RESPONSE OF ENERGETIC MATERIALS TO THERMAL HAZARDS

Eugene S. Hertel, Jr., William W. Erikson, Michael J. Kaneshige,
Anita M. Renlund, Robert G. Schmitt, and Arthur C. Ratzel, III
Sandia National Laboratories*
Albuquerque, New Mexico 87185

ABSTRACT

Sandia has the responsibility to verify the safety of devices that contain energetic materials under a range of hazardous environments including fires. The energetic materials involved include a variety of explosives, pyrotechnics, and solid propellants. Over the past several years, we have developed a program to study energetic materials using an approach that combines modeling with advanced experimental techniques. In this paper, we review a number of experimental techniques and related modeling efforts used at Sandia to address the problem of energetic material cookoff. Our posture has consistently been that the final result of a cookoff event (i.e. reaction violence) is a strong function of the state of the material (temperature, porosity, etc.) at the time of ignition. Thus, we have focused efforts on understanding material behavior leading up to ignition.

The experimental program includes a number of tests that are used to assess the thermal and mechanical state of thermally decomposing material. The hot-cell experiments consist of heating small pellets of energetic material while simultaneously measuring one-dimensional stress and strain behavior. A triaxial device has also been employed, yielding information on the complete stress-strain state under heating. The Sandia Instrumented Thermal Ignition (SITI)[1,2] experiment has been developed to provide time-resolved temperature measurements within heated energetic materials. The SITI apparatus captures the thermal runaway leading to ignition and it has been modified to make in-situ measurements of evolved gas pressure.

Modeling efforts have paralleled the experiments. Pre-ignition decomposition chemistry models have been developed for a number of different energetic materials using SITI and other data. These have been implemented into codes, and applied to various geometries. Models for the coupled thermo-mechanical behavior have been developed and implemented. A variety of post-ignition combustion models have been developed to describe the enhanced combustion of thermally damaged energetic materials and the deflagration to detonation transition (DDT).

INTRODUCTION

Cookoff of energetic materials (EMs), including high explosives, solid rocket propellants, and gun propellants is an important problem for the DOE and DoD. Cookoff concerns affect operations and handling of munitions and can have a major impact on life cycle costs. Although there are some qualitative differences between “fast” and “slow” cookoff, and separate qualification tests are typically prescribed, fundamentally the same types of physical processes occur in both types. The applicable physical and chemical processes involved in a cookoff event are described here.

The first process is heat transfer. During an accident event, energy transfer occurs between a source (typically a fire) and a target system (munition, rocket, or other device containing propellant and/or high explosive). That energy transfer manifests itself in a rise of temperature in the target through thermal conduction, convection, and radiation.

The next process is chemical reaction. The organic materials that make up the energetic materials chemically decompose, generating heat and gas (decomposition products) while undergoing a thermo-mechanical process that can give rise to internal damage. A major difference between fast and

* Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy’s National Nuclear Security Administration under contract DE-AC04-94AL85000. This work is also supported by the Joint Munitions Program, a collaborative effort between the DOE nuclear weapons laboratories and the DoD.

slow cookoff is the level of thermal penetration that occurs in the energetic material. In a slow cookoff event, most of the energetic material is affected by the temperature rise and can undergo a damage process. The result of the damage is an increase in internal porosity (surface area). In a fast cookoff event, the thermal penetration and damage is generally limited to a small fraction of the energetic material. As the heating continues, the exponential nature of temperature-dependent chemistry leads to a thermal runaway or ignition state.

Chemical reactions continue as the energetic material burns. Once ignition occurs, the model system becomes a race where chemical energy release and pressure generation compete with confinement provided by either an external container or the self-induced inertial confinement of the mass of energetic material. The details of how the chemical energy and combustion process interact with the damaged energetic material determine the final results; the ultimate result of a cookoff insult (violence of reaction) is due to the tradeoff between confinement dynamics and energy and pressure generation. Combustion rates are strong functions of pressure and burning surface area, so reaction rates will continue to grow as the flame spreads and pressure increases. In a damaged material, pressure enhanced combustion can lead to shock driven flows and possibly detonation. Weak confinement typically fails before this can occur and pressure is relieved resulting in little or no violence. However, when the confinement is substantial, there can be adequate time for significant combustion acceleration and the system response can be a violent explosion or detonation.

An illustration of the range of violence which can be achieved is shown in Figure 1; these are examples of the results from a series of pipe bomb cookoff experiments conducted at Naval Air Warfare Center China Lake for a program in which Sandia participated.[3,4] Here, Figure 1 (a) represents a mild pressure burst event; (b) shows a somewhat more violent result; and (c) shows results from a detonation-like event (note: these tests were performed with different explosive materials and the temperature histories also were varied from test-to-test).

