0.00E+00	1.000000000E-03	1.00000000E-03	0.00000000E+00
1.00E-03	1.000349421E-03	1.00034945E-03	2.89911294E-08
2.00E-03	1.000786797E-03	1.00078689E-03	9.62788491E-08
3.00E-03	1.000349490E-03	1.00034945E-03	-3.95746853E-08
4.00E-03	9.999995208E-04	1.00000000E-03	4.79181257E-07
5.00E-03	9.998368842E-04	9.99836887E-04	2.69988588E-09
6.00E-03	9.996774516E-04	9.99677541E-04	8.96274622E-08
7.00E-03	9.998369431E-04	9.99836887E-04	-5.61667153E-08
8.00E-03	9.999999103E-04	1.00000000E-03	8.96546353E-08

As expected, the level of agreement exhibited in the table is, in general, a few parts in 10^8, similar to the level of agreement exhibited by the C_5 and C_6 coefficients.

Continuing with the closed form solution investigation, if one assumes that $C_4=C_5=C_6=0$, then a simple closed form solution for the internal energy due to the first four terms can be developed, which exhibits the following form:

$$E = -\{C_0(V-1) + C_1(\ln V - V + 1) + C_2(-1/V - 2\ln V + V) + C_3(-1/(2V^2) + 3/V + 3\ln V - V - 1.5)\} + E_0$$

where V is the final volume of the cube and E_0 is the initial internal energy. This solution takes advantage of the fact that the initial volume of the cube is 1 cm^3. Note that the C_2 term contributes to the internal energy only when the tension-limited excess compression is non-zero.

The internal energy resulting from each of the four terms, extracted from the code output using GRIZ, was compared to the results of the closed form solution. The following table displays the results for the internal energy resulting from the C_1 term as a function of time.

Table 95. Exact and Numerical Integration results for the Internal Energy from the C_1 term

Time	Code (GRIZ)	*Closed Form*	(*Closed* - GRIZ)/GRIZ
0.00E+00	1.000000E-09	1.0000000E-09	0.0000000E+00
1.00E-03	5.608092E-08	5.6080925E-08	9.6391507E-08
2.00E-03	2.213349E-07	2.2133493E-07	1.2195607E-07
3.00E-03	5.608092E-08	5.6080925E-08	9.6391507E-08
4.00E-03	1.000000E-09	1.0000000E-09	0.0000000E+00
5.00E-03	1.477006E-08	1.4770057E-08	-1.9319866E-07
6.00E-03	5.608091E-08	5.6080911E-08	1.2779578E-08
7.00E-03	1.477006E-08	1.4770057E-08	-1.9319866E-07
8.00E-03	1.000000E-09	1.0000000E-09	0.0000000E+00

The agreement between the code results and the closed form solution is better than 2 parts in 10^7 and is similar to the results from coefficients C_0, C_2 and C_3. These results are also similar to the level of agreement exhibited by the results for the last three terms of this EOS.

The internal energy resulting from the combination of the four terms, extracted from the code output using GRIZ, was compared to the results of the closed form solution. The following table displays these results as a function of time.

Table 96. Exact and Numerical Integration results for Internal Energy from the C_0 - C_3 terms

Time	Code (GRIZ)	*Closed Form*	(*Closed* - GRIZ)/GRIZ
0.00E+00	1.0000000E-09	1.0000000E-09	0.0000000E+00
1.00E-03	6.9793750E-08	6.9793744E-08	-8.5787025E-08
2.00E-03	3.5540810E-07	3.5540812E-07	4.7938045E-08
3.00E-03	6.9793750E-08	6.9793744E-08	-8.5787025E-08
4.00E-03	1.0000000E-09	1.0000000E-09	-2.8865805E-09
5.00E-03	1.4916910E-08	1.4916911E-08	4.3050380E-08
6.00E-03	5.8600770E-08	5.8600763E-08	-1.1509280E-07
7.00E-03	1.4916910E-08	1.4916911E-08	4.3050380E-08
8.00E-03	1.0000000E-09	1.0000000E-09	0.0000000E+00

The agreement between the code results and the closed form solution is better than 2 parts in 10^7 and is similar to the level of agreement exhibited by the results for the last three terms of this EOS. This establishes confidence in the numerical integration performed by the code to determine the internal energy.

Finally, a convergence study[2] was performed on the internal energy integration calculation for EOS Form 1 and these results should be applicable to EOS Form 15 as well. A series of seven simulations was run with successively smaller time-step values that varied between 5.0e-5 and 8.9e-11. Each simulation was run to the first peak in the compression. The final value of the internal energy for each of the first seven cubes was extracted using GRIZ. Using the energy from the simulation with the smallest time-step size as the “exact” answer, the error (difference in values) for each cube/term was calculated and examined as a function of the time-step size. For each term, the error looked like *error* = $C\,\Delta t^2$, where C is some constant and Δt is the time-step size. Therefore, the integration of the internal energy is second order accurate as the error is quadratic in Δt.

The pressure is the more important quantity being determined from the equation-of-state and the agreement between the code results and those obtained from the theoretical equation is better than 5 parts in 10^7, as exhibited earlier. This level of agreement is similar to that exhibited by the code results for the internal energy and the closed form solutions. Finally, as established by the convergence study, the agreement between the closed form solutions for the internal energy and the code results can be improved by decreasing the time step, which would also improve the agreement between the code predictions for the pressure and the theoretical result

This establishes the implementation of Equation-of-State Form 15 in DYNA3D. The equation-of-state is performing as expected, in that the pressure in the cubes increases as they are compressed and decreases as they are expanded. The behavior of each of the terms in the equation-of-state has been examined and found to be performing as expected and with good accuracy. The behavior of the equation-of-state as a whole has been examined and is performing as expected and with good accuracy.

Equation-of-State Form 16

Equation-of-State Form 16 has been removed from the code as a result of the creation of this test suite and the subsequent analysis performed. The results of the testing and analysis performed on EOS Form 16 may be found in Appendix B.

Equation-of-State Form 17

Equation-of-State Form 17 is a Pore Collapse model (a modification of EOS Form 11) intended for use only with Material Model 64. It uses two curves: the virgin loading curve and the completely crushed curve, as shown in the figure below (taken from the EOS Form 11 section of

Figure 48. Illustration of EOS Form 11 from the DYNA3D manual

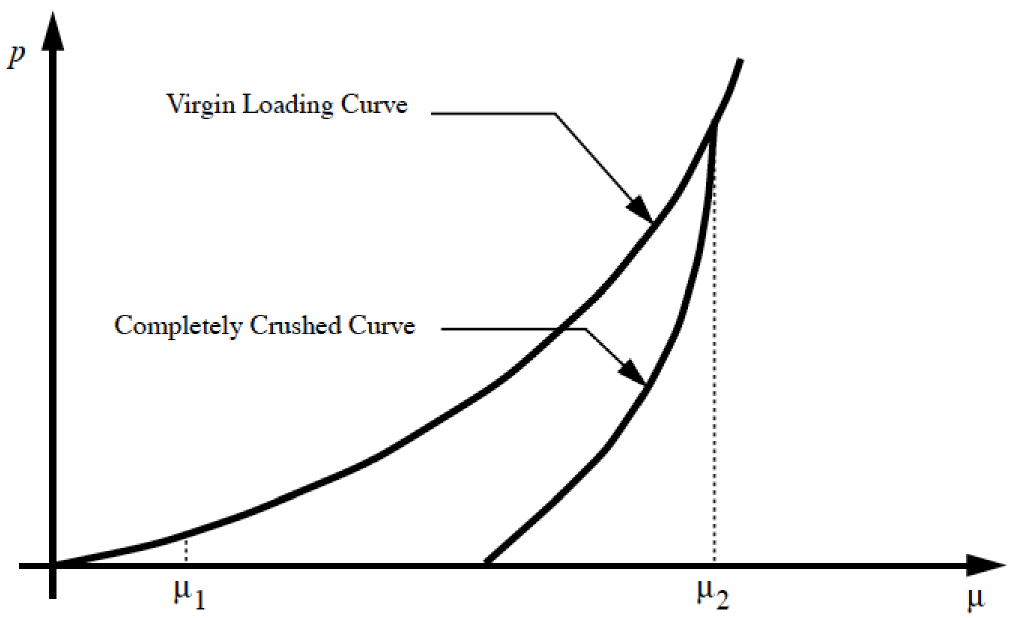


Figure 43
Pressure vs. excess compression for the Pore Collapse equation-of-state. The partially crushed curve lies between the Virgin Loading Curve and the Completely Crushed Curve.

DYNA3D manual). The loading curves are entered into the model by defining the pressures as a function of the excess compression, μ (related to the density by $\mu = \rho/\rho_0 - 1$). Note that μ is positive in compression and negative in tension.

The model requires the definition of two critical points: the excess compression required for pore collapse to begin (μ_1) and the excess compression required for the material to be completely crushed (μ_2). Unloading occurs along the virgin loading curve until the excess compression exceeds μ_1. Once the excess compression exceeds μ_1, unloading occurs along a partially crushed path between the virgin and completely crushed curves defined by:

$$p_{pc}\left(\mu\right) = p_{cc}\left(\frac{\left(1+\mu_B\right)\left(1+\mu\right)}{1+\mu_{\max}} - 1\right)$$

where

$$\mu_B = p_{cc}^{-1}(p_{\max})$$

is the excess compression corresponding to a pressure of p_{max} on the completely crushed curve.

Prior to discussing the calculations using EOS Form 17, a few code issues need to be addressed and these are not necessarily readily apparent to the user. First, in order to eliminate issues with the work performed by the bulk viscosity, the two input coefficients for the bulk viscosity on the material card were set to 1.0e-20 in each of the 3 cubes. Failing to do so results in the work performed on the cube being dominated by contributions from the bulk viscosity. Finally, the code version used for this test was version 15.2.0 revision 1.3368.

The implementation of the model in DYNA3D uses a monotonic cubic spline to model the virgin loading and completely crushed curves. Previous testing of this equation-of-state model[3] revealed that cubic spline routines available for use in EXCEL returned results that differed from each other by as much as several per cent when applied to the same data sets. This makes characterization of the code results difficult if one is to rely on the values returned by these routines. Therefore, the decision was made to test this EOS model using two sets of input curves. The first set of curves would define linear relationships between the pressure and the excess compression for both the virgin loading and completely crushed curves. This would allow the pressure to be calculated exactly from the excess compression without relying on an interpolation to check the code result. The second set of curves were provided by Jerry Lin for the initial testing of this EOS model and resemble the curves that appear in the figure on the previous page. This testing requires the use of a cubic spline routine to compare to the code results. In addition, the pressure in this EOS model is defined to be independent of the internal energy and so each set of input curves was tested twice using different initial values for the internal energy to verify this independence.

