

## **Temperature dependent ductile material failure constitutive modeling with validation experiments**

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### **Abstract**

A unique quasi-static temperature dependent low strain rate constitutive finite element failure model is being developed at Sandia National Laboratories [1]. The model is used to predict ductile tensile failure initiation using a tearing parameter methodology and assessed for accuracy against validation experiments. Experiments include temperature dependent tensile testing of 304L stainless steel and a variety of aluminum alloy round specimens to generate true-stress true-strain material property specifications. Two simple geometries including pressure loaded steel cylinders and thread shear mechanisms are modeled and assessed for accuracy by experiment using novel uncertainty quantification techniques.

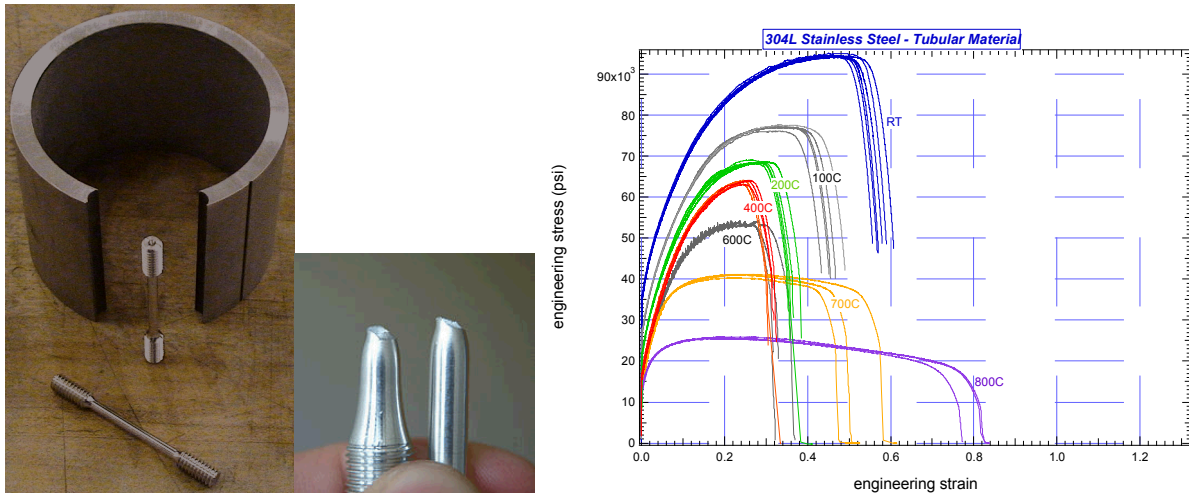
### **Finite element material characterization modeling**

Finite element (FE) analysis with validation testing is performed to predict quasi-static failure initiation of ductile materials when subjected to high pressures at elevated temperature. Two structure types are chosen to envelope load and displacement modes of failure. The structures include a simple stainless steel cylinder (pipe bomb) that is pressurized and heated and an aluminum Acme thread geometry that is extended and heated to failure.

A unique FE quasi-static temperature dependent constitutive model [2] has been developed and uses a tearing parameter methodology for failure initiation. Model inputs require experimental derived tensile test hardening data taken at temperatures in the range of the desired failure prediction. The structural response is then validated by tests.

The elastic-plastic constitutive model incorporating temperature dependence was developed for use in Sandia's quasi-static finite element modeling software, Adagio [3]. The model requires a temperature dependent true stress-true strain hardening curve definition to failure plus temperature dependent elastic constant specifications. Elastic constants can be obtained in the open literature but the hardening curve data is characterized through experimental tensile tests at elevated temperature [4]. Pipe bomb tensile-test material samples were cut and machined from a common 304L stainless steel tubular stock. The resulting engineering stress strain curves are shown, Figure 1.

Validation-experiment pipe vessels were machined from the same batch of tube stock material to match the tensile test data. As shown, the strength degrades with increasing temperature. From room temperature to 600 C, the ductility at failure decreases. After 600C, it increases for this particular material.