Figure 1. Examples of cookoff responses: (a) mild pressure burst [PBXN-109, 3°C/hr], (b) moderate violence [PBX9501, 195°C hold] (c) high violence, detonation-like response [LX-10 at low pressing density, 3°C/hr].

The Sandia National Laboratories modeling approach mirrors our understanding of the key phenomena and the required numerical techniques necessary to accurately capture the phenomena. Our numerical approach is broken into two main temporal domains based principally on the critical time scales of the problem: (1) the pre-ignition phase with its long (minutes to hours) time scales and (2) the post-ignition phase with its short (microseconds to milliseconds) time scales.

During the first, pre-ignition phase, the energetic material is subjected to a thermal load over time scales from minutes to hours. For this phase an appropriate numerical approach is an implicit, finite element technique where thermal conduction, thermal radiation, quasi-static mechanics, and finite-rate chemistry can be modeled accurately. Specific codes at Sandia for this include Calore,[5] Adagio,[6] and Calagio (Calore and Adagio coupled together) and all are based on the Sierra numerical infrastructure.

The second, post-ignition phase involves dynamic processes where the key phenomena (combustion, dynamic mechanics, gas dynamics, and shock waves) occur on the time scale of microseconds to milliseconds. There are a couple of possible numerical techniques for the second phase

but all are based on explicit solutions of the appropriate conservation equations. Conventional finite element techniques with and without multimaterial remeshing schemes (typically referred to as Lagrangian and arbitrary Lagrangian Eulerian) and finite difference/volume schemes (typically referred to as Eulerian) have been applied.[7] All methods have their strengths and weaknesses, but Sandia has focused our efforts on the Eulerian code CTH[8] due to several factors: a natural mechanism for the development of free surfaces, the ability to handle very large deformations, and a simple (but accurate) numerical structure which has led to a focus on the subgrid physics. The nature of CTH has allowed us to implement a suite of subgrid physics models for pressure driven combustion, multiphase flow, and confinement effects that allow a solution through the dynamic combustion phases. Tools to map results from the finite element codes into CTH have also been developed and exercised on slow cookoff problems.

Sandia's hazards program is a tightly coupled experimental-computational effort focused on developing a suite of validated models that can be used to analyze risk and consequence assessment of ordnance systems. Our focus has been to develop and improve sub-models for energetic material decomposition kinetics, mechanical response, ignition, combustion, rapid energy release (detonation), and system response. Our model development effort is focused on phenomenology elucidated by well conducted experiments. The next sections will include a discussion of the key aspects of our program, experiments, model development, and validation.

EXPERIMENTS FOR DISCOVERY AND MODEL DEVELOPMENT

THERMOMECHANICAL BEHAVIOR

A variety of experimental devices have been used to study the cookoff of energetic materials. One of the earliest used at Sandia is known as a "hot cell." These devices consist of a small pellet of explosive material confined between pistons on the top and bottom and a metal sleeve around the perimeter. The piston/sleeve system is contained in a metal load frame. The metal sleeve is heated to desired temperatures and force and displacement measurements of the pistons are made. The principal outputs from hot cell experiments are measurements of displacement and/or load response as a function of temperature and either load or displacement variations. These data ultimately yield properties such as bulk and shear moduli, creep behavior, and thermal expansion coefficients. Data from hot cell experiments have been used in the past to develop constitutive models for heated and thermally damaged energetic materials.[9] Over the years, modifications were made to the original device[10] to allow for scaled-up measurements,[11,12] feedback control,[12] Raman spectroscopic measurements,[13,14] and ultrasonic acoustic measurements.[13,14,15] A photograph of the Scale-Up Hot Cell is shown in Figure 2.

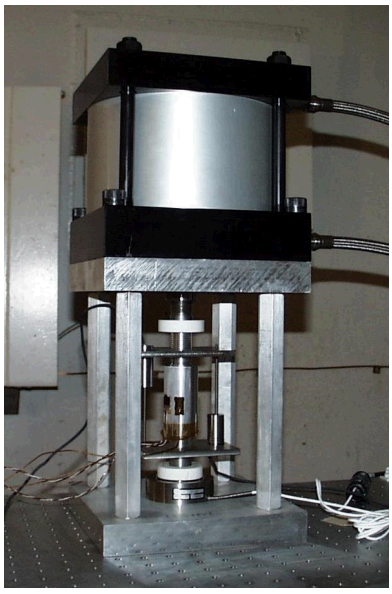

Figure 2. Scale-Up Hot Cell

The response of a number of energetic materials under heating has been studied extensively in both the small- and large-scale hot cells. The character of the materials can be established. For instance, it was observed that PBXN-109 behaves nearly hydrostatically when loaded one-dimensionally, implying a very low shear modulus, in contrast to other materials such as pressed HMX. Bulk modulus, Poisson's ratio, and the coefficient of thermal expansion (CTE) measurements can also be derived from the data. For PBXN-109, it was found that bulk modulus decreases significantly with increases in temperature (the material softens from ~3.4 GPa at 39°C to ~2.3 GPa at 145°C). Poisson's ratio was determined to be ~0.49, very near the 0.5 limit which would be expected with a low shear modulus. CTE of ~108x10^{-6}/°C was measured. The Scale up Hot Cell was also modified by fitting it with a pressure transducer in one piston

to measure gas pressure. By varying the piston displacement and measuring the commensurate change in gas pressure an estimate of evolved gas volume can be made.