The first set of curves to be tested uses 10 points to define a linear relationship between the excess compression and the pressure for both the virgin loading curve and the completely crushed curve. The defining points are given in the following table:

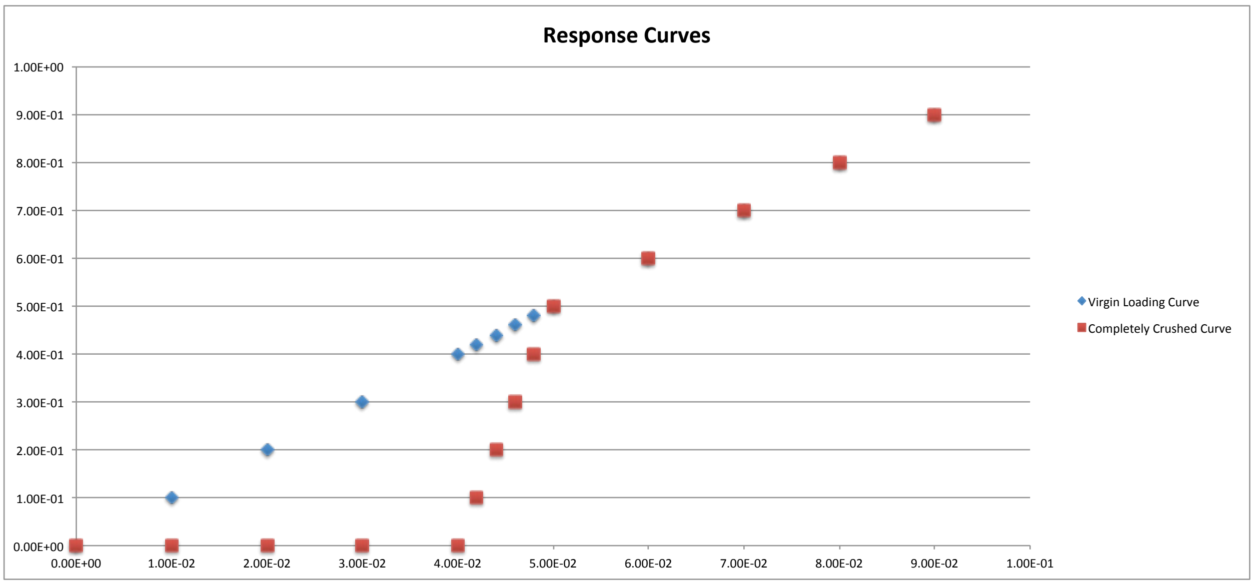
Table 97. Linear response curves used for testing EOS Form 17

Virgin Loading Curve		Completely Crushed Curve	
μ	*p*	μ	*p*
0.000000E+00	0.000000E+00	4.000000E-02	0.000000E+00
1.000000E-02	1.000000E-01	4.200000E-02	1.000000E-01
2.000000E-02	2.000000E-01	4.400000E-02	2.000000E-01
3.000000E-02	3.000000E-01	4.600000E-02	3.000000E-01
4.000000E-02	4.000000E-01	4.800000E-02	4.000000E-01
5.000000E-02	5.000000E-01	5.000000E-02	5.000000E-01
6.000000E-02	6.000000E-01	6.000000E-02	6.000000E-01
7.000000E-02	7.000000E-01	7.000000E-02	7.000000E-01
8.000000E-02	8.000000E-01	8.000000E-02	8.000000E-01
9.000000E-02	9.000000E-01	9.000000E-02	9.000000E-01

For these linear curves, $\mu_1 = 0.01$ and $\mu_2 = 0.05$. These response curves will be tested using Cubes 1 and 2, with Cube 1 having an initial internal energy of $1x10^{-6}$ and Cube 2 an initial internal energy of $1x10^{-3}$. These linear response curves can be calculated exactly in the spreadsheet model.

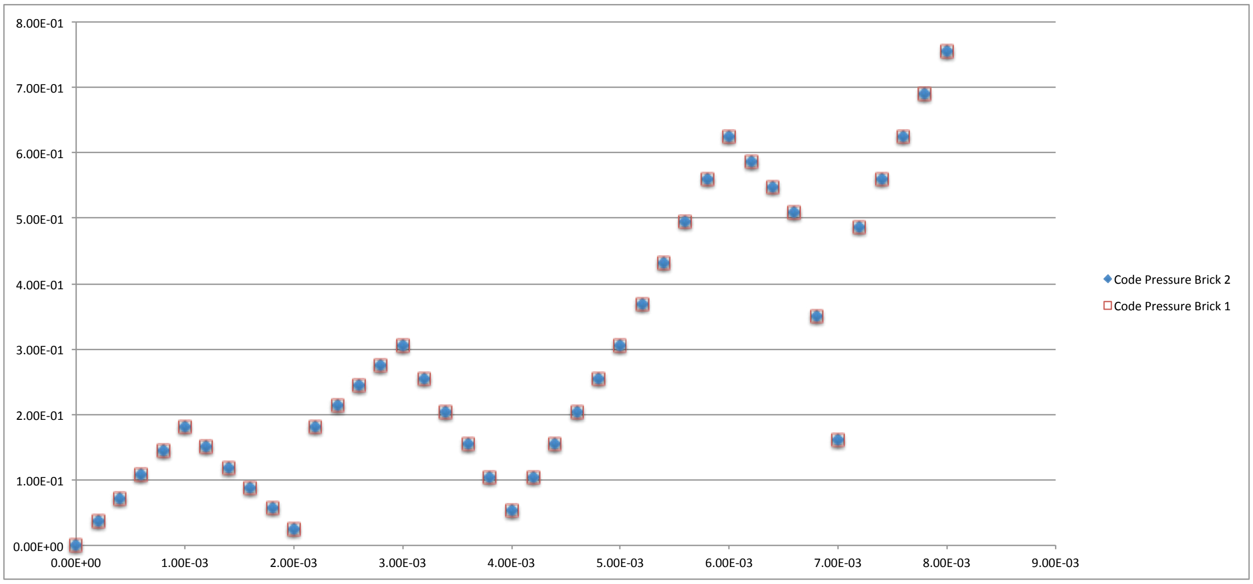
The following plot illustrates that these response curves yield a result which resembles the earlier figure from the DYNA3D manual. However, the use of these curves actually represents an overtest in terms of physical reality, in that actual curves would not display such a pronounced kink when the two curves merge. This will illuminate an issue with the cubic spline routines used in the code, which will be discussed below.

Figure 49. Linear response curves used for testing Cubes 1 and 2



Given the definition of the pressure in this equation-of-state model, one would expect Cubes 1 and 2 to return the same pressures as a function of time, which is the result obtained. The pressures for these 2 cubes are shown in the following plot as a function of time. Note that the cubes are loaded 4 times and unloaded 3 times, with two of the load/unload cycles occurring below $\mu=\mu_2$. As the plot demonstrates, at least at the level of the graph norm, the two cubes are returning the same pressure.

Figure 50. Cubes 1 and 2 pressures from testing EOS Form 17 with linear response curves



The following table makes this point more forcefully, and also reveals the issue with the cubic spline routines mentioned earlier.

Table 98. Code pressures returned for Cubes 1 and 2 from testing EOS Form 17

Time	Analytic Pressure	C1 Pressure	(An - C1)/C1	C2 Pressure	(An-C2)/C2
0.00E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00
2.00E-04	3.608657E-02	3.608657E-02	-6.770342E-13	3.608657E-02	8.000964E-13
4.00E-04	7.234699E-02	7.234699E-02	-1.216155E-13	7.234699E-02	6.759829E-13
6.00E-04	1.087823E-01	1.087823E-01	-7.450319E-14	1.087823E-01	2.472383E-13
8.00E-04	1.453935E-01	1.453935E-01	-7.292367E-14	1.453935E-01	-3.136481E-13
1.00E-03	1.821818E-01	1.821818E-01	-5.576046E-14	1.821818E-01	-1.546362E-13
1.20E-03	1.506962E-01	1.506962E-01	-2.273915E-12	1.506962E-01	-4.052380E-12
1.40E-03	1.192359E-01	1.192359E-01	-6.958921E-13	1.192359E-01	-5.904084E-12
1.60E-03	8.780086E-02	8.780086E-02	-1.014112E-12	8.780086E-02	-1.029649E-11
1.80E-03	5.639113E-02	5.639113E-02	-4.629856E-12	5.639113E-02	-9.189081E-12
2.00E-03	2.500666E-02	2.500666E-02	-1.148414E-11	2.500666E-02	-3.405813E-11
2.20E-03	1.821818E-01	1.821818E-01	-6.086422E-13	1.821818E-01	-1.267408E-12
2.40E-03	2.129747E-01	2.129747E-01	-6.735112E-13	2.129747E-01	-8.003158E-13
2.60E-03	2.438918E-01	2.438918E-01	-3.805566E-13	2.438918E-01	-7.987820E-13
2.80E-03	2.749339E-01	2.749339E-01	-3.046781E-13	2.749339E-01	-1.039419E-12
3.00E-03	3.061015E-01	3.061015E-01	-3.169977E-13	3.061015E-01	-9.408377E-13
3.20E-03	2.554132E-01	2.554132E-01	2.716732E-14	2.554132E-01	7.317790E-13
3.40E-03	2.047904E-01	2.047904E-01	-8.207795E-13	2.047904E-01	1.537742E-12
3.60E-03	1.542329E-01	1.542329E-01	-1.481601E-12	1.542329E-01	2.603104E-12

3.80E-03	1.037408E-01	1.037408E-01	-5.968984E-13	1.037408E-01	5.032568E-12
4.00E-03	5.331371E-02	5.331371E-02	-5.158971E-12	5.331371E-02	1.126649E-11
4.20E-03	1.037408E-01	1.037408E-01	-6.023965E-12	1.037408E-01	6.851891E-13
4.40E-03	1.542329E-01	1.542329E-01	-3.160976E-12	1.542329E-01	-2.000242E-12
4.60E-03	2.047904E-01	2.047904E-01	-1.865728E-12	2.047904E-01	-1.104041E-12
4.80E-03	2.554132E-01	2.554132E-01	-1.339240E-12	2.554132E-01	-2.666527E-12
5.00E-03	3.061015E-01	3.061015E-01	2.981375E-13	3.061015E-01	-1.162083E-12
5.20E-03	3.688160E-01	3.688160E-01	-2.819086E-13	3.688160E-01	-1.149609E-12
5.40E-03	4.320403E-01	4.307048E-01	3.100694E-03	4.307048E-01	3.100694E-03
5.60E-03	4.957797E-01	4.957797E-01	-3.300798E-13	4.957797E-01	-1.048127E-12
5.80E-03	5.600394E-01	5.600394E-01	-3.326470E-13	5.600394E-01	-1.014593E-12
6.00E-03	6.248247E-01	6.248247E-01	-2.048714E-13	6.248247E-01	-9.346259E-13
6.20E-03	5.858901E-01	5.858901E-01	-1.464784E-13	5.858901E-01	-8.479829E-13
6.40E-03	5.471455E-01	5.471455E-01	-1.743013E-13	5.471455E-01	-9.528740E-13
6.60E-03	5.085898E-01	5.085898E-01	-2.220054E-13	5.085898E-01	-8.768886E-13
6.80E-03	3.511088E-01	3.511088E-01	-1.738494E-12	3.511088E-01	-5.247419E-12
7.00E-03	1.602014E-01	1.602014E-01	-3.322497E-12	1.602014E-01	-1.379052E-11
7.20E-03	4.788983E-01	4.868939E-01	-1.642173E-02	4.868939E-01	-1.642173E-02
7.40E-03	5.600394E-01	5.600394E-01	-2.246061E-13	5.600394E-01	-8.478733E-13
7.60E-03	6.248247E-01	6.248247E-01	-1.099873E-13	6.248247E-01	-7.661800E-13
7.80E-03	6.901411E-01	6.901411E-01	-7.705625E-14	6.901411E-01	-6.523238E-13
8.00E-03	7.559939E-01	7.559939E-01	3.377690E-15	7.559939E-01	-6.422017E-13

As the table illustrates, the analytic model and the code are in excellent agreement and the differences in the pressures returned by Cubes 1 and 2 are very small, as expected, since the internal energy does not play a role in determining the pressure in the equation-of-state model.

