

TABLE OF CONTENTS

OBJECTIVE STATEMENT

TECHNICAL APPROACH

IMPACT OF THE PROPOSED WORK

RELEVANCE

GENERAL WORK PLAN

DATA SHARING

SCIENTIFIC/TECHNICAL/MANAGEMENT

REFERENCES

OBJECTIVE STATEMENT:

The Sandia objective will be a focus on Task 3: “Development and validation of test approaches for assessment of material flammability under microgravity and partial gravity conditions.” The approach to be applied in executing this objective will be typical of Sandia: 1) fundamental, or micro-scale studies utilizing precision measurements, 2) macro-studies involving larger or multiple samples under specified environmental conditions, and 3) model studies to rationalize results for expanded application.

In proceeding through test method development and validation, wireless sensors will be utilized to collect information for a large number of potentially flammable specimens or flammable conditions with respect to gas composition and total pressure when exposed to an incipient ignition situation. Associated with this experimental approach will be chemical and mathematical modeling studies which focus on quantifying controlling parameters including offgas identification and reaction rate constants. This information will be incorporated into appropriate chemical (Chemkin) and mathematical models (technique developed by a Co-I) with the goal of projecting performance of materials in real use scenarios, i.e., manned space station. It will be the ultimate goal to examine the fundamentals of flammability and seek to represent material response in terms of generalized boundary conditions, similar to efforts at NASA WSTF.

It is expected that the effect of gravity and orientation will be illuminated experimentally using the Sandia centrifuge facilities and results will be examined by a corresponding CFD model to verify that sufficiently descriptive physics is included in a commercially available code (Star-CCM+). The centrifuge testing is also anticipated to replicate launch G loading/vibration to verify that the test apparatus, which can potentially be flown on ISS, will survive launch.

TECHNICAL APPROACH:

A typical approach in examining flammability of materials for spacecraft is to conduct an experiment at normal gravity which specifies an ignition source applied to the bottom of a prescribed size of material under consideration and to note the upward flame spread. While the size and orientation is realistic, the effect of non-standard gravity is absent. NASA has noted in this solicitation that there is concern that under some situations, low or zero gravity may exacerbate risk of flammability so there is a prospect to actually fly experiments on the International Space Station (ISS) and conduct material flammability tests. However, because of: a) the desire to examine multiple materials simultaneously exposed to abnormal environments, b) robust design for simplicity of installation, data collection methods, and launch survival, and c) the need to conduct experiments in a inhabited environment, a simplified but compact and contained experimental bundle is proposed. By encapsulating each material in an individually sealed Pyrex ampoule with an installed Micro Electro-Mechanical System (MEMS) wireless (and battery-less) sensor with antenna, it will be possible to monitor quantities such as temperature, pressure, and offgas composition during heating of the bundle onboard the ISS. The need for an individual battery for each ampoule would significantly compromise the sensor functioning lifetime and vulnerability so a Standing Acoustic Wave system (SAWs) which is externally excited and returns a signal related to the property of interest, will be proposed. The figure below indicates temperature measurement which was obtained from a MEMS/SAWs couple.