For some materials, such as HMX, the deviatoric material behavior plays a significant role in its overall mechanical response.[16] For instance, the compressive strength may be significantly higher if motion in the lateral direction is confined. In order to study these effects a triaxial mechanical testing system with a heated environmental chamber was acquired. This system will allow for the stress in axial and lateral directions to be controlled independently and more complete mechanical models to be developed and parameterized.

WALL STRAIN

One of the ultimate goals of thermal explosion modeling is to develop a method to predict the violence of reaction. Unfortunately, reaction violence is not an easily diagnosed quantity and we must rely on indirect measurements to help understand the important processes. To this end, wall strain has been a principal diagnostic of violence of reaction and considerable effort has been expended by researchers at several facilities in choosing appropriate methods of strain measurements. Various configurations of strain gage techniques (fast versus slow sampling rates; individual gages versus series gage connections, standard versus high elongation gages) have been attempted. We have also investigated two types of fiber optic interferometry as well as a resistance wire technique with some degree of success.

THERMOCHEMICAL BEHAVIOR

To support the critical pre-ignition phase of cookoff, a new experimental technique was developed to examine thermal decomposition leading to ignition.[1,2] In this experiment, the basic concept is to measure temperatures in the interior of an energetic material while it is undergoing thermal decomposition. SITI is similar conceptually to the radial cookoff experiments performed at Los Alamos,[17] except that SITI is sealed gas tight and the original LANL experiments were open to the environment. In SITI, two 1” diameter x 0.5” thick cylinders of energetic material are placed within aluminum confinement. Nine thermocouples are strung between the two layers of energetic material in a staggered format such that the beads lie at specified radii from the center of the explosive. The two aluminum pieces are bolted together. A layer of gasket material between the aluminum halves maintains a gas-tight seal while maintaining electrical isolation for the thermocouples. Thermocouples are also attached to the exterior of the aluminum in three locations. The device is heated electrically with a rope heater wrapped around the exterior. A feedback loop is used to control the heater power such that desired temperature histories can be achieved. Early tests verified that the spatial temperature profile produced in SITI is circumferentially symmetric.[1] Figure 3 shows a cutaway drawing of the SITI apparatus.

SITI experiments have proven to be very beneficial in the model validation process, because internal as well as external temperatures are measured. Simulations can thus use external temperatures as boundary conditions and compare temperature histories at locations within the energetic material with SITI measurements. SITI tests using PBXN-109 were performed as part of a recent joint DoD/DOE model validation project.[2] In those experiments, the aluminum confinement material was heated quickly to a specified hold temperature which was then maintained through thermal runaway and ignition. It was observed that self-heating (verified when interior temperatures exceeded the boundary temperature) occurred much more quickly in the experiment than had been

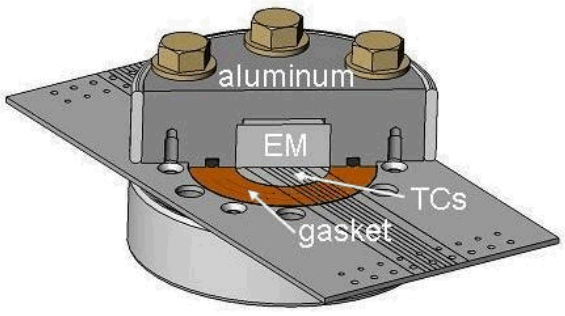

Figure 3. Cutaway drawing of the Sandia Instrumented Thermal Ignition experimental apparatus.

predicted by the PBXN-109 chemical decomposition model. This had occurred because the model had included an endothermic first reaction step. Once the model was adjusted to remove the endothermicity of the first step, SITI temperatures could be matched quite well.

The SITI apparatus has also been adapted to examine other effects. The device has been fitted with a pressure transducer in attempt to measure both the gas generation rate from decomposition and the effect of pressure on cookoff. Leaving the device unsealed led to a significant change in time-to-explosion for certain energetic materials, but has less effect with others. Attempts have also been made to measure post-ignition burn front propagation in SITI by using thermocouples as break wires. SITI data can be used to extract thermal property (conductivity, specific heat) as a function of temperature, particularly at low temperatures when thermal decomposition is minimal. SITI experiments have been conducted on a number of explosive materials including PBXN-109, PBX 9501, LX-10-2, Composition B, and neat HMX, RDX, TNT, and Nitromethane. AP composite and modern high-performance solid propellants have also been tested in the apparatus.