However, there are two time points where the analytic model and the code do not agree well. The second of these is at a time of $7.2\text{x}10^{-3}$ and the discrepancy at this time as actually expected, as this point is near μ_2, which means the cubic spline in the code is drawing a smooth curve around the kink in the response curve, so it is not surprising that a disagreement is obtained at this point. The other issue occurs at a time of $5.4\text{x}10^{-3}$ and uncovering the cause of this discrepancy illustrates an issue with the cubic splines and how they are used in the code.

To improve the speed of the code, three cubic spline fits are actually employed by the code. There is a fit for the virgin loading curve, the completely crushed curve and the inverse of the completely crushed curve, which is required for loading and unloading at points between μ_1 and μ_2. The code uses the partially crushed curve defined by the earlier equation for loading and unloading for all $\mu_1<\mu<\mu_2$ and it turns out that the fits to the completely crushed curve and its inverse are not always mathematical inverses of each other, i.e.,

$$\mu = p_{cc}^{-1}\left(p_{cc}\left(\mu\right)\right)$$

does not hold for all values of μ between all of the input data pairs. This can cause the code to return a loading that does not agree exactly with the expected value and is the reason for the discrepancy between the analytical model and the code result at a time of 5.4×10^{-3}.

Having established that the implementation of this equation-of-state model can indeed match the results of a simplified response curve, the following, more realistic response curves provided by Jerry Lin were used to test the EOS model.

Table 99. Generalized response curves used for testing EOS Form 17

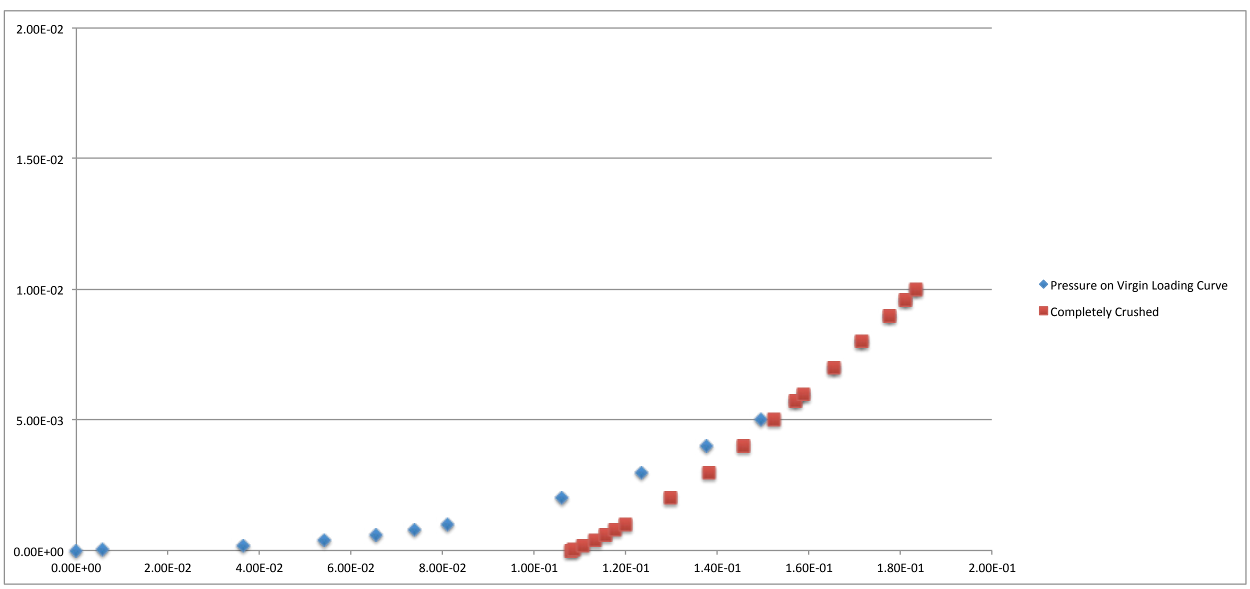
Virgin Loading Curve		Completely Crushed Curve	
μ	*p*	μ	*p*
0.00000000E+00	0.00000000E+00	1.08030000E-01	0.00000000E+00
5.63830000E-03	4.30000000E-05	1.08600000E-01	4.30000000E-05
3.63890000E-02	2.00000000E-04	1.10630000E-01	2.00000000E-04
5.40830000E-02	4.00000000E-04	1.13110000E-01	4.00000000E-04
6.53400000E-02	6.00000000E-04	1.15470000E-01	6.00000000E-04
7.39140000E-02	8.00000000E-04	1.17730000E-01	8.00000000E-04
8.09860000E-02	1.00000000E-03	1.19910000E-01	1.00000000E-03
1.06040000E-01	2.00000000E-03	1.29690000E-01	2.00000000E-03
1.23510000E-01	3.00000000E-03	1.38130000E-01	3.00000000E-03
1.37480000E-01	4.00000000E-03	1.45630000E-01	4.00000000E-03
1.49370000E-01	5.00000000E-03	1.52440000E-01	5.00000000E-03
1.56970000E-01	5.71370000E-03	1.56970000E-01	5.71370000E-03
1.58720000E-01	6.00000000E-03	1.58720000E-01	6.00000000E-03
1.65330000E-01	7.00000000E-03	1.65330000E-01	7.00000000E-03
1.71620000E-01	8.00000000E-03	1.71620000E-01	8.00000000E-03
1.77640000E-01	9.00000000E-03	1.77640000E-01	9.00000000E-03
1.81140000E-01	9.60000000E-03	1.81140000E-01	9.60000000E-03
1.83430000E-01	1.00000000E-02	1.83430000E-01	1.00000000E-02
2.09720000E-01	1.50000000E-02	2.09720000E-01	1.50000000E-02
2.32960000E-01	2.00000000E-02	2.32960000E-01	2.00000000E-02
2.50000000E-01	2.40000000E-02	2.50000000E-01	2.40000000E-02
2.71130000E-01	3.00000000E-02	2.71130000E-01	3.00000000E-02
2.86000000E-01	3.50000000E-02	2.86000000E-01	3.50000000E-02
3.00350000E-01	4.00000000E-02	3.00350000E-01	4.00000000E-02
3.27680000E-01	5.00000000E-02	3.27680000E-01	5.00000000E-02
3.78540000E-01	7.00000000E-02	3.78540000E-01	7.00000000E-02
4.48380000E-01	1.00000000E-01	4.48380000E-01	1.00000000E-01
5.56280000E-01	1.50000000E-01	5.56280000E-01	1.50000000E-01
6.68470000E-01	2.00000000E-01	6.68470000E-01	2.00000000E-01

7.72960000E-01	2.50000000E-01	7.72960000E-01	2.50000000E-01
8.48410000E-01	3.00000000E-01	8.48410000E-01	3.00000000E-01
8.97070000E-01	3.50000000E-01	8.97070000E-01	3.50000000E-01
9.39820000E-01	4.00000000E-01	9.39820000E-01	4.00000000E-01
1.01220000E+00	5.00000000E-01	1.01220000E+00	5.00000000E-01
1.12250000E+00	7.00000000E-01	1.12250000E+00	7.00000000E-01
1.20480000E+00	9.00000000E-01	1.20480000E+00	9.00000000E-01
1.23910000E+00	1.00000000E+00	1.23910000E+00	1.00000000E+00
1.36860000E+00	1.50000000E+00	1.45720000E+00	2.00000000E+00
1.45720000E+00	2.00000000E+00		

For these generalized curves, $\mu_1 = 0.0056383$ and $\mu_2 = 0.15697$. These response curves will be tested using Cubes 3 and 4, with Cube 3 having an initial internal energy of 1×10^{-6} and Cube 4 an initial internal energy of 1×10^{-3}. These generalized response curves cannot be calculated exactly in the spreadsheet model, requiring instead the use of a cubic spline to model them. Based on the earlier testing of this EOS model[3], this is expected to result in a poorer match between the spreadsheet model and the code results.

The following plot illustrates that these generalized response curves yield a result which greatly resembles the earlier figure from the DYNA3D manual. Note that the plot is displaying only the bottom part of the curves in order to accentuate the difference between the two curves. Note also that these curves join much more smoothly than the two linear curves used in the earlier tests for this EOS model and the cubic splines should not have as large an effect near the junction point as was observed in the earlier tests. The testing of the EOS model will focus on this part of the curves.

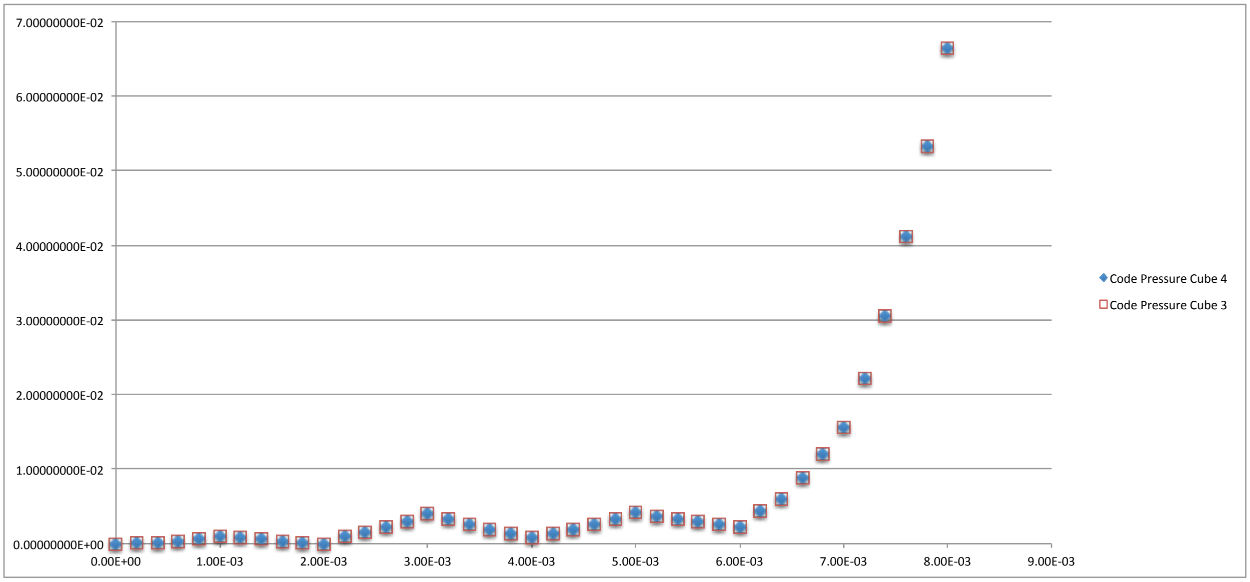
Figure 51. Generalized response curves used for testing Cubes 3 and 4



Given the definition of the pressure in this equation-of-state model, one would expect

Cubes 3 and 4 to return the same pressures as a function of time, which is the result obtained. The pressures for these 2 cubes are shown in the following plot as a function of time. Note that the cubes are loaded 4 times and unloaded 3 times, with three of the load/unload cycles occurring below $\mu=\mu_2$. As the plot demonstrates, at least at the level of the graph norm, the two cubes are returning the same pressure.

Figure 52. Cubes 3 and 4 pressures from testing EOS Form 17 with generalized response curves



The following table makes this point more forcefully, and also demonstrates the reduced agreement between the spreadsheet model and the code results that was expected due to the use of a cubic spline routine in the spreadsheet model.