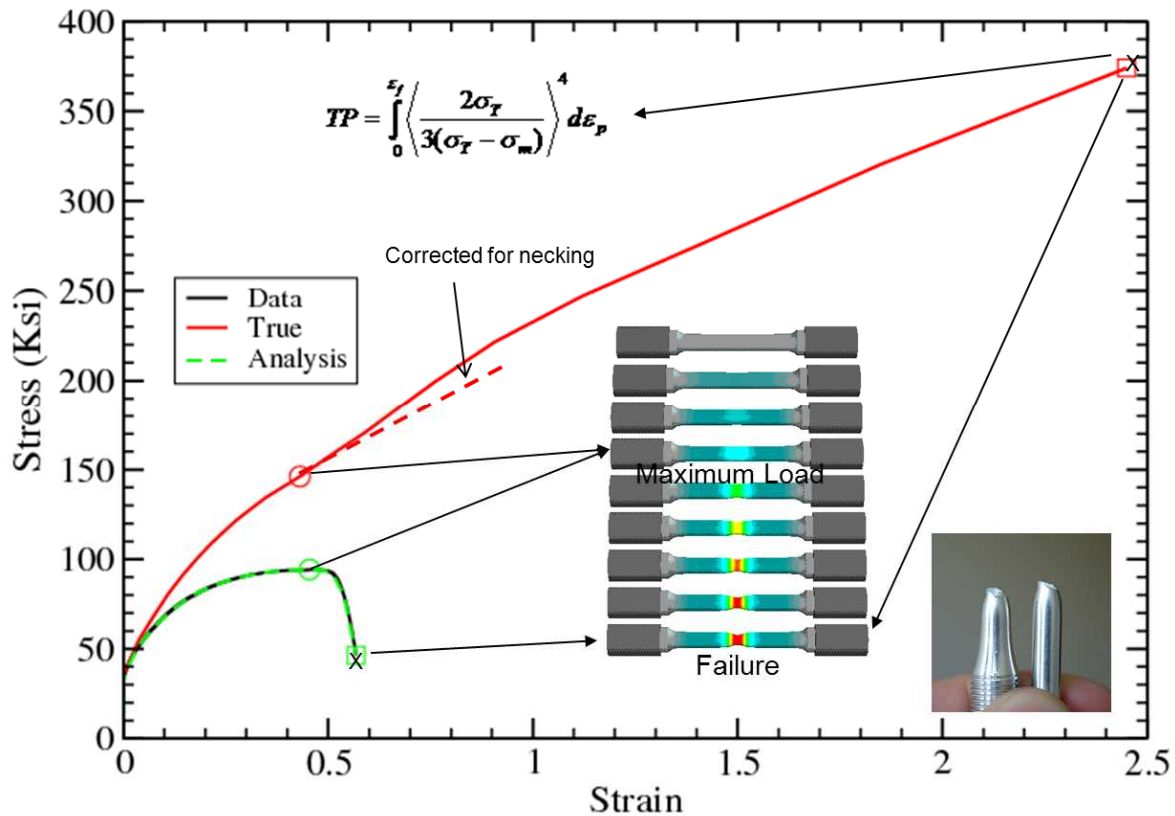
**Figure 1 - Cylinder tensile-test material samples were cut and machined from the same 304L stainless steel tubular stock that the validation-experiment pipe vessels were machined from. Measured stress-strain response-to-failure curves plotted from cylinder pull-tests at a strain rate of 0.001/s for the labeled temperatures (note: “RT” in the plot stands for “room temperature”, nominally 25C).**

For each measured stress-strain curve, an advanced optimization technique is used to solve an inverse finite element tensile necking problem to calculate true stress/true strain response and will later be used system model input. An example is presented in Figure 2.

Given the engineering stress strain response of a tensile test [4], the round tensile specimen is modeled using finite elements. A displacement controlled FE calculation is then performed to simulate the tensile test. The simulation predicts no necking through yield but as the specimen begins to harden, true stress/log strain necking response is estimated and checked against the original averaged engineering stress/strain. Iteratively, true stress and log strain can be computed to failure. This is referred to as solving the inverse problem. A tearing parameter method is used to track failure progress. At failure, a critical tearing parameter is calculated to be used in pipe bomb models. This procedure is repeated at every temperature. The inverse problem and solution procedures & results are more fully documented in [2].