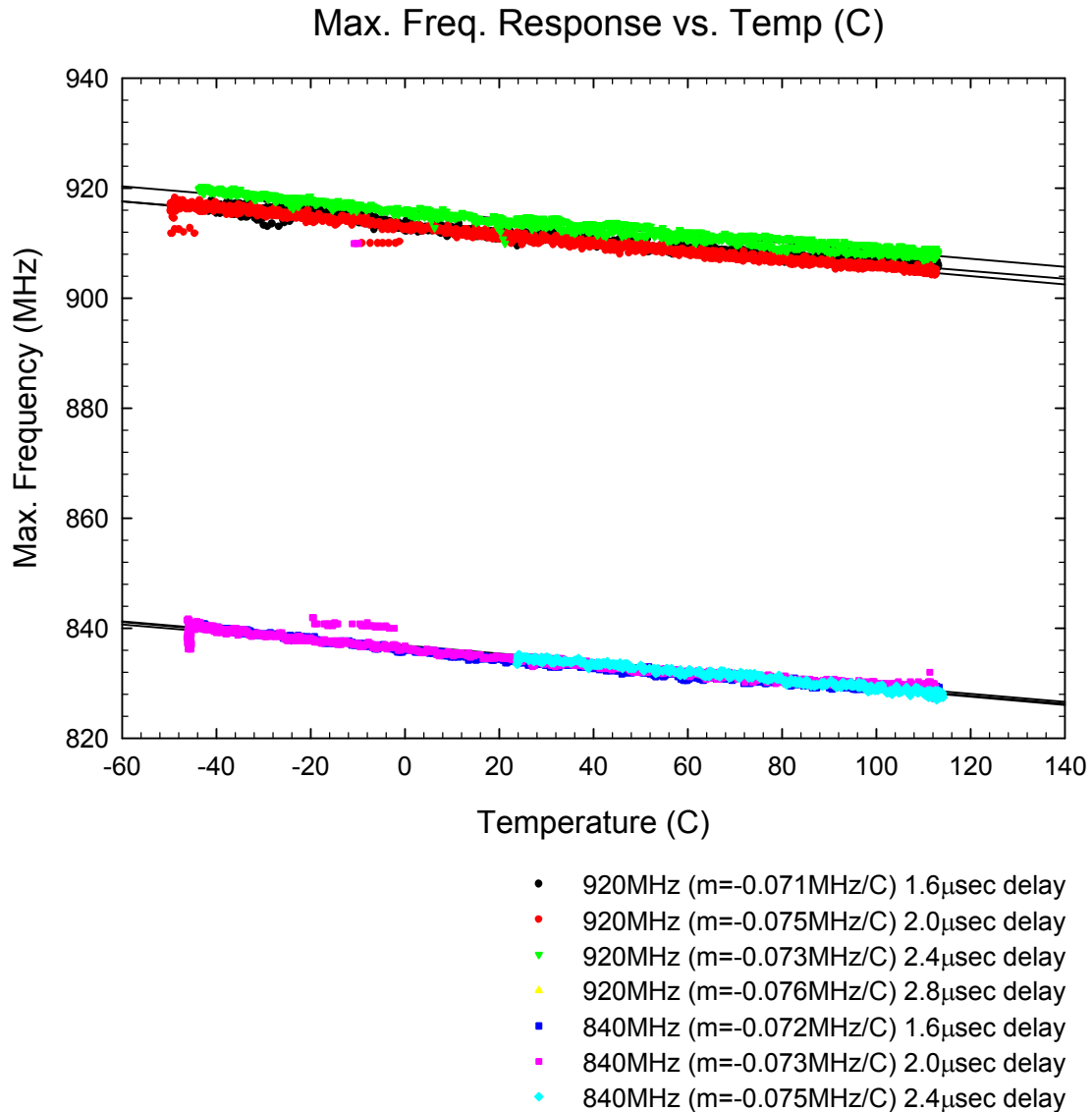


Figure 1. Temperature-Frequency for MEMS/SAWs Device

It should also be possible to vary oxidizer gas composition and total pressure for any samples to provide the effect of reduced gravity on minimum oxygen threshold. Performance of and communication with MEMS devices in sealed ampoules have been demonstrated at Sandia National Laboratories. An ampoule comprising a sealed Pyrex container with an enclosed MEMS/SAWs and attached antenna is show next. This is followed by figure which shows a comparison of communication between the enclosed device and a similar device in open air.