Table 100. Code pressures returned for Cubes 3 and 4 from testing EOS Form 17

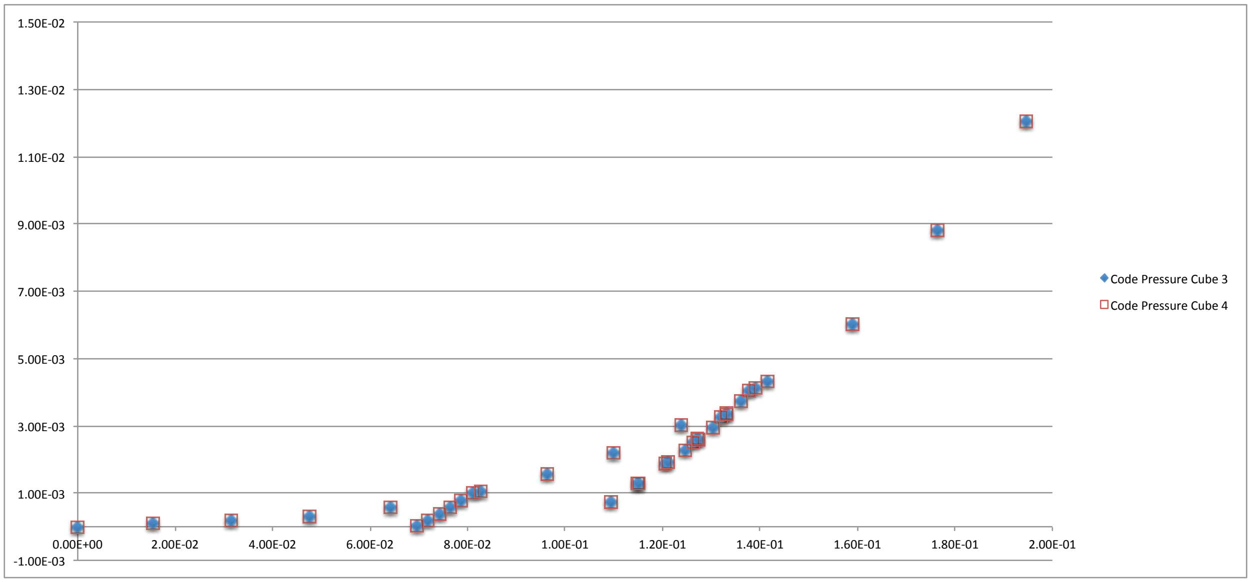
Time	Analytic Pressure	C3 Pressure	(An - C3)/C3	C4 Pressure	(An-C4)/C4
0.00E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00
2.00E-04	9.645977E-05	9.474809E-05	1.806554E-02	9.474809E-05	1.806554E-02
4.00E-04	1.672482E-04	1.677360E-04	-2.908515E-03	1.677360E-04	-2.908515E-03
6.00E-04	3.109244E-04	3.132531E-04	-7.433834E-03	3.132531E-04	-7.433834E-03
8.00E-04	5.748602E-04	5.751803E-04	-5.564665E-04	5.751803E-04	-5.564665E-04
1.00E-03	9.999946E-04	9.999943E-04	2.925077E-07	9.999943E-04	2.925099E-07
1.20E-03	7.831329E-04	7.831286E-04	5.507326E-06	7.831286E-04	5.507330E-06
1.40E-03	5.750693E-04	5.750983E-04	-5.050622E-05	5.750983E-04	-5.050621E-05
1.60E-03	3.767314E-04	3.767335E-04	-5.594242E-06	3.767335E-04	-5.594227E-06
1.80E-03	1.882123E-04	1.881993E-04	6.902560E-05	1.881993E-04	6.902562E-05
2.00E-03	8.231522E-06	8.230771E-06	9.126185E-05	8.230771E-06	9.126211E-05
2.20E-03	1.057329E-03	1.059971E-03	-2.492685E-03	1.059971E-03	-2.492685E-03
2.40E-03	1.549730E-03	1.562714E-03	-8.308592E-03	1.562714E-03	-8.308592E-03

2.60E-03	2.198989E-03	2.192369E-03	3.019260E-03	2.192369E-03	3.019260E-03
2.80E-03	3.014766E-03	3.014835E-03	-2.297077E-05	3.014835E-03	-2.297077E-05
3.00E-03	4.030104E-03	4.027933E-03	5.390382E-04	4.027933E-03	5.390382E-04
3.20E-03	3.215352E-03	3.240665E-03	-7.810815E-03	3.240665E-03	-7.810815E-03
3.40E-03	2.499214E-03	2.523526E-03	-9.634170E-03	2.523526E-03	-9.634170E-03
3.60E-03	1.847859E-03	1.869343E-03	-1.149277E-02	1.869343E-03	-1.149277E-02
3.80E-03	1.258571E-03	1.279072E-03	-1.602833E-02	1.279072E-03	-1.602833E-02
4.00E-03	7.297018E-04	7.470227E-04	-2.318661E-02	7.470227E-04	-2.318661E-02
4.20E-03	1.280905E-03	1.301610E-03	-1.590705E-02	1.301610E-03	-1.590705E-02
4.40E-03	1.897540E-03	1.919052E-03	-1.121000E-02	1.919052E-03	-1.121000E-02
4.60E-03	2.581446E-03	2.606043E-03	-9.438089E-03	2.606043E-03	-9.438089E-03
4.80E-03	3.335888E-03	3.361754E-03	-7.694298E-03	3.361754E-03	-7.694298E-03
5.00E-03	4.128556E-03	4.118987E-03	2.323112E-03	4.118987E-03	2.323112E-03
5.20E-03	3.755325E-03	3.712124E-03	1.163770E-02	3.712124E-03	1.163770E-02
5.40E-03	3.363498E-03	3.321409E-03	1.267231E-02	3.321409E-03	1.267231E-02
5.60E-03	2.989107E-03	2.949365E-03	1.347491E-02	2.949365E-03	1.347491E-02
5.80E-03	2.631686E-03	2.594397E-03	1.437267E-02	2.594397E-03	1.437267E-02
6.00E-03	2.290757E-03	2.254829E-03	1.593411E-02	2.254829E-03	1.593411E-02
6.20E-03	4.349821E-03	4.324582E-03	5.836294E-03	4.324582E-03	5.836294E-03
6.40E-03	6.021134E-03	6.020208E-03	1.537848E-04	6.020208E-03	1.537848E-04
6.60E-03	8.810522E-03	8.810483E-03	4.400700E-06	8.810483E-03	4.400698E-06
6.80E-03	1.202203E-02	1.204345E-02	-1.778218E-03	1.204345E-02	-1.778218E-03
7.00E-03	1.566475E-02	1.565860E-02	3.926142E-04	1.565860E-02	3.926142E-04
7.20E-03	2.213134E-02	2.212437E-02	3.150547E-04	2.212437E-02	3.150547E-04
7.40E-03	3.047556E-02	3.046505E-02	3.451182E-04	3.046505E-02	3.451182E-04
7.60E-03	4.126745E-02	4.127381E-02	-1.540618E-04	4.127381E-02	-1.540618E-04
7.80E-03	5.325636E-02	5.326140E-02	-9.449795E-05	5.326140E-02	-9.449795E-05
8.00E-03	6.639880E-02	6.639596E-02	4.287370E-05	6.639596E-02	4.287370E-05

As the table illustrates, the analytic model and the code exhibit markedly poorer agreement than that exhibited in the testing using the linearized response curves, a result that was expected based on the requirement to use cubic splines in both the analytical model and the code. Note that the agreement between the spreadsheet model and the code results exhibits marked improvement in the vicinity of the entered data pairs in the response curves, as would be expected from the behavior of cubic splines.

As expected, the differences in the pressures returned by Cubes 3 and 4 are smaller than the number of significant digits displayed in the table, since, by definition, the internal energy does not play a role in determining the pressure in this equation-of-state model. In addition, as the following plot demonstrates, these cubes are loading and unloading in the manner expected from this EOS model.

Figure 53. Cubes 3 and 4 pressures as a function of excess compression



As the plot demonstrates, for $\mu_1<\mu<\mu_2$, the cubes unload and reload along a line that lies between the virgin loading curve and the completely crushed curve. In addition, both cubes exhibit the same behavior, as expected.

The code results for the internal energy can also be examined for the equation-of-state model. Given the use of cubic splines in the code to determine the behavior of this EOS model, there is no closed form solution for the internal energy returned by this model. Given the use of linear response curves in Cubes 1 and 2 and the excellent agreement obtained for the pressure between the analytic model and the code, one would expect to obtain good agreement for the internal energies in Cubes 1 and 2. The requirement to use cubic splines in the analytic model for Cubes 3 and 4 degrades the agreement obtained for the pressures and one would expect that to also affect the results obtained for the internal energy.

The following table gives the results for the internal energy for Cube 1, which had an initial internal energy of $1.0\text{x}10^{-6}$. The code results for the internal energy were extracted using GRIZ, which limits the accuracy to 7 significant figures.

Table 101. Internal energies for Cube 1 from testing EOS Form 17

Time	Code (GRIZ)	EXCEL Integration	(EXCEL - GRIZ)/GRIZ
0.00E+00	1.00000000E-06	1.00000000E-06	0.000000E+00
2.00E-04	6.58000200E-05	6.58000156E-05	-6.618777E-08
4.00E-04	2.60200300E-04	2.60200249E-04	-1.942089E-07
6.00E-04	5.84201300E-04	5.84201264E-04	-6.233230E-08
8.00E-04	1.03780400E-03	1.03780400E-03	-2.915011E-09
1.00E-03	1.62101000E-03	1.62100977E-03	-1.435633E-07
1.20E-03	1.52232300E-03	1.52232317E-03	1.099541E-07
1.40E-03	1.44226600E-03	1.44226597E-03	-2.061316E-08
1.60E-03	1.38083800E-03	1.38083817E-03	1.227213E-07

1.80E-03	1.33804000E-03	1.33803976E-03	-1.793816E-07
2.00E-03	1.31387100E-03	1.31387074E-03	-1.991245E-07
2.20E-03	1.62101000E-03	1.62100977E-03	-1.434241E-07
2.40E-03	2.20601800E-03	2.20601811E-03	4.968109E-08
2.60E-03	2.88103100E-03	2.88103092E-03	-2.824079E-08
2.80E-03	3.64605000E-03	3.64604957E-03	-1.192449E-07
3.00E-03	4.50107500E-03	4.50107561E-03	1.345998E-07
3.20E-03	4.23683500E-03	4.23683443E-03	-1.344698E-07
3.40E-03	4.02013000E-03	4.02013026E-03	6.526612E-08
3.60E-03	3.85096300E-03	3.85096306E-03	1.478035E-08
3.80E-03	3.72933300E-03	3.72933278E-03	-5.936694E-08
4.00E-03	3.65523900E-03	3.65523940E-03	1.099970E-07
4.20E-03	3.72933300E-03	3.72933278E-03	-5.936694E-08
4.40E-03	3.85096300E-03	3.85096306E-03	1.478035E-08
4.60E-03	4.02013000E-03	4.02013026E-03	6.526610E-08
4.80E-03	4.23683500E-03	4.23683443E-03	-1.344699E-07
5.00E-03	4.50107500E-03	4.50107561E-03	1.345998E-07
5.20E-03	6.48115700E-03	6.48115703E-03	4.513066E-09
5.40E-03	8.81996100E-03	8.82129139E-03	1.508381E-04
5.60E-03	1.15134500E-02	1.15214979E-02	6.989997E-04
5.80E-03	1.45737500E-02	1.45817988E-02	5.522829E-04
6.00E-03	1.79941700E-02	1.80022195E-02	4.473409E-04
6.20E-03	1.58987000E-02	1.59067512E-02	5.064072E-04
6.40E-03	1.39328800E-02	1.39409299E-02	5.777643E-04
6.60E-03	1.20967000E-02	1.21047498E-02	6.654514E-04
6.80E-03	1.05424100E-02	1.05596761E-02	1.637772E-03
7.00E-03	9.64913500E-03	9.66640222E-03	1.789509E-03
7.20E-03	1.15148600E-02	1.15247308E-02	8.572206E-04
7.40E-03	1.45737400E-02	1.45817989E-02	5.529706E-04
7.60E-03	1.79941700E-02	1.80022195E-02	4.473419E-04
7.80E-03	2.17747300E-02	2.17827884E-02	3.700822E-04
8.00E-03	2.59154800E-02	2.59235371E-02	3.108988E-04

As the table demonstrates, the agreement between the analytic model and the code is as good as can be expected, given the 7 digit output from GRIZ, until $t = 5.4 \times 10^{-3}$. This is the first time point when the analytic model and the code disagree noticeably for the pressure due to the manner in which the cubic splines are employed by the code. This feeds through into the numerical integration performed by the code to determine the internal energy and the analytic mode and code never re-establish good agreement for the internal energy after that.