Once the material characterization has been defined for an applicable range of temperatures, it is formatted as input into a thermo-elastic plastic constitutive model and used to predict the failure response of a pressurized cylindrical steel vessel at high temperature. In this case, a critical tearing parameter is used to define a point in which the code will automatically delete elements, thus establishing the pressure, temperature and location of failure initiation.

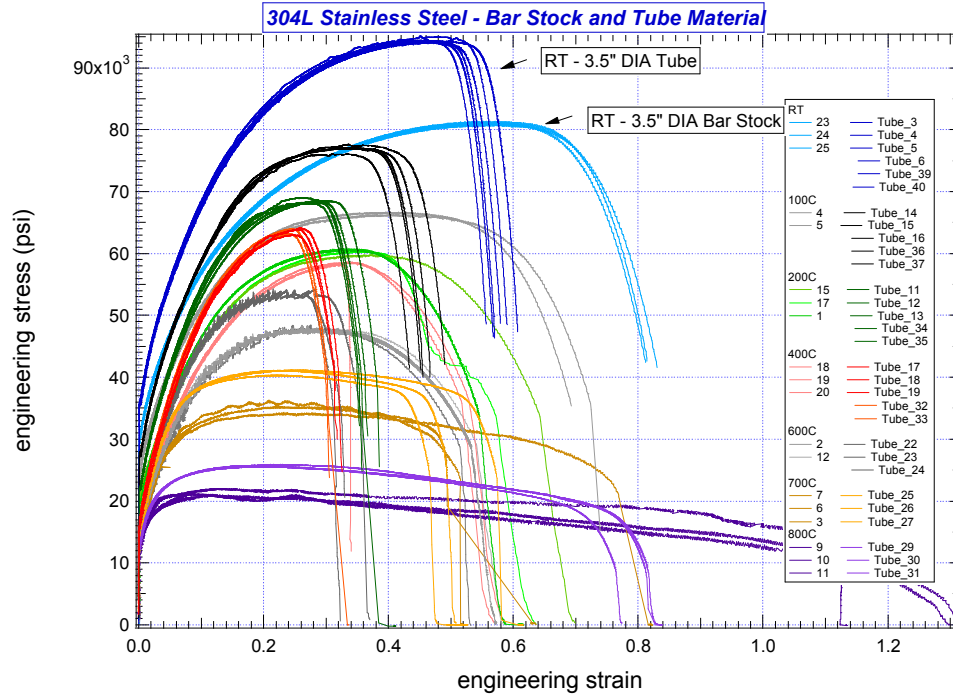
True stress and log strain response for a given material at elevated temperatures is unique. For example, tensile tests have shown that extruded 304L bar stock has an ultimate strength of nearly 20% less than extruded tubing. It is also about 25% more ductile, Figure 3. Additionally, some aluminum alloys including 6061-T651, 6061-T6, 7075-T651, 7075-T7351, 7079 and 7050-T74 have been tested and characterized to tensile failure at elevated temperature. The 304L tube stock is used for pipe bomb and aluminums for thread shear modeling and simulation.



**Figure 2 - Example of various stress-strain curves pertaining to experimental and modeled response in a given tensile-test. Red curve is Cauchy-Stress/Logarithmic-Strain “True” curve conditioned to the constitutive model. The curve is inversely calculated using the constitutive model and a FE model of pulled cylinder such that when the curve is used with the constitutive model in the FE simulations the calculated green stress-strain curve matches the experimentally measured black stress-strain curve from the pull test. See [9] for the set of derived curves at each temperature.**

#### Finite element validation modeling

Two quasi-static verification models were created for validation to experiments. They include the pipe bomb pipe bomb and thread shear geometries. Figure 4 shows the pipe bomb geometry. Figure 5 and 6 show the pipe bomb and thread shear finite element models, respectively. Thread shear validation modeling is just beginning; therefore pipe bomb work will be discussed herein.