MODEL DEVELOPMENT

Our model development activities parallel our understanding of the physical processes described in the introduction. Modeling and simulation play an important role in our cookoff work. As was described earlier, an overall goal is to be able to predict cookoff response in a variety of conditions. For this to happen, the models must be validated by appropriate experimental evidence. On the other hand, modeling and analysis can also contribute to experiments by providing insight to improve procedures (help with placing diagnostics, estimating time requirements, provide feedback for data quality, etc.). This is possible if simulations are completed in a timely manner. Thus, experiments and modeling are tightly coupled. We feel that this tight coupling is critical to fully realizing the potential of the experiments and improving the quality of the data that is ultimately obtained. At the same time it serves as a quality check for the modeling.

PRE-IGNITION CHEMISTRY MODELING

Prior to ignition, the slow cookoff of energetic materials involves thermal and chemical processes which occur over a very long period of time (on the order of hours). However, the resulting cookoff explosion is characterized by processes associated with combustion and dynamic failure. These occur at very fast time scales (on the order of microseconds to milliseconds). In order to achieve efficient computations while maintaining high fidelity physical representations, the modeling effort was separated into two regimes: (1) pre-ignition and (2) post-ignition. Models describe the various physicochemical processes associated with each regime. These models are implemented into appropriate numerical codes.

The simplest level of pre-ignition modeling involved simulating the heat transfer to the apparatus and energy release associated with decomposition of the energetic materials. These simulations are performed using finite element models of the experiments. Thermal and chemical models require a number of inputs, including material thermal properties (density, conductivity, specific heat) and a description of the chemical reaction mechanism. Various chemical reaction descriptions have been explored over the last several years. A commonly used representation of thermal decomposition is the one originally developed by McGuire and Tarver[18] (see Equation 1). Our approach has often been to utilize a sequential reaction scheme such as Equation 1 and then adjust rate constant parameters such that results from a one-dimensional code would fit One-Dimensional Time to eXplosion (ODTX) data. The resulting models are implemented into finite element codes for representing the cookoff experiment geometries. A major problem with this approach is that the parameter sets as fitted to ODTX data are not unique. SITI was developed to provide a more stringent data set for material characterization.

$$A \xrightarrow{k_1} B \xrightarrow{k_2} C \xrightarrow{k_3} D \qquad (1)$$

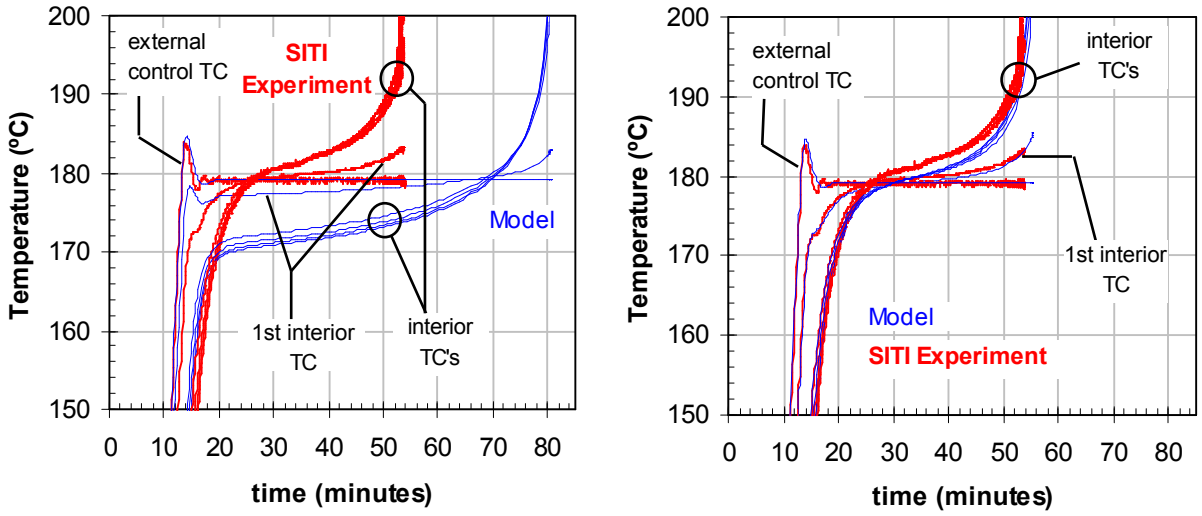

Figure 5. Simulated temperatures and SITI experiment measurements for PBXN-109. Left graph is original chemistry model; right graph is new model. Red lines = experiment; blue lines = model.