The following table gives the results for the internal energy for Cube 2, which had an initial internal energy of $1.0x10^{-3}$. The code results for the internal energy were extracted using GRIZ, which limits the accuracy to 7 significant figures.

Table 102. Internal energies for Cube 2 from testing EOS Form 17

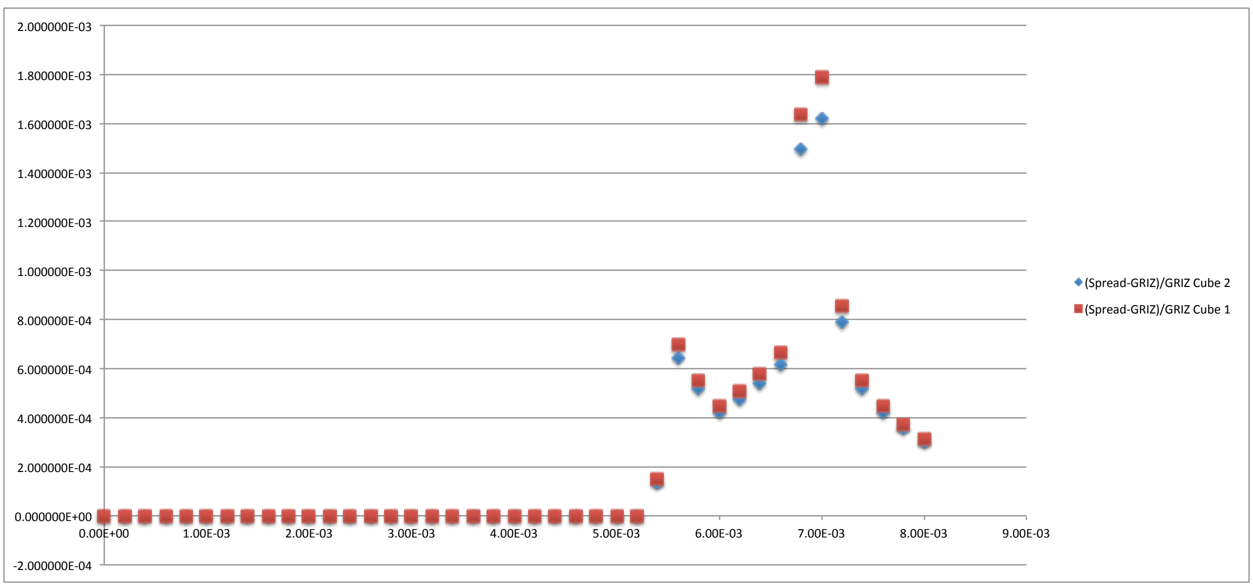
Time	Code (GRIZ)	EXCEL Integration	(EXCEL - GRIZ)/GRIZ
0.00E+00	1.00000000E-03	1.00000000E-03	0.000000E+00
2.00E-04	1.06480000E-03	1.06480002E-03	1.469276E-08
4.00E-04	1.25920000E-03	1.25920025E-03	1.981153E-07
6.00E-04	1.58320100E-03	1.58320126E-03	1.664889E-07
8.00E-04	2.03680400E-03	2.03680400E-03	-1.485270E-09
1.00E-03	2.62001000E-03	2.62000977E-03	-8.882312E-08
1.20E-03	2.52132300E-03	2.52132317E-03	6.638805E-08
1.40E-03	2.44126600E-03	2.44126597E-03	-1.217796E-08
1.60E-03	2.37983800E-03	2.37983817E-03	7.120576E-08
1.80E-03	2.33704000E-03	2.33703976E-03	-1.027024E-07
2.00E-03	2.31287100E-03	2.31287074E-03	-1.131165E-07
2.20E-03	2.62001000E-03	2.62000977E-03	-8.873703E-08
2.40E-03	3.20501800E-03	3.20501811E-03	3.419556E-08
2.60E-03	3.88003100E-03	3.88003092E-03	-2.096957E-08
2.80E-03	4.64505000E-03	4.64504957E-03	-9.359921E-08
3.00E-03	5.50007500E-03	5.50007561E-03	1.101519E-07
3.20E-03	5.23583500E-03	5.23583443E-03	-1.088129E-07
3.40E-03	5.01913000E-03	5.01913026E-03	5.227565E-08
3.60E-03	4.84996300E-03	4.84996306E-03	1.173588E-08
3.80E-03	4.72833300E-03	4.72833278E-03	-4.682392E-08
4.00E-03	4.65423900E-03	4.65423940E-03	8.638694E-08
4.20E-03	4.72833300E-03	4.72833278E-03	-4.682392E-08
4.40E-03	4.84996300E-03	4.84996306E-03	1.173587E-08
4.60E-03	5.01913000E-03	5.01913026E-03	5.227563E-08
4.80E-03	5.23583500E-03	5.23583443E-03	-1.088130E-07
5.00E-03	5.50007500E-03	5.50007561E-03	1.101519E-07
5.20E-03	7.48015700E-03	7.48015703E-03	3.910329E-09
5.40E-03	9.81896100E-03	9.82029139E-03	1.354916E-04
5.60E-03	1.25124500E-02	1.25204979E-02	6.431913E-04
5.80E-03	1.55727500E-02	1.55807988E-02	5.168536E-04
6.00E-03	1.89931700E-02	1.90012195E-02	4.238117E-04
6.20E-03	1.68977000E-02	1.69057512E-02	4.764682E-04
6.40E-03	1.49318800E-02	1.49399299E-02	5.391096E-04
6.60E-03	1.30957000E-02	1.31037498E-02	6.146877E-04

6.80E-03	1.15414100E-02	1.15586761E-02	1.496010E-03
7.00E-03	1.06481400E-02	1.06654022E-02	1.621148E-03
7.20E-03	1.25138600E-02	1.25237308E-02	7.887874E-04
7.40E-03	1.55727400E-02	1.55807989E-02	5.174972E-04
7.60E-03	1.89931700E-02	1.90012195E-02	4.238127E-04
7.80E-03	2.27737300E-02	2.27817884E-02	3.538481E-04
8.00E-03	2.69144800E-02	2.69225371E-02	2.993590E-04

As the table demonstrates, the agreement between the analytic model and the code is as good as can be expected, given the 7 digit output from GRIZ, until t = 5.4×10^{-3}. This is the first time point when the analytic model and the code disagree noticeably for the pressure due to the manner in which the cubic splines are employed by the code. This feeds through into the numerical integration performed by the code to determine the internal energy and the analytic mode and code never re-establish good agreement for the internal energy after that.

An interesting behavior is revealed by the following plot, which shows the normalized difference between the spreadsheet numerical integration for the internal energy and the code result for both Cubes 1 and 2.

Figure 54. Normalized differences for internal energy for Cubes 1 and 2



Despite a difference of three orders of magnitude in the initial value of the internal energy for Cubes 1 and 2, the normalized difference between the spreadsheet model and the code result for the internal energy returned by these cubes bear a striking resemblance to each other. This is in fact not a surprise, as the internal energy developed in Cube 1 becomes on the order of the initial value of the internal energy in Cube 2 by a time of 8×10^{-4}, which is very early in the calculation.

The following table gives the results for the internal energy for Cube 3, which had an initial internal energy of 1.0×10^{-6}, and used the generalized response curve. The code results for the internal energy were extracted using GRIZ, which limits the accuracy to 7 significant figures.

Table 103. Internal energies for Cube 3 from testing EOS Form 17

Time	Code (GRIZ)	EXCEL Integration	(EXCEL - GRIZ)/GRIZ
0.00E+00	1.00000000E-06	1.00000000E-06	0.00000000E+00
2.00E-04	1.80596600E-06	1.81834290E-06	6.85333928E-03
4.00E-04	3.76389600E-06	3.78468534E-06	5.52335536E-03
6.00E-04	7.21363400E-06	7.22450966E-06	1.50765277E-03
8.00E-04	1.36197600E-05	1.36257020E-05	4.36281390E-04
1.00E-03	2.49320600E-05	2.49449455E-05	5.16823285E-04
1.20E-03	2.31866400E-05	2.31992987E-05	5.45947248E-04
1.40E-03	2.18555100E-05	2.18681132E-05	5.76659425E-04
1.60E-03	2.09219300E-05	2.09345716E-05	6.04228454E-04
1.80E-03	2.03674900E-05	2.03801699E-05	6.22555405E-04
2.00E-03	2.01753100E-05	2.01880737E-05	6.32641486E-04
2.20E-03	2.65476100E-05	2.65584147E-05	4.06993806E-04
2.40E-03	4.12512200E-05	4.11533325E-05	-2.37296131E-03
2.60E-03	6.21536600E-05	6.19990312E-05	-2.48784760E-03
2.80E-03	9.09356200E-05	9.08311699E-05	-1.14861638E-03
3.00E-03	1.29561600E-04	1.29379950E-04	-1.40203197E-03
3.20E-03	1.13292300E-04	1.13231911E-04	-5.33034463E-04
3.40E-03	1.00351900E-04	1.00403496E-04	5.14152566E-04
3.60E-03	9.04622400E-05	9.06165804E-05	1.70613070E-03
3.80E-03	8.33530400E-05	8.36055806E-05	3.02977104E-03
4.00E-03	7.87731600E-05	7.91099118E-05	4.27495558E-03
4.20E-03	8.35865900E-05	8.38354097E-05	2.97678973E-03
4.40E-03	9.11455900E-05	9.12921790E-05	1.60829511E-03
4.60E-03	1.01735000E-04	1.01773427E-04	3.77713985E-04
4.80E-03	1.15657800E-04	1.15579024E-04	-6.81110061E-04
5.00E-03	1.33197500E-04	1.33020950E-04	-1.32547455E-03
5.20E-03	1.24404000E-04	1.24127655E-04	-2.22134977E-03
5.40E-03	1.16493200E-04	1.16120975E-04	-3.19525282E-03
5.60E-03	1.09429200E-04	1.08964184E-04	-4.24946861E-03
5.80E-03	1.03173000E-04	1.02621365E-04	-5.34669971E-03
6.00E-03	9.76918200E-05	9.70574704E-05	-6.49337440E-03
6.20E-03	1.41428900E-04	1.41287212E-04	-1.00182933E-03
6.40E-03	2.07937900E-04	2.07809627E-04	-6.16882897E-04
6.60E-03	3.03560900E-04	3.03453104E-04	-3.55104477E-04
6.80E-03	4.36807700E-04	4.36588506E-04	-5.01808113E-04
7.00E-03	6.12227800E-04	6.11870197E-04	-5.84101645E-04

7.20E-03	9.78664600E-04	9.78420002E-04	-2.49930118E-04
7.40E-03	1.47821100E-03	1.47769636E-03	-3.48152163E-04
7.60E-03	2.15277200E-03	2.15237042E-03	-1.86542489E-04
7.80E-03	3.02791800E-03	3.02745324E-03	-1.53491620E-04
8.00E-03	4.11831000E-03	4.11781346E-03	-1.20570041E-04

As the table demonstrates, the agreement between the analytic model and the code is not as good as that exhibited by the results from Cubes 1 and 2. Given the use of cubic splines in the spreadsheet model, as well as the code, to determine the behavior of the response curve, this was to be expected. In addition, there is no point in time during the simulation after which the agreement between the spreadsheet model and the code has clearly degraded, as was observed in the results from Cubes 1 and 2.