**Figure 3. – Engineering stress/strain response of 304L bar stock tensile tests through elevated temperature and a comparison of bar stock and tube stock at room temperature.**

### Finite element modeling to validation experiments

The pipe bomb consists of a 3" O.D tube that is machined down to a .020" wall thickness at the center, Figure 4. Other thicknesses including .035 and .05 thicknesses are also investigated. It is 14" in length.

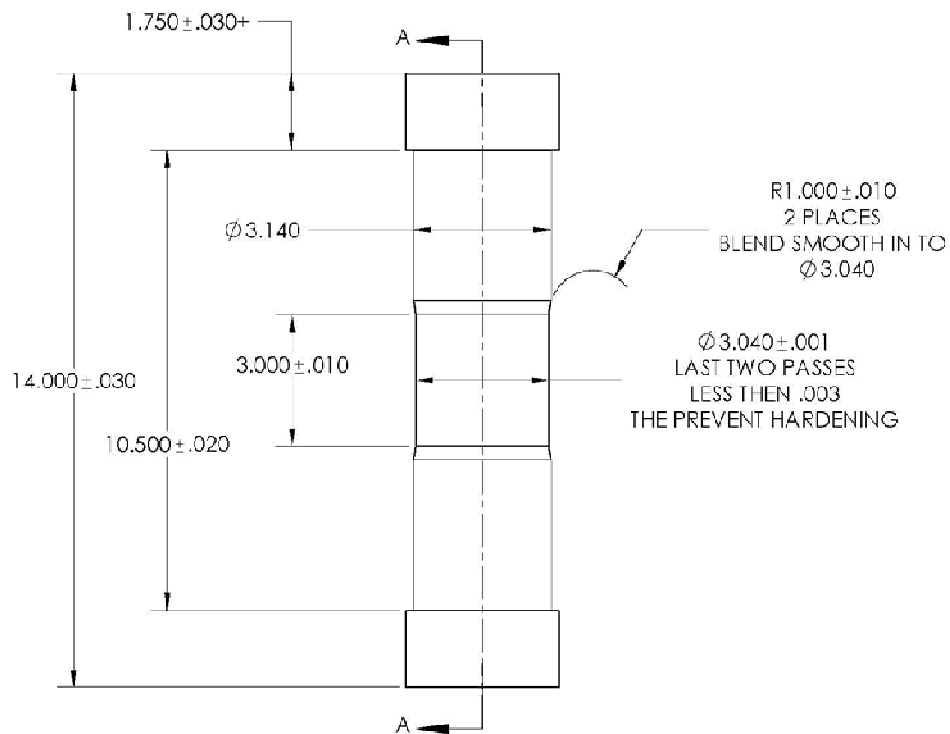
A finite element model of the pipe bomb and thread shear validation experiments are shown in Figures 5 and 6, respectively. In Figure 5, a thermo-mechanical  $\frac{1}{4}$  symmetric section of the experiment is modeled.

The ends are clamped and it is centrally heated by an external source. An internal steel slug is used to minimize gaseous energy due to pressurization for safety purposes. A variety of pressurization and temperature ramp rates were used to validate the model to experiment, however one particular scenario in which the tube is spot heated to 700C, then pressurized to failure will be discussed.