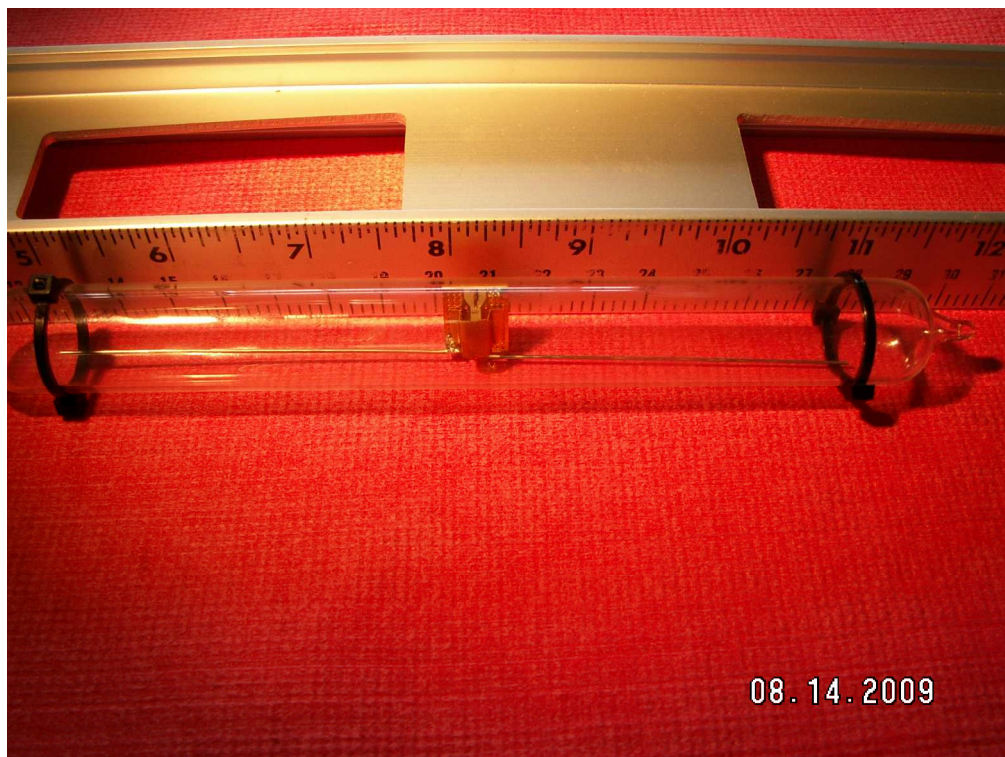


Figure 2. MEMS/SAWs Device sealed in Pyrex Ampoule

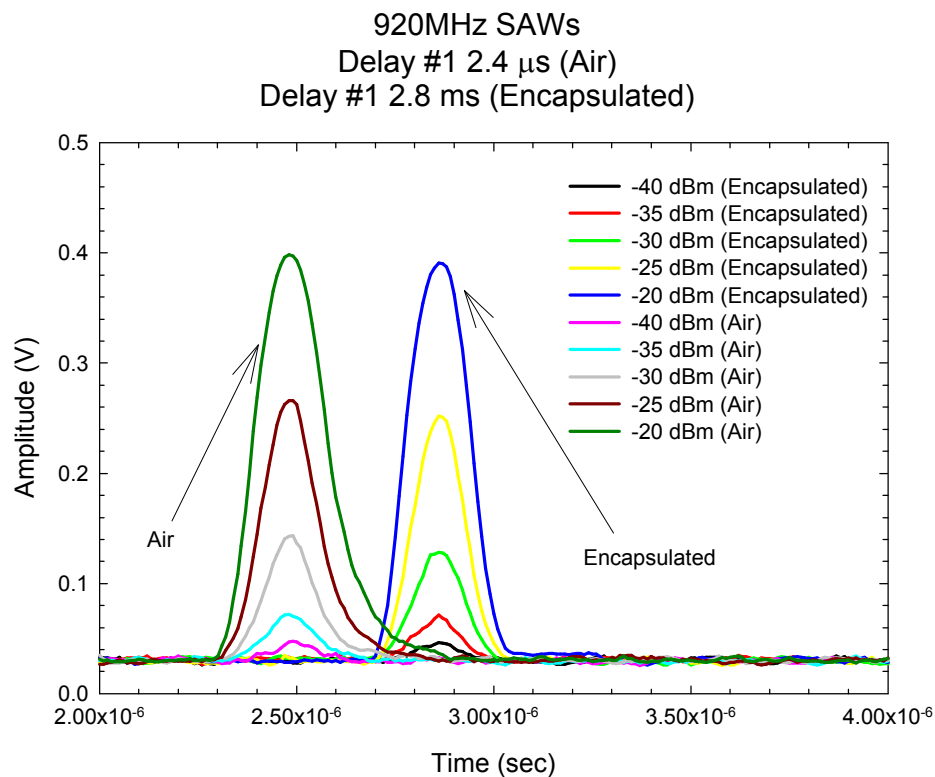


Figure 3. Demonstration of Communication for MEMS/SAWs Device Sealed in Pyrex

A number of tests with MEMS/SAWs devices have indicated the ability of the interrogator to discriminate between multiple signals which will facilitate communication between the individual experiments and the interrogator/data retrieval and storage system.

By using the MEMS/SAWs for sensing and communication with an interrogator, it will be possible to bundle multiple specimens in a very confined volume. The target number of specimens and/or different gas environments is order of 100, and these can be imbedded in an aluminum billet for heat distribution, and occupy a volume of less than 0.5 cubic feet. The drilled nests for specimen insertion can be with minimal tolerance, and covered with a nonflammable cover which will transmit RF and secure specimens in the billet. The billet can be heated at the back using an electric resistive heater, and the entire assembly will be insulated to minimize power consumption and to assist in minimizing temperature variation throughout the samples. The testing can commence by energizing the power supply at a specified rate and monitoring the response of each sample to indicate internal pressure, temperature and offgas composition, e.g. CO, CO₂, or O₂ depletion, depending on ease of development of the appropriate sensor. It may be desirable to use a heat conductive material or paste between the drilled ports in the billet and ampoules to overcome contact resistance to heat transfer and also provide some cushioning for launch survival.