The following table gives the results for the internal energy for Cube 4, which had an initial internal energy of $1.0\text{x}10^{-3}$, and used the generalized response curve. The code results for the internal energy were extracted using GRIZ, which limits the accuracy to 7 significant figures.

Table 104. Internal energies for Cube 4 from testing EOS Form 17

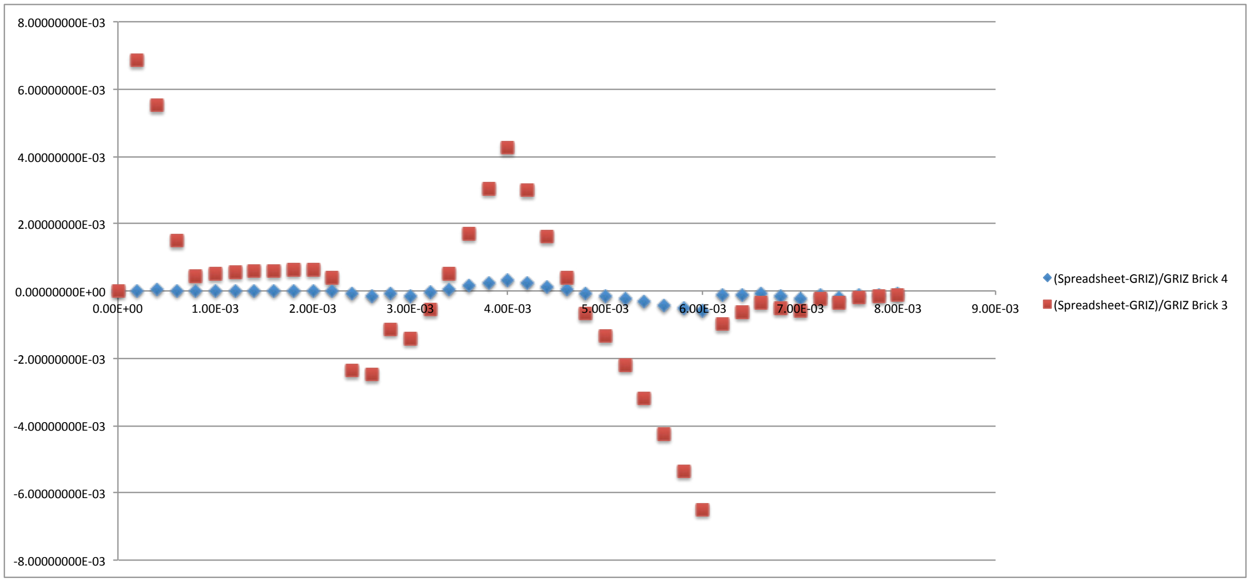
Time	Code (GRIZ)	EXCEL Integration	(EXCEL - GRIZ)/GRIZ
0.00E+00	1.00000000E-03	1.00000000E-03	0.00000000E+00
2.00E-04	1.00080600E-03	1.00081834E-03	1.23329574E-05
4.00E-04	1.00276400E-03	1.00278469E-03	2.06283185E-05
6.00E-04	1.00621400E-03	1.00622451E-03	1.04447516E-05
8.00E-04	1.01262000E-03	1.01262570E-03	5.63098480E-06
1.00E-03	1.02393200E-03	1.02394495E-03	1.26428993E-05
1.20E-03	1.02218700E-03	1.02219930E-03	1.20317291E-05
1.40E-03	1.02085600E-03	1.02086811E-03	1.18657093E-05
1.60E-03	1.01992200E-03	1.01993457E-03	1.23260604E-05
1.80E-03	1.01936700E-03	1.01938017E-03	1.29196705E-05
2.00E-03	1.01917500E-03	1.01918807E-03	1.28277605E-05
2.20E-03	1.02554800E-03	1.02555841E-03	1.01552610E-05
2.40E-03	1.04025100E-03	1.04015333E-03	-9.38884504E-05
2.60E-03	1.06115400E-03	1.06099903E-03	-1.46038029E-04
2.80E-03	1.08993600E-03	1.08983117E-03	-9.61800945E-05
3.00E-03	1.12856200E-03	1.12837995E-03	-1.61311041E-04
3.20E-03	1.11229200E-03	1.11223198E-03	-5.39618477E-05
3.40E-03	1.09935200E-03	1.09940356E-03	4.69035901E-05
3.60E-03	1.08946200E-03	1.08961665E-03	1.41948754E-04
3.80E-03	1.08235300E-03	1.08260565E-03	2.33424766E-04
4.00E-03	1.07777300E-03	1.07810998E-03	3.12662433E-04
4.20E-03	1.08258700E-03	1.08283548E-03	2.29521573E-04

4.40E-03	1.09014600E-03	1.09029225E-03	1.34153017E-04
4.60E-03	1.10073500E-03	1.10077349E-03	3.49712701E-05
4.80E-03	1.11465800E-03	1.11457909E-03	-7.07915096E-05
5.00E-03	1.13219700E-03	1.13202102E-03	-1.55434546E-04
5.20E-03	1.12340400E-03	1.12312768E-03	-2.45965273E-04
5.40E-03	1.11549300E-03	1.11512100E-03	-3.33483761E-04
5.60E-03	1.10842900E-03	1.10796421E-03	-4.19322777E-04
5.80E-03	1.10217300E-03	1.10162139E-03	-5.00473723E-04
6.00E-03	1.09669200E-03	1.09605750E-03	-5.78560926E-04
6.20E-03	1.14042900E-03	1.14028724E-03	-1.24305147E-04
6.40E-03	1.20693800E-03	1.20680965E-03	-1.06340930E-04
6.60E-03	1.30256100E-03	1.30245313E-03	-8.28133269E-05
6.80E-03	1.43580800E-03	1.43558853E-03	-1.52852765E-04
7.00E-03	1.61122800E-03	1.61087022E-03	-2.22052274E-04
7.20E-03	1.97766500E-03	1.97742003E-03	-1.23868974E-04
7.40E-03	2.47721100E-03	2.47669638E-03	-2.07740048E-04
7.60E-03	3.15177200E-03	3.15137044E-03	-1.27406748E-04
7.80E-03	4.02691800E-03	4.02645327E-03	-1.15406773E-04
8.00E-03	5.11731000E-03	5.11681348E-03	-9.70272232E-05

As the table demonstrates, the agreement between the analytic model and the code is not as good as that exhibited by the results from Cubes 1 and 2. Given the use of cubic splines in the spreadsheet model, as well as the code, to determine the behavior of the response curve, this was to be expected. In addition, there is no point in time during the simulation after which the agreement between the spreadsheet model and the code has clearly degraded, as was observed in the results from Cubes 1 and 2. Finally, the normalized difference between the spreadsheet model and the code results is, in the early part of the simulation, generally about an order of magnitude better than the results from Cube 3.

This last point is made more clear by the following plot, which displays the normalized differences for the internal energy from Cubes 3 and 4. Given that the initial value of the internal energy in Cube 4 is three orders of magnitude larger than that of Cube 3, it is expected that the normalized difference from Cube 4 would be considerably smaller than that of Cube 3 until the internal energy developed in Cube 3 becomes on the order of the initial value used for Cube 4, which occurs at $t \sim 7.4 \times 10^{-3}$.

Figure 55. Normalized differences for internal energy for Cubes 3 and 4



This establishes the implementation of Equation-of-State Form 17, a modification of EOS Form 11 intended for use only with Material Model 64, in DYNA3D. The equation-of-state is performing as expected, in that the pressure in the cubes increases as they are compressed and decreases as they are expanded. The behavior of the equation-of-state as a whole has been examined using both linearized response curves, which may represent an over test of the model but demonstrates that good agreement can be achieved between the code and an analytic model, and generalized response curves, which are more physically realistic but harder to capture in an analytic model due to the use of cubic spline fits. Equation-of-State Form 17 is performing as expected and with good accuracy.

Author's Note: An important issue was revealed in the testing of Equation-of-State Form 17. The testing of this equation-of-state should have returned results essentially identical to those obtained from the testing of EOS Form 11. This was not the case and this testing revealed that some variables were not being passed correctly to the relevant subroutines. As of code version 15.2.0 revision 1.3368, this issue has been corrected.

Equation-of-State Form 18

Equation-of-State Form 18 is an interface to the LEOS database. According to the LEOS development team, all of the EOS models in the LEOS database on the open side are based on QEOS type calculations and none are based on simple analytic models. Therefore, a comparison of the code results to an analytic model is not possible for EOS Form 18. The test will consist of a simulation that uses three cubes to return the results from the Al table (eos # 130 in the LEOS database), the stainless steel table (eos # 3010) and the water table (eos # 2010).

Prior to discussing the calculations using EOS Form 18, a few code issues need to be addressed and these are not necessarily readily apparent to the user. First, in order to eliminate issues with the work performed by the bulk viscosity, the two input coefficients for the bulk viscosity on the material card were set to 1.0e-20 in each of the 3 cubes. Failing to do so results in the work performed on the cube being dominated by contributions from the bulk viscosity. Finally, the code version used for this test was version 15.2.0 revision 1.3368.

Due to the use of metallic equations-of-state, the displacements used in this simulation were reduced dramatically from previous tests. The cubes are compressed slightly and then put into tension for the second half of the simulation, as shown in the following table.

Table 105. Displacements used for testing EOS Form 18

Time	Displacement
0.00E+00	0.0000E+00
1.00E-03	5.0000E-07
2.00E-03	1.0000E-06
3.00E-03	5.0000E-07
4.00E-03	2.3359E-21
5.00E-03	-5.0000E-07
6.00E-03	-1.0000E-06
7.00E-03	-5.0000E-07
8.00E-03	-7.1780E-21

The following table lists the pressures from the 3 cubes as a function of time for this simulation.