For PBXN-109, the original reaction mechanism (based on that of RDX) led to inconsistencies with SITI data. Modifications were made to the parameter set based on the insight gained from a careful investigation of SITI data. The McGuire and Tarver functional form was maintained, but the endothermicity of the first reaction step was removed and rate constants re-adjusted to match ODTX data. Once these changes were made, simulation results were more consistent with SITI data and agreement with pipe bomb experiments was improved as well.[2] Figure 4 shows the improvement of the new model for PBXN-109 over the old. In that figure, the left hand graph shows the comparison of the original model with SITI; the right hand graph shows the newer model. Improvement was achieved for other experiments as well, as shown in Figure 5, which shows the overall time to ignition for simulations compared to a number of experiments. In that graph, perfect agreement between model and experiment is represented by the diagonal line from lower left to upper right corner.

With the development of SITI, our original approach to developing reaction models has been modified. First SITI allows us to determine temperature dependent thermal diffusivity of the explosive material by fitting models to the temperature traces during the initial heat up. Then models are fit which match not only the time to ignition but also the time - temperature histories of the SITI thermocouples. The overall process of model development has been summarized in a recent document.[19]

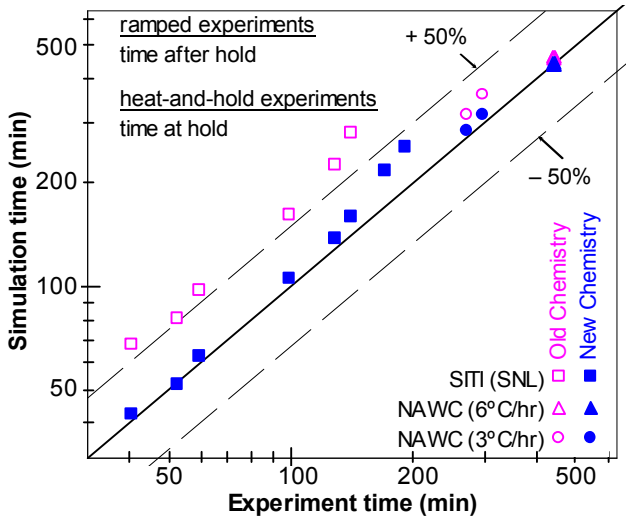

Figure 4. Time-to-ignition comparison of simulation and experiment for two reaction models for PBXN-109.

COUPLED MECHANICS

A simple thermochemical analysis can yield insight into time-to-ignition and extent of reaction at the time of ignition. However, other important parameters such as the gas pressure and the stress/strain state of energetic constituents require a more involved modeling approach. The approach taken at Sandia has been to couple a thermal analysis code with a quasi-static mechanics code.[20] This can be done in two ways: (1) one-way coupling, in which the mechanical environment is affected by temperature field but that mechanical state does not influence heat transfer; and (2) two-way coupling in which mechanical and thermal environments both influence each other. One-way coupling allows the thermal simulation to be performed independently prior to a subsequent mechanical simulation which uses the temperature field as an input. This is computationally much more efficient. Two-way coupling involves using two codes simultaneously to solve the thermal and stress/strain fields. Temperature information is passed from the thermal code to the mechanics code; pressure/stress state and displacement data are passed from the mechanics code to the thermal code. Both of these types of calculations have been performed. However, because the potential mechanical effects (e.g. the effect of pressure on reaction rate, changes in heat transfer at material contact points due to gaps closing, etc.) were not clear, most coupled thermochemical mechanical simulations have been performed with one-way coupling.

Recent experiments conducted with SITI (and other devices) have shown that reaction rate, changes in heat transfer at material contact for certain energetic materials, and the presence of leaks in the confinement can lead to significant changes in time to ignition, compared to a hermetically sealed system. Moreover, for some materials the amount of free volume in the system affects the time to ignition. These suggest that for these materials, decomposition reaction rates are influenced by pressure and/or the concentration of some chemical species. In order to model this response, we have recently begun implementing pressure dependent chemistry[21] and are investigating the use of porous flow models coupled to the thermochemical calculations to describe the pre-ignition evolution of gas associated with decomposition.

Calculating the mechanical state of the explosive-confinement system requires a constitutive model for each material. For steel, we have used an elastic-plastic constitutive model (more complicated models could be used but we have focused on simplicity to test the numerics of coupling). The energetic material behavior is typically more complicated and can include such phenomena as phase change and volumetric and deviatoric creep for the solid component. Porosity is important in the combustion process and pores in the explosive are assumed to be filled with gas. The amount of gas is allowed to evolve as a function of chemical decomposition level (e.g. some fraction of species C and D from Equation 1 are assumed to be gas). Mean stress is a porosity-weighted average of the mechanical stress and the gas pressure in the pores. Obtaining an appropriate set of model parameters involves a significant level of experimental and modeling effort. Because of this, the coupled-mechanics calculations have been used for demonstrations of potential capability rather than as a predictive capability. Further work is clearly warranted in this area.