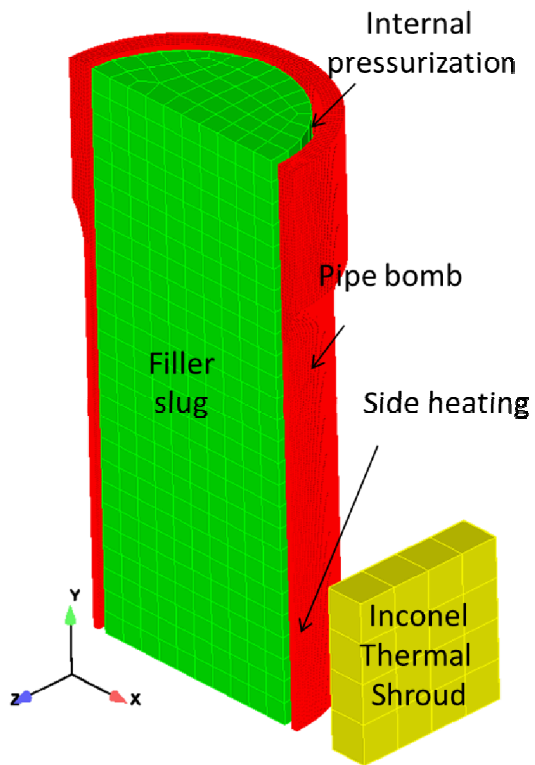
Upon pressurization to failure, the material at the hot spot begins to displace toward the heat source. As it deforms, the wall thickness thins out and failure initiation occurs. Figure 6 shows the experimental setup and an example specimen during a pipe bomb validation test.

In quasi-statics [3], the model must be non-accelerating with no rigid body modes to be statically determinate. As the hot spot displaces toward the heating shroud, instability begins to develop and the model becomes ill conditioned, requiring a significant reduction in the solution time step to continue. Then, as the pressure incrementally increases, the equivalent plastic strain exponentially increases and the tearing parameter approaches critical. In these simulation calculations, adaptive time steps are typically driven to the nanosecond range or smaller in order to obtain convergent solutions with several hundred percent plastic strain and tearing parameters near 10. Given a set of code convergence tolerances, iteration limits and solution updates, the calculation will continue until static instability is reached. At this point, failure is assumed to have initiated. In some cases, element deletion occurs by exceeding the critical tearing parameter, however, in most cases failure is determined by an ill

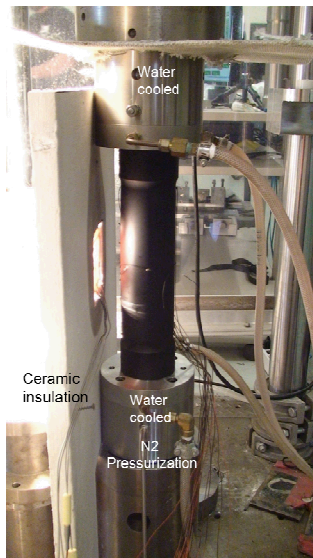
conditioning. Addition work is ongoing and has been demonstrated that failure propagation can be shown by restarting the calculation with an explicit dynamics solver (Presto) [5].



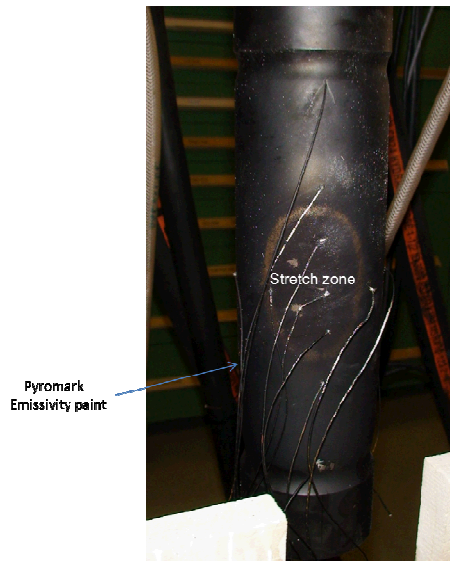
**Figure 4 –Pipe bomb geometry and manufactured test article.**