The sequence of subtasks is summarized next: 1) project planning, coordination and selection of materials, 2) fundamental chemistry, 3) flammability modeling, 4) development of the appropriate capability of MEMS sensors, 5) validation of the sensor functions of single and multiple MEMS device(s), and 6) centrifuge testing and 7) final test assessment and reporting. Each of these activities will be briefly discussed next with details to follow in general plan of work.

1) Project planning, coordination and sample selection: This effort is intended to lay out the tasks ahead and establish a medium of coordination and communication within the team. It is anticipated that materials selection and sampling conditions will be addressed before any of the experimental work begins, as well as specification of the measurements which will need to be made with MEMS devices so that development specific to that task can commence.

2) Fundamental chemistry: While development and verification of the capability provided above is ongoing, other, more fundamental testing of these candidate materials can commence. By using TGA with offgas separation and analysis via GC/MS of candidate samples in a gaseous environment of choice, it will be possible to first characterize and screen candidate materials.

3) Mathematical & computational modeling: Such information, if experiments are properly selected, can first allow for empirical determination of global reaction kinetics, e.g., Arrhenius constants, and that information can be used with an analytic model which accounts for internal heat generation, reactant depletion, and heat diffusion. With this model, it should be possible to consider boundary conditions for which ignition of bulk materials subject to surface heating, might be expected. This model is not anticipated to include gravitational or orientation effects; such complications will be left to a CFD model. Additionally, with TGA offgas analysis, it should be possible to make a preliminary attempt at identifying more detailed reaction kinetics which can be used in conjunction with Chemkin to build a detailed overall reaction model. This model can be

used to examine results of DSC measurements in various atmospheres to determine the level of predictability. Chemkin can use as input, the experimental temperature profile, and execute the calculations in constant pressure mode, corresponding to conditions existing in TGA and DSC.

4) MEMS sensor development: The measurement of both temperature and pressure by MEMS devices has already been demonstrated, but not for a single device. Gas composition of CO, CO₂ or O₂ depletion is optimistically believed achievable. However, development of the specific sensor and technique remain to be demonstrated. And combination of all sensors to be used into a single crystal needs to be demonstrated. Additionally, the present the antenna has not been optimized for minimum space requirements. This also could reduce volume occupied by each of the ampoules which will be incorporated with the test bundle.

5) Hardware testing and validation of sensor function: A critical step in the development of MEMS devices is to insure that they will make a reliable measurement of the expected quantity within acceptable accuracy, and with needed discrimination between multiple sensors. To develop confidence in this approach, many single and low multiple tests will be performed with Pyrex sealed samples and subjected to temperature excursions. The interrogation, separation sensitivity, data storage, sample survivability, uniformity of ampoule dimensions and other functions will be investigated. It is expected that these experimental results can be compared to the analytic chemistry results by use of Chemkin. In other words, Chemkin will be used with detailed reaction kinetics in a constant pressure calculation applied to TGA and DSC results, but for the same kinetics model, the calculation can be carried out for a constant volume process so that results such as pressure or O₂ depletion can be compared to experimental results from ampoule testing.

6) Centrifuge testing: This activity is intended to provide preliminary information related to influence on gravity of samples to be tested, and the ability to stimulate SAWs devices remotely, and to evaluate the launch survival capability of the package which is intended to house multiple specimens.

PERCEIVED IMPACT:

Material flammability, unfortunately, is not a material property and this has led to many test methods which attempt to quantify the propensity of a material to ignite under a specified set of conditions. Generally, results are used to rank-order different materials according to results of these specific tests. A number of ASTMs and other standard methods have been proposed and utilized to make measurements of flash point, auto-ignition temperature, flammability limits, oxygen consumption index, smoke point, etc. A few attempts have been made to define ignition or flammability of gases in terms of fundamental properties. Among these are the work of Sheldon, who proposed a minimum heat release per unit volume of combustibles [1] and Melhem, who proposed the criteria of a minimum adiabatic reaction temperature [2], both for gas phase reactions. However, many flammable materials naturally exist in a condensed phase; either liquid or solid. This state confounds the material response by introducing other factors such as heat diffusion, latent heat, mixing with oxidizer gas, etc. Recent literature documents attempts for predicting solid materials flammability [3,4,5], and still other literature has focused on testing procedures [6], the effect of gravity on material flammability [7] and

threshold oxygen concentration [8]. It is hoped that a complete set of parameters can be identified, sufficient for non-dimensionalization utilizing Pi group analysis, leading to the development of generalization of minimum flammability conditions for condensed phase ignition. Obviously, prior literature, e.g., [3,4,5] will be closely considered in this attempt.