POST-IGNITION MODELING

As mentioned previously, post-ignition processes occur over much faster time scales than the slow decomposition processes prior to ignition and require different numerical techniques for their efficient solution. At Sandia, we have implemented combustion models into hydrodynamics codes to describe the deflagration of explosives. A flame-sheet model in which mass, momentum, and energy are conserved across a discontinuity has been developed and compared against experiments.[7,22,23] One side of the discontinuity is unreacted material; the other is completely reacted. The flame sheet is allowed to propagate through the domain at a rate determined by the local pressure, temperature, and/or specific surface area (i.e. damage state). The flame is generally initiated by inserting a small “bubble” of reaction products and allowing it to propagate. The principal material characteristic for this model is a burning rate. We believe that the burning rate of pristine material is significantly different than that of thermal degraded material. An example showing a model of burn propagation and confinement failure in a cookoff scenario is shown in Figure 6.

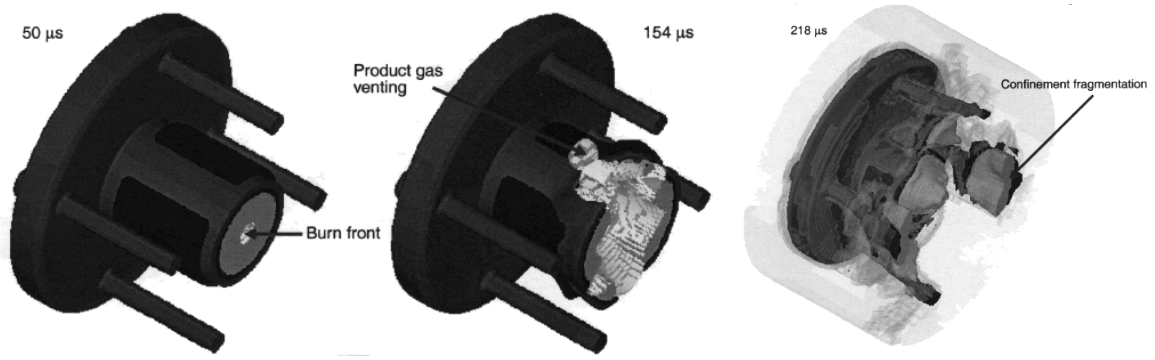

Figure 6. Combustion model showing, initiation, gas venting, and confinement fragmentation of the Variable Confinement Cookoff Test (VCCT) from reference 23.

A number of unknown parameters are needed to describe the post-ignition burn. Parameter sensitivity has been studied for ignition bubble size, constant burning rates, and pressure-dependent burning rates.[7] Comparisons were made with measured wall strains from small scale tests. The outcome of the parametric study was that wall strain histories could be reproduced with "enhanced" pressure-dependent burns of the form $r_{burn}=k\times AP^n$, where k is a constant "enhancement factor," and AP^n is the pristine material burning rate. An example of this process is given in Figure 7 which compares model strains with measurements.[24] Reproducing the strain histories does not imply that an enhanced pressure-dependent burn is the only way to describe the phenomena; clearly without additional data this can not be stated as a fact (e.g. the pressure exponent may change at elevated pressures or convective combustion may occur). Moreover, even if burning enhancement does occur, such as by the creation of additional surface area through thermal damage, it is unlikely that a constant value would be applicable throughout the entire material. For instance, during combustion, pressure-driven material compaction could cause gaps to close up precluding flame spread into some areas.

Agreement of post-ignition modeling results with strain measurements gives hope that reaction violence can be addressed. However, there is still much to do before we can say that reaction violence is predictable. The combustion processes occurring in thermally damaged explosive materials clearly must be better understood. In addition, it is important to understand the behavior of inert confinement materials under fast loading. Reaction violence depends on fracture and fragmentation behavior of the confinement; these aspects have been largely ignored.

Combustion model development is continuing at Sandia National Laboratories. A set of combustion models based on a level-set front tracking approach has been implemented into CTH and has been used to model a number of cookoff scenarios.[25,26] Variations of this model have been used successfully to model shock-to-detonation transition and deflagration-to-detonation transition. The level-set burn model has also been used to describe distributed combustion following behind a rapidly propagating flame front. These techniques appear promising and further development will be conducted.