**Figure 5. – Finite element model of the pipe bomb validation experiment,  $\frac{1}{4}$  symmetry.**

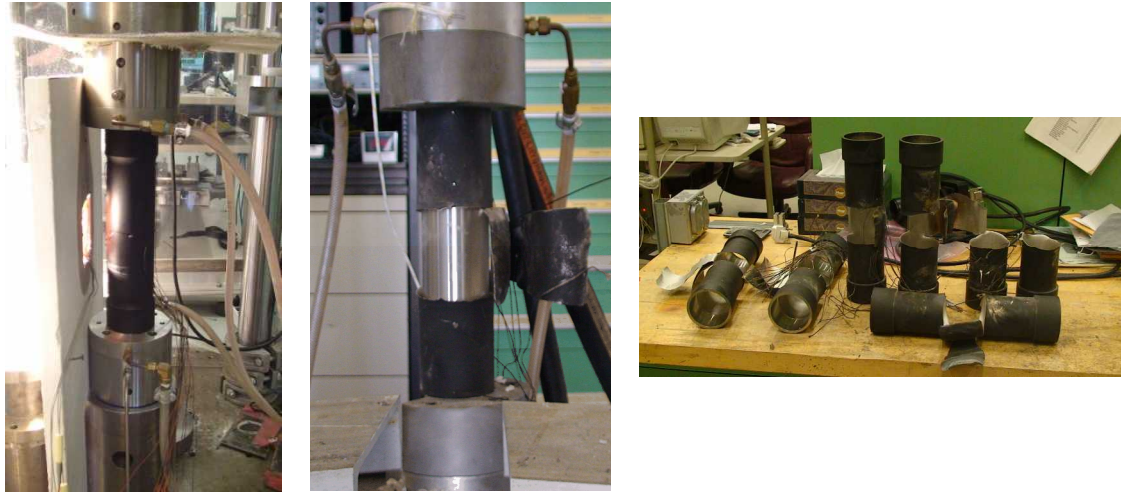


**Side view of Specimen during heating**



**Specimen bulged and deformed after heating and pressurization**

**Figure 6 – Experimental setup and example specimen deformation during a pipe bomb validation test.**

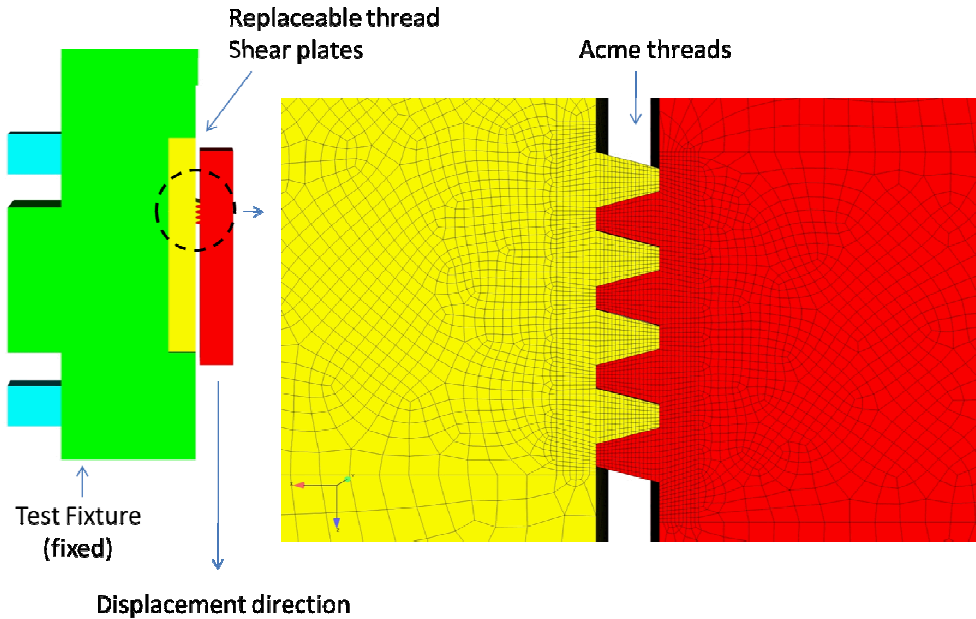


**Figure 7 –Pressure loaded stainless steel “pipe bomb” validation experiment, resulting post-test failure and validation of repeated failure modes.**

Figure 7 show the experimental setup for a pipe bomb validation experiment. During an experiment, the center section is heated and pressurized, causing high deformation at the heated zone as shown. Failure initiation occurs at the hot spot and propagates axially, then circumferentially as shown, Figure 8. Similarly, the pipe bomb models predict this response, but with 20-30% later failure times, as quasi-static finite element solutions are highly dependent on mesh quality, number of elements through the center thickness and a variety of code tolerance settings.