Table 106. Pressures returned from testing EOS Form 18

Time	Cube 1 Pressure	Cube 2 Pressure	Cube 3 Pressure
0.00E+00	1.90458855E+03	-3.60091078E+01	2.60127968E+05
1.00E-03	2.21151870E+06	4.79275521E+06	3.55769522E+05
2.00E-03	4.42117656E+06	9.58565901E+06	4.51413383E+05
3.00E-03	2.21151870E+06	4.79275521E+06	3.55769523E+05
4.00E-03	1.90458469E+03	-3.59957748E+01	2.60127969E+05
5.00E-03	-2.20934724E+06	-4.72965609E+06	1.62934310E+05

6.00E-03	-4.42055511E+06	-9.45915447E+06	6.57428338E+04
7.00E-03	-2.20934724E+06	-4.72965609E+06	1.62934310E+05
8.00E-03	1.90457053E+03	-3.60281525E+01	2.60127970E+05

As the table demonstrates, the cubes are behaving as expected, in that the pressure increases as the cubes are compressed and decreases as the cubes are put into tension. Also, the cubes return to essentially the initial pressure when the displacement returns to zero. Finally, the pressure in the steel cube is larger in compression than the pressure in the Al or water cube due to the higher density of steel.

This establishes the implementation of Equation-of-State Form 18, an interface to the LEOS database of equations-of-state. The equation-of-state is performing as expected, in that the pressure in the cubes increases as they are compressed and decreases as they are expanded. Equation-of-State Form 18 is performing as expected.

Appendix A

Equation-of-State Form 2 Testing with ω=0

The form of the JWL eos is as follows:

$$p = A(1\text{-}\omega/(R_1 V)) \exp(\text{-}R_1 V) + B(1\text{-}\omega/(R_2 V)) \exp(\text{-}R_2 V) + \omega E/V,$$

where V is the relative volume and E is the internal energy. Removing the dependence on the internal energy (ω=0) also greatly simplifies the eos model and may require future investigation, e.g., let the code calculate the internal energy and then import that back into the spreadsheet to do the full eos model calculation.

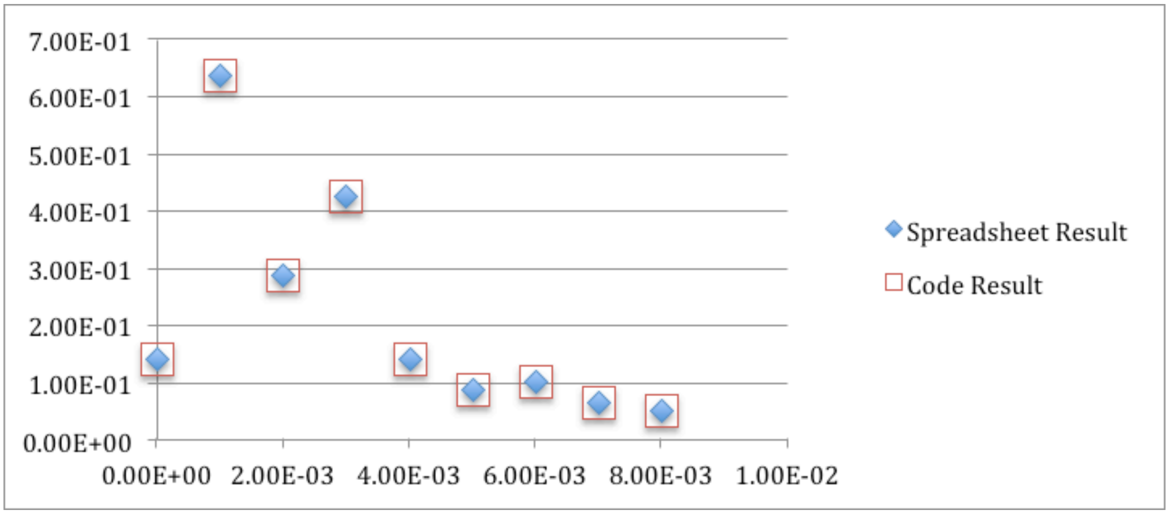
A listing of JWL coefficients was investigated online (JWL Equation of State Coefficients for High Explosives, Lee, Finger and Collins, 1973) and supplied the coefficients for a typical material, except that ω was set 0 to remove the dependence on the internal energy. Note that in addition to removing any dependence on the internal energy, setting ω = 0 also changes the dependence of the first two terms on the relative volume. The input coefficients used were: A = 8.684, B = 0.18711, R_1 = 4.60, and R_2 = 1.25.

This simplified test of EOS Form 2 returned excellent results (as demonstrated in the table below), with the code and analytic forms agreeing to better than 5 parts in 10^7 over the range of densities tested by this problem.

Table A-1. Simplified test results for EOS Form 2

Time	Displacement	Volume	Analyt Pressure	Code Pressure	(Code-Analyt)/Analyt
0.00E+00	0.0000E+00	1.00E+00	1.408981E-01	1.4090E-01	-3.842985E-07
1.00E-03	-4.0000E-01	6.00E-01	6.380102E-01	6.3801E-01	-3.466793E-08
2.00E-03	-2.0000E-01	8.00E-01	2.878702E-01	2.8787E-01	-1.240375E-07
3.00E-03	-3.0000E-01	7.00E-01	4.249688E-01	4.2497E-01	5.073887E-08
4.00E-03	0.0000E+00	1.00E+00	1.408981E-01	1.4090E-01	-3.842985E-07
5.00E-03	1.5000E-01	1.15E+00	8.822517E-02	8.8225E-02	-7.431108E-08
6.00E-03	1.0000E-01	1.10E+00	1.024137E-01	1.0241E-01	4.337202E-07
7.00E-03	2.5000E-01	1.25E+00	6.685966E-02	6.6860E-02	7.348629E-08
8.00E-03	3.5000E-01	1.35E+00	5.206009E-02	5.2060E-02	4.082513E-08

This agreement is also demonstrated in the following plot of the pressures as a function of time:



Note that choosing ω = 0 makes this EOS model positive definite in the pressure and does not allow for negative pressures under tension.

Appendix B

Equation-of-State Form 16 has been removed from the code as a result of the creation of this test suite and the subsequent analysis performed. The results of the testing and analysis performed on EOS Form 16 are included here for completeness.

Equation-of-State Form 16

The next model to be tested was Equation-of-State Form 16, a modification of EOS Form 2 intended for use with Material Model 68. This equation-of-state is a JWL expression often used for high-explosive detonation products. This EOS has the following form:

$$p = A(1 - \omega/(R_1 V)) \exp(-R_1 V) + B(1 - \omega/(R_2 V)) \exp(-R_2 V) + \omega E/V$$

where p is the pressure, V is the relative volume and E is the specific internal energy. A, B, ω, R_1 and R_2 are material dependent coefficients.

Equation-of-State Form 16 was tested using 4 cubes, one for each of the 'terms' and one for the full equation-of-state model. However, unlike Equation-of-State Form 1 which separated into terms easily, the manner in which each term of EOS Form 16 depends on ω prevents this equation-of-state model from being cleanly separated, unless ω is set to 0, in which case the dependence of the first two terms on the relative volume is modified. Therefore, the decision was made to test terms 1 and 3 with the first cube, terms 2 and 3 with the second cube and term 3 alone with the third cube. The full equation-of-state was tested using the fourth cube. The 4 cubes use the same compression and expansion as that used for the testing of EOS Form 1.

As it turns out, for the material coefficients chosen for this test of EOS Form 16, the contribution to the pressure from term 3 is orders of magnitude smaller than the contributions from terms 1 and 2, validating this testing choice. In addition, tests of EOS Form 2 (similar to EOS Form 16) with ω set to zero have already been conducted and discussed elsewhere[3].

Prior to discussing the calculations using EOS Form 16, a few code issues need to be addressed and these are not necessarily readily apparent to the user. First, in order for the terms dependent on the internal energy to perform as expected, it is required to have an initial energy present in the simulation, so the initial internal energy was set to a value of 1.0e-3 in all of the cubes. In addition, in order to eliminate issues with the work performed by the bulk viscosity, the two input coefficients for the bulk viscosity on the material card were set to 1.0e-20 in each of the 4 cubes. Failing to do so results in the work performed on the cube being dominated by contributions from the bulk viscosity. Finally, the code version used for this test was version 15.2.0 revision 1.3364.

Input coefficients for Equation-of-State Form 16 for a representative were taken from a 1973 paper by Lee, et. al.[4]. The following table gives the value of the input coefficients for each of the four cubes used in the test suite.

Table B-1. Input coefficients for the testing of EOS Form 16

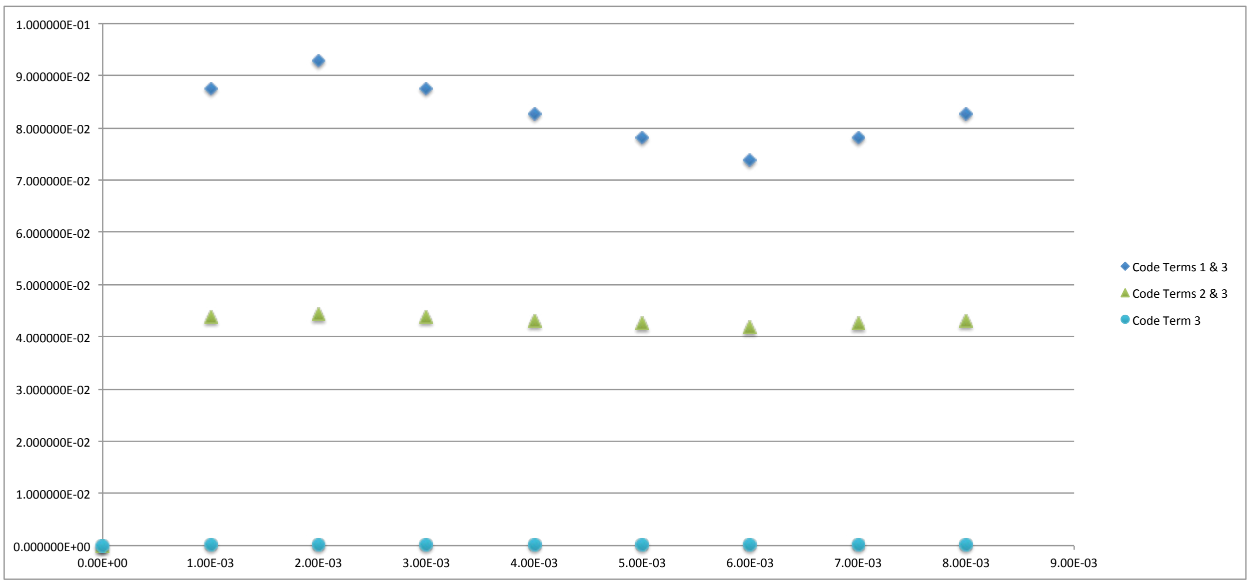
Cube	A	B	R_1	R_2	ω
1	8.684	0	4.6	1.25	0.25

2	0	1.8711e-1	4.6	1.25	0.25
3	0	0	4.6	1.25	0.25
4	8.684	1.8711e-1	4.6	1.25	0.25

Note that the R_1 and R_2 coefficients were set for each cube to avoid divide by zero problems in the code.