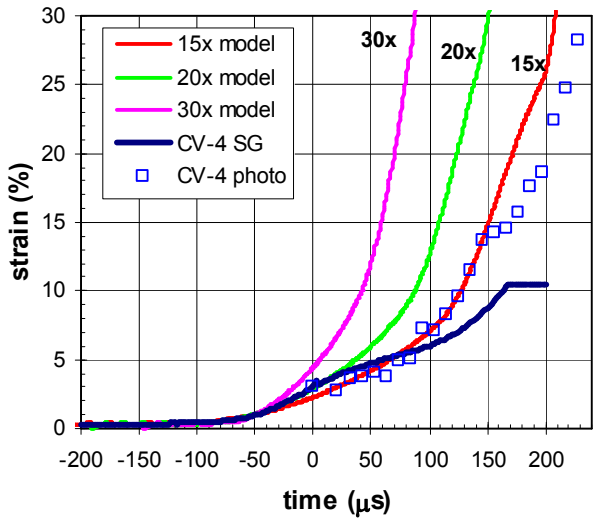

Figure 7. Simulation results compared with strain gage (SG) and photographic (photo) strain measurements from reference 24.

CONCLUSIONS AND FUTURE WORK

Development of practical models for truly predictive analysis of cookoff is an ongoing challenge. However, small-scale real-time in situ measurements are able to provide unique physical insight into the governing mechanical, thermal, and chemical processes, leading to scalable models. We have exercised these techniques on several programs and have developed reasonably good pre-ignition models for ideal (or nearly ideal) explosives. These models were applied to several experimental configurations with good success. Internal temperature measurements are very advantageous (even necessary) in model development and validation. These data are required in addition to well-defined boundary conditions.

We have demonstrated a simple post-ignition combustion model based on a pressure-dependent burn ($k \times AP^n$). Wall strain history can be reproduced by using this model but currently it should not be considered predictive. Violence can be inferred from these strain histories but as yet we do not claim a predictive capability. More physically complete models for combustion, flame spread, and the transition to detonation have also been developed and implemented into hydrodynamics codes. Additional testing and development of these models in the cookoff regime is needed.

We believe that there are still many unknowns associated with explosives which have been heated and thermally damaged. There is a need for some clever experiments to address these. Information on basic material properties (conductivity, specific heat, etc. as a function of temperature) is still needed for many materials. More information is needed on the combustion behavior of energetic materials, especially in the degraded (in-situ) state. Important aspects include: the mechanism for flame spread, burning rates (as a function of pressure and damage level), interaction with damage/cracks, etc. To predict violence of reaction, the failure characteristics of the confinement are important for assessing and predicting violence. We have made great strides in understanding cookoff phenomena but more progress is needed before truly predictive models are available.

REFERENCES

[1] Kaneshige, M. J., Renlund, A. M., Schmitt, R. G., and Erikson, W. W., "Cook-off Experiments for Model Validation," *20th JANNAF PSHS Meeting*, Destin, FL, 2002.

[2] Kaneshige, M. J., Renlund, A. M., Schmitt, R. G., and Erikson, W. W., "Cook-off Experiments for Model Validation at Sandia National Laboratories," *Twelfth International Detonation Symposium*, San Diego, CA, 2002.

[3] Atwood, A. I., Curran, P. D., Decker, M. W., and Boggs, T. L., "Experiments for Cookoff Model Validation," *19th JANNAF PSHS Meeting*, Monterey, CA, November, 2000

[4] Atwood, A. I., Curran, P. D., Lee, K. B. and Bui, D. T., "Experimental Progress on a Cookoff Model Validation Effort," *20th JANNAF PSHS Meeting*, Destin, FL, Apr. 2002

[5] Bova, S. W., Okusanya, T. O., Newman, C. K., Glass, M. W., and Copps, K. D., "Calore A Computational Heat Transfer Program," SAND2005-0623, Sandia National Laboratories, October 10, 2005.

[6] Adagio Development Team, "Adagio/Andante User Reference Manual," Sandia National Laboratories, July 29, 2005.

[7] Erikson, W. W. and Schmitt, R. G. "Pre- and Post-Ignition Modeling of Validation Cookoff Experiments," *20th JANNAF PSHS, Meeting*, Destin FL, Apr. 2002.

[8] Hertel, E. S., et al., "CTH: A Software Family for Multi-Dimensional Shock Physics Analysis," Proceedings of the 19th International Symposium on Shock Waves, Vol. 1, edited by R. Brun and L. D. Dumitrescu, pp. 377-382, July 1993.

[9] Schmitt, R. G., Wellman, G. W., Renlund, A. M., and Miller, J. C., "A Constitutive Model for Confined HMX during Cookoff," *17th JANNAF PSHS Meeting*, Tucson, AZ, Dec. 1998.

[10] Renlund, A. M., Miller, J. C., Trott, W. M., Erickson, K. L., Hobbs, M. L., Schmitt, R. G., Wellman, G. W., and Baer, M. R., "Characterization of Thermally Degraded Energetic Materials," *Eleventh International Detonation Symposium*, Snowmass, CO, Aug. 30 – Sep. 4, pp. 127-134, 1998.