Two iterative solvers can be used for pipe bomb pressurization breach at elevated temperature. These include the finite element tearing and interconnecting (FETI) [6] and conjugate gradient (CG) [7] solvers. The FETI solver is generally used for solving problems in the linear range whereas CG is best for non-linear solutions. Typically, CG can take two orders of magnitude more CPU time to find a solution that FETI. For typical pipe bomb solutions, FETI will tend to over predict failure by around 10% as compared to CG; however FETI has successfully predicted relative failure trends and is useful in screening calculations. For validation, CG is used. Table 1 lists suggested solver settings that should be used as a baseline for high temperature pressurization breach simulations.





**Figure 8 – Finite element model of the thread shear validation experiment.**

Solver resolution settings	FETI	CG
Target relative residual	1.00E-06	1.00E-06
Acceptable relative residual	1.00E-04	1.00E-04
Max iterations	1000	5000
Min iterations	3	3
Adaptive time step settings		
Max cutback	10	10
cutback factor	0.5	0.5
Growth factor	1.5	1.1
Iteration window	100	1000
Target iterations	400	35000
Max multiplier	100	100
Min multiplier	1.00E-12	1.00E-09

**Table 1 – Code settings that control simulation accuracies.**

Table 2 lists results of an isothermal pipe bomb screening simulation study used to rank tensile test data in terms of high and low material strengths. As shown, tensile test repeats were done at 20, 100, 200, 400, 600, 700 and 800 C respectively. The failure pressures (Pmax) are listed for each simulation. For example, six sets of tensile tests were done at 20C. Case try5-rt tensile test data produced a higher pipe bomb failure pressure than the other curves at this temperature. Case try40-rt produced the lowest failure pressure. Similarly, a status of high and low strength simulation runs were ranked for all of the tensile



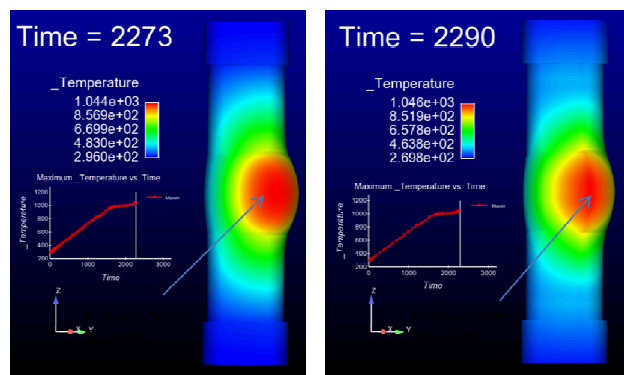
tests. Other quantities of interest include minimum simulation time step acquired for failure and maximum equivalent plastic strain (EQPS) and corresponding tearing parameter values.

The calculations were performed on Sandia's Red Sky [8] computer using 192 processors using a FETI [6] preconditioning solver with adaptive time stepping. Compute times were generally less than 0.4 hours except as noted. Figure 9 shows a result of a fully coupled simulation.

Fully coupled thermo-mechanical and temperature mapped validation simulations are in progress to explore prediction extrapolations and temperature mapping techniques. Figure 9 depicts a result of a study to determine the effect of temperature mapping from a fully coupled simulation (or validation experiment) to an interpolated simulation. High/low material rankings were used to predict failure pressures at high temperature with variations in emissivities, an important step to quantify the error involved in temperature mapping from experiment to model [9,10].