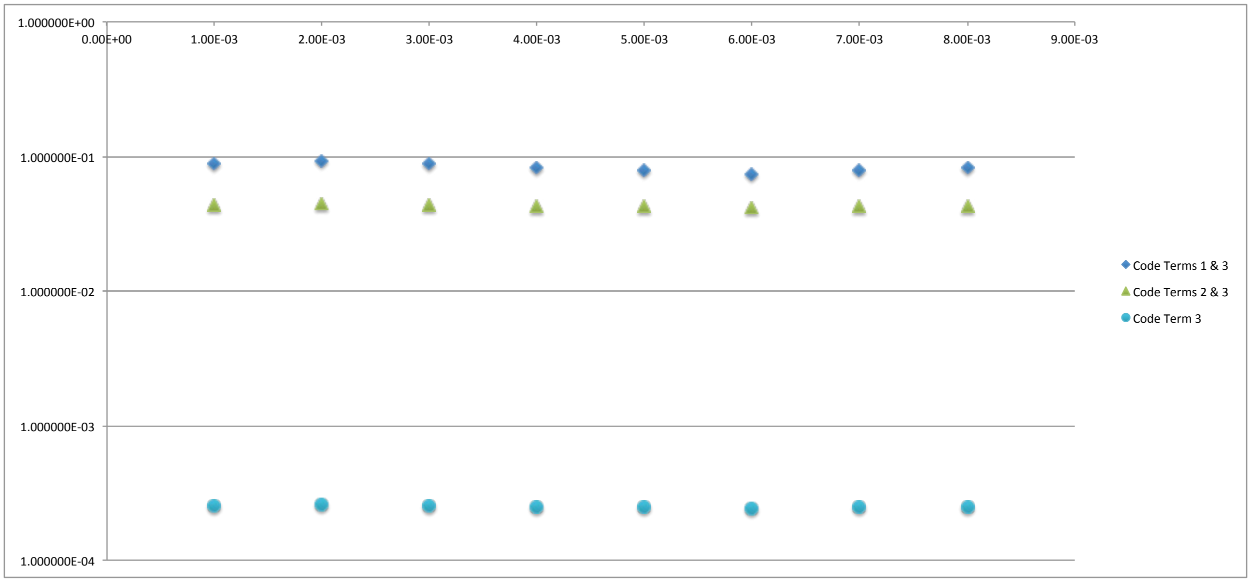
The following plot displays the pressure from each of the three individual terms tested for EOS Form 16, as returned by the code, as a function of time for this simulation.

Figure B-1. Code pressure for the three terms as a function of time



As the plot demonstrates, the pressures returned by the first two terms differ by approximately a factor of two, while the contribution of the third term is orders of magnitude smaller. A log plot makes the difference between these terms more easily understood:

Figure B-2. Code pressure for the three terms as a function of time



It is clear from this version of the plot that the contributions to the pressure from the first two terms (as tested) are approximately two orders of magnitude larger than the contribution from the third term.

The following observations may be made from the code output. In all of the cubes, the pressure increases as the cube is compressed and decreases as the cube is expanded, as expected. As asserted earlier, the pressure from Cube 3 (Term 3 only) is about 2 orders of magnitude smaller than the pressures resulting from Cubes 1 (Terms 1 and 3) and 2 (Terms 2 and 3). Finally, note that with this choice of input coefficients, the pressure appears to be positive definite.

Using the normalized difference defined by equation 1, the agreement between the pressures for the second 'term' as calculated using the reference expression and the results returned by the code is demonstrated in the following table as a function of time.

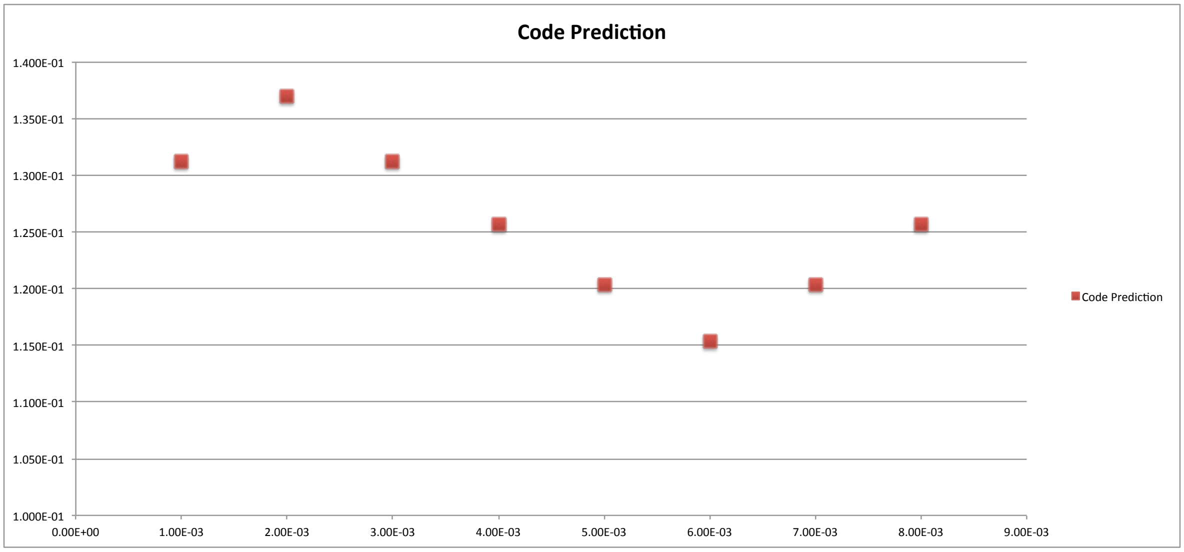
Table B-2. Reference and Code Pressures for the second term of EOS Form 16

Time	*Reference Pressure*	*Code Pressure*	*(Reference - Code)/Code*
0.00E+00	0.0000000E+00	0.0000000E+00	0.00000000E+00
1.00E-03	4.3784672E-02	4.3784672E-02	1.31820115E-09
2.00E-03	4.4435504E-02	4.4435504E-02	-1.01792817E-09
3.00E-03	4.3784672E-02	4.3784672E-02	1.31818515E-09
4.00E-03	4.3136330E-02	4.3136330E-02	-1.06081293E-10
5.00E-03	4.2490632E-02	4.2490632E-02	2.11502961E-10
6.00E-03	4.1847728E-02	4.1847728E-02	-1.15369312E-11
7.00E-03	4.2490632E-02	4.2490632E-02	2.11531213E-10
8.00E-03	4.3136330E-02	4.3136330E-02	-1.06025636E-10

As the table clearly demonstrates, the code pressures are in excellent agreement with the reference results, with the level of agreement being better than 2 parts in 10^9. This level of agreement is typical of the three individual terms tested in this simulation. Note that, unlike the results of the testing of EOS Form 2, the initial pressure in this testing is zero due to the use of an HE material model.

Now that the behavior of each of the individual terms in the expression for Equation-of-State Form 16 has been examined, the behavior of the full expression for this EOS can be investigated. The following plot displays the pressure as a function of time for EOS Form 16.

Figure B-3. Code Pressure for EOS Form 16 as a function of time



Note that the pressure is behaving as one would expect, as the pressure increases when the cube is compressed, decreases as the cube is expanded and then returns to the initial pressure as the cube is relaxed back to its original configuration. Note also that with the present choice of input coefficients, the pressure returned by EOS Form 16 is positive definite.

The following table compares the reference pressure to the code results as a function of time.

Table B-3. Reference and Code Pressures for Equation-of-State Form 16

Time	*Reference Pressure*	*Code Pressure*	*(Reference - Code)/Code*
0.00E+00	0.000000000E+00	0.00000000E+00	0.0000000E+00
1.00E-03	1.311924892E-01	1.31192489E-01	-6.4708255E-10
2.00E-03	1.369396360E-01	1.36939636E-01	-9.0623046E-10
3.00E-03	1.311924892E-01	1.31192489E-01	-6.4704426E-10
4.00E-03	1.256824421E-01	1.25682442E-01	5.8312519E-11
5.00E-03	1.204011320E-01	1.20401132E-01	1.3140666E-11
6.00E-03	1.153403825E-01	1.15340382E-01	8.9323278E-10
7.00E-03	1.204011320E-01	1.20401132E-01	1.3082458E-11
8.00E-03	1.256824421E-01	1.25682442E-01	5.8344319E-11

As the table clearly demonstrates, the code predictions are again in excellent agreement with the reference results, with the level of agreement being better than 9 parts in 10^{10}. Note that, unlike the results of the testing of EOS Form 2, the initial pressure in this testing is zero due to the use of an HE material model. These results establish confidence in the pressures returned by the implementation of Equation-of-State Form 2 in DYNA3D.

The code results for the internal energy can also be investigated for this equation-of-state. Unfortunately, due to the form of this EOS (ω present in each term and E only in the third term), a simple closed form solution can only be generated for the third term, using the assumption that A=B=0. Making such an assumption leads to the following expression for the internal energy due to the third term:

$$E = \exp(-\omega \ln V + \ln E_0)$$

where V is the final volume of the cube and E_0 is the initial internal energy. This solution takes advantage of the fact that the initial volume of the cube is 1 cm^3.

The predictions of this closed form solution for the internal energy due to the third term can be compared to the code results as extracted using GRIZ, which again limits the comparison to 7 significant figures. This is done in the following table.

Table B-4. Exact and Code Internal Energies for the third term in EOS Form 16

Time	Code (GRIZ)	*Closed Form*	(*Closed* - GRIZ)/GRIZ
0.00E+00	1.00000000E-03	1.0000000E-03	0.000000E+00
1.00E-03	1.00301100E-03	1.0030105E-03	-4.599701E-07
2.00E-03	1.00604200E-03	1.0060423E-03	3.084640E-07
3.00E-03	1.00301100E-03	1.0030105E-03	-4.599701E-07
4.00E-03	1.00000000E-03	1.0000000E-03	2.168404E-16
5.00E-03	9.97010500E-04	9.9701046E-04	-3.847118E-08
6.00E-03	9.94041700E-04	9.9404169E-04	-5.741633E-09
7.00E-03	9.97010500E-04	9.9701046E-04	-3.847118E-08
8.00E-03	1.00000000E-03	1.0000000E-03	2.168404E-16

As expected, the agreement between the closed form solution for the third term and the code results is at the level of ~ 4 parts in 10^7, which is limited by the number of significant figures in the output provided by GRIZ.

Finally, the internal energy returned by the code for Equation-of-State Form 16 can be compared to a numerical integration performed using EXCEL (*Reference Energy*) to determine the sensitivity of this result to differences in the numerical integration scheme. This is done in the following table.

Table B-5. Reference and Code Internal Energies for EOS Form 16

Time	Code (GRIZ)	*Reference Energy*	(*Reference* - GRIZ)/GRIZ
0.00E+00	1.00000000E-03	1.00000000E-03	0.000000E+00
1.00E-03	2.53481600E-03	2.53481682E-03	3.223784E-07

2.00E-03	4.12407900E-03	4.12407982E-03	1.981169E-07
3.00E-03	2.53481600E-03	2.53481692E-03	3.631048E-07
4.00E-03	9.99999500E-04	1.00000041E-03	9.068224E-07
5.00E-03	-4.82148000E-04	-4.82147431E-04	-1.180607E-06
6.00E-03	-1.91336300E-03	-1.91336271E-03	-1.528894E-07
7.00E-03	-4.82148000E-04	-4.82147522E-04	-9.913354E-07
8.00E-03	9.99999500E-04	9.99999629E-04	1.293263E-07

The agreement between these two numerical integration schemes is better than 1 parts in 10^6, which is about what would be expected, given the limitations of the GRIZ output.

This establishes the implementation of Equation-of-State Form 16 in DYNA3D. The equation-of-state is performing as expected, in that the pressure in the cubes increases as they are compressed and decreases as they are expanded. The behavior of each of the terms in the equation-of-state has been examined and found to be performing as expected and with good accuracy. The behavior of the equation-of-state as a whole has been examined and is performing as expected and with good accuracy.

Note that as a result of the creation of this test suite, and the subsequent analysis of the EOS models, Equation-of-State Form 16 has been removed from the code.