[11] Renlund, A. M., Kaneshige, M. J., Schmitt, R. G., and Wellman, G. W. “Mechanical Response and Decomposition of Thermally Degraded Energetic Materials: Experiments and Model Simulations,” *18th JANNAF PSHS Meeting*, Cocoa Beach, FL, 1999.
[12] Kaneshige, M. J., Renlund, A. M., and Schmitt, R. G., “Mechanical Response of Heated PBXN-109,” *19th JANNAF PSHS Meeting*, Monterey, CA, Nov. 2000.
[13] Tappan, A. S., Renlund, A. M., Gieske, J. H. and Miller, J. C., “Raman Spectroscopic and Ultrasonic Measurements to Monitor the HMX β-δ Phase Transition,” *18th JANNAF PSHS Meeting*, Cocoa Beach, FL, 1999.
[14] Tappan, A. S., Renlund, A. M., Gieske, J. H. and Miller, J. C., “Real-Time Raman Spectroscopic and Ultrasonic Measurements to Monitor the HMX β-δ Phase Transition and Physical Changes in Thermally Damaged Energetic Materials,” *19th JANNAF PSHS Meeting*, Monterey, CA, 2000.
[15] Tappan, A. S., Renlund, A. M., Miller, J. C., Casstevens, J. E. and Oliver, M. S., “Real-Time Ultrasonic Characterization of Thermally-Damaged Energetic Materials Approaching Cookoff,” *20th JANNAF PSHS Meeting*, Destin, FL, 2002.
[16] Schmitt, R. G., Wellman, G. W., Renlund, A. M., and Miller, J. C., “A Constitutive Model for Confined HMX during Cookoff,” *17th JANNAF PSHS Meeting*, Tucson, AZ, Dec. 1998.
[17] Dickson, P. M., Asay, B. W., Henson, B. F., Fugard, C. S. and Wong, J., “Measurement of phase change and thermal decomposition kinetics during cookoff of PBX 9501,” *American Physical Society 1999 Conference on Shock Compression of Condensed Matter*, Snowbird, UT, June 28-July 2 1999. Also “Measurement of phase change and thermal decomposition kinetics using the Los Alamos Radial Cookoff Test,” Los Alamos National Laboratory report *LA-UR-99-3272*.
[18] McGuire, R. R. and Tarver, C. M., “Chemical Decomposition Models for the Thermal Explosion of Confined HMX, TATB, RDX, and TNT Explosives,” *Seventh Symposium (International) on Detonation*, NSWC MP 82-334, pp. 56-64, 1981.
[19] Dodd, A. B. and Kaneshige, M. J., “Cook-Off Model Development and Analysis of Energetic Materials Using Sandia Instrumented Thermal Ignition (SITI) Experimental Data,” *13th International Detonation Symposium*, Norfolk, VA, July, 2006.
[20] Erikson, W. W., Schmitt, R. G., Atwood, A. I., and Curran, P. D., “Coupled Thermal-Chemical-Mechanical Modeling of Validation Cookoff Experiments,” *19th JANNAF PSHS Meeting*, Monterey, CA, November, 2000.
[21] Hobbs, M. L. and Kaneshige, M. J., “Modeling HMX Ignition Using an Enthalpy Formulation,” *13th International Detonation Symposium*, Norfolk, VA, July, 2006.
[22] Schmitt, R. G. and Baer, T. A., “Millisecond Burning of Confined Energetic Materials During Cookoff,” *16th JANNAF PSHS Meeting*, West Palm Beach, FL, Oct. 1997.
[23] Schmitt, R. G., Baer, T. A., Renlund, A. M., and Margolis, S. B., “Modeling Burn Rate Phenomena of Damaged Energetic Materials,” *11th International Detonation Symposium,* Snowmass, CO, Aug. 1998.
[24] Sandusky, H. W., Chambers, G. P., Erikson, W. W., and Schmitt, R. G. “Validation Experiments for Modeling Slow Cook-off” *12th International Detonation Symposium*, San Diego, CA, Aug. 2002.
[25] Schmitt, R. G., Erikson, W. W., Asay, B., Dickson, P., Henson, B., Smilowitz, L., and Tellier, L., “Application of a Multiphase Mixture Theory with Coupled Damage and Reaction to the LANL Large-Scale Annular Cookoff Experiment,” *19th JANNAF PSHS Meeting*, Monterey, CA, Nov. 2000.
[26] Schmitt, R. G., Taylor, P. A., and Hertel, E. S. “Application of a Multiphase Mixture Theory with Coupled Damage and Reaction to Energetic Material Response,” *12th International Detonation Symposium*, San Diego, CA, Aug. 2002.