Case	T_max	P_max (psi)	dt (sec)	EQPS_max*	Tearing*	Status	# Procs	cpu-hrs	res	Adaptive
try3-rt	20	1484.5	1.60E-11	0.601	2.14		192	0.368	1.00E-06	feti
try4-rt	20	1482.8	9.00E-13	0.571	2.03		192	0.308	1.00E-06	feti
try5-rt	20	1485.2	9.00E-13	0.575	2.04	high	192	0.324	1.00E-06	feti
try6-rt	20	1485	9.00E-13	0.549	1.54		192	0.348	1.00E-06	feti
try39-rt	20	1483.9	9.00E-13	0.587	2.09		192	0.402	1.00E-06	feti
try40-rt	20	1474.8	9.00E-13	0.555	1.96	low	192	0.309	1.00E-06	feti
try14-100	100	1227.1	1.00E-11	0.586	2.09	high	192	0.441	1.00E-06	feti
try15-100	100	1208.7	9.00E-13	0.528	1.86	low	192	0.546	1.00E-06	feti
try16-100	100	1225.3	9.00E-13	0.561	1.99		192	0.31	1.00E-06	feti
try36-100	100	1226.3	8.60E-12	0.559	1.98		192	0.335	1.00E-06	feti
try37-100	100	1222.9	1.60E-08	0.549	1.95		192	0.284	1.00E-06	feti
try11-200	200	1102.1	1.70E-09	0.529	1.66	high	192	0.335	1.00E-06	feti
try12-200	200	1085.8	9.00E-13	0.426	1.26		192	2.62	1.00E-06	feti
try13-200	200	1088.6	1.30E-06	0.469	1.43		192	2.26	1.00E-06	feti
try34-200	200	1089.9	9.00E-13	0.442	1.32		192	0.453	1.00E-06	feti
try35-200	200	1081.7	9.00E-13	0.402	1.17	low	192	0.342	1.00E-06	feti
try17-400	400	1010.3	1.00E-12	0.394	1.06		192	0.393	1.00E-06	feti
try18-400	400	1007.2	1.00E-12	0.386	1.02		192	0.325	1.00E-06	feti
try19-400	400	1005.7	3.00E-09	0.432	1.2		192	0.312	1.00E-06	feti
try32-400	400	1001.9	1.00E-12	0.373	0.986	low	192	2.479	1.00E-06	feti
try33-400	400	1014	1.00E-12	0.384	1.03	high	192	0.369	1.00E-06	feti
try22-600	600	869.2	1.00E-12	0.409	1.1	low	192	0.361	1.00E-06	feti
try23-600	600	880.1	4.00E-07	0.49	1.39		192	2.54	1.00E-06	feti
try24-600	600	884.7	1.20E-09	0.523	1.52	high	192	0.359	1.00E-06	feti
try25-700	700	705.1	1.00E-12	0.617	1.88	high	192	0.431	1.00E-06	feti
try26-700	700	694.8	1.00E-12	0.605	1.84	low	192	0.431	1.00E-06	feti
try27-700	700	695.5	1.00E-12	0.606	1.83		192	0.443	1.00E-06	feti
try29-800	800	448	3.50E-11	0.501	1.32		192	0.476	1.00E-06	feti
try30-800	800	440.8	1.00E-12	0.632	1.82	low	192	0.431	1.00E-06	feti
try31-800	800	448.8	1.00E-12	0.645	1.89	high	192	0.414	1.00E-06	feti

**Table 2 - Predicted pipe bomb pressurization failure results at isothermal temperature using 304L material characterization true stress/ log strain tensile test data.**



Coupled experiment calculation  
High strength, Nominal Emissivity  
with TC outputs for self check (right)

TC interpolation check calculation  
Using coupled TC outputs (left)



**Figure 9 - Uncertainty on thermocouple mapping algorithm with hi/low material ranking and emissivity variance for the pipe bomb.**

## Results

Run case	Time Seconds	Temp K	Pressure psi	TP ref
Coupled High 0.86	2273.50	1043.64	1183.09	4.12
Coupled Low 0.86	2204.50	1040.90	1110.06	5.28
Coupled High 0.7	2310.40	988.96	1222.16	4.03
Coupled Low 0.7	2259.70	977.26	1168.49	3.28
Interp High 0.86	2290.10	1043.55	1200.66	4.36
Interp Low 0.86	2231.10	1040.77	1138.21	5.93
Interp High 0.7	2328.60	988.89	1241.41	4.39
Interp Low 0.7	2274.90	977.18	1184.58	3.52

## ACKNOWLEDGEMENTS

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