RELEVANCE OF THE PROPOSED WORK:

For purposes attendant to this solicitation, the safety of astronauts onboard ISS is of paramount importance. Disasters in the history of manned spaceflight have seen the loss of life and have had a significant dampening effect on the initiative of continuing manned missions. Even the loss of an unmanned space package can also be disappointing and costly. Hence any anomalies which are determined to be specific to low gravity conditions can be of interest for both civilian and military purposes. In addition, for both the general public and industrial activities, safety and material standards can potentially be improved and refined as the fundamentals of material flammability are better understood and modeled. Any significant developments during this study will be dutifully disclosed to both NASA and the general public, once the results have been verified, scrutinized and reviewed.

GENERAL WORK PLAN:

In order to make the limited funding provided in this solicitation achieve as much information as possible, the involvement of two of the higher education institutions in New Mexico has been sought. Faculty at these institutions with unique qualifications and/or laboratory facilities have been identified and enlisted. It is the intention, where possible, to use subcontract funding to support students and faculty research. Other tasks specific to Sandia National Laboratories unique capabilities have been assigned internally, as needed.

Effort at New Mexico State University:

Analytic Chemistry:

Chemical analysis of samples to be studied will be carried out in the Department of Chemistry under the supervision of Dr Antonio Lara. In fulfilling the tasks of the proposed work, material specimens which either are in current use, or of potential use in the crew quarters and work area of the manned space station, will be investigated as to their propensity for flammability under the expected space station environment. While the number of specimens is not specified, it is anticipated that there will be a significant number different materials which are at least representative of possible choices. Foams, plastics, insulating materials (specifically electric wiring but potentially thermal, as well), fabrics, polymers, etc. are but a few generic classes under consideration. In addition to direct experimental data, it is anticipated that the collected information will be utilized in models which seek to characterize flammability in general, and which can be used with more comprehensive models to consider other contributing properties which could impact flammability, e.g., solid heat diffusion, effect of oxidizing atmosphere, effect of orientation, effect of gravity, effect of type of heat source and heating rate, etc. This latter modeling effort will be the responsibility of researchers at New Mexico Institute of

Mining and Technology; hence experimental information will be provided to both Sandia, and to NMT as their subcontractor.

In order to provide both reaction information and heat release information, data will be collected for the various samples with two different systems: the DSC and the TGA with GC/MS. The DSC is a differential scanning calorimeter and will indicate the temperature and the corresponding energetics during a heating profile and subject to a prescribed environment. If the material sublimates and absorbs energy in the process, then this property will be identified. If at another temperature, there is exothermic reaction, then that property will likewise be identified. This information will provide input to the energy equation which models large specimen response to a mathematically defined heating boundary condition. TGA is thermogravimetric analysis and will be used to determine temperature at which the material outgases. This will be an indicator of the propensity of the material to decompose. By coupling with GC/MS for the offgas analysis, it will be possible to determine the chemical nature of the resulting gas. It is anticipated that variables for DSC and TGA with GC/MS will include not only the specimen type, but also the environmental gas composition (including inert), the total pressure up to local barometric, and the heating rate. These results will presumably represent a uniform temperature sample, but by using the Semenov analysis, can provide global reaction rate parameters, e.g., frequency factor, reaction order and activation energy. Additionally, the identification of the offgases, can allow incorporation of reaction pathways for oxidation of those components. Then by combining individual rate constants into a chemical kinetics code such as Chemkin, it should be possible to replicate the test conditions and verify the global reaction rate parameters. This approach will assist in generalizing results of the materials studied to other similar materials which might eventually become candidates as spacecraft materials. In addition to the global reaction rate parameters, the energetic measurements from DSC will support analytic consideration of the consequence of certain boundary conditions which could contribute to either smoldering or outright ignition of materials under realistic conditions.

Since variable gas environments can be imposed on both TGA and DSC enclosures, it will be possible to examine threshold oxygen concentration, and total pressure and correlate the data obtained to similar information which has been reported in the literature.

Hardware design, fabrication and testing Additionally, testing of individual samples and communication with the interrogation system, will be conducted in the Mechanical Engineering Department of New Mexico State University under the supervision of Dr Burl Donaldson. Equipment available includes various constant temperature baths and controllers, as well as high temperature heat sources.

In order to support the large batch testing proposed at Sandia, several individual tasks will need to be first conducted to demonstrate the equipment capability and testing procedure. Samples which have passed through the chemical analysis will be sealed in a glass or Pyrex® ampoule, along with the latest MEMS device available. The MEMS should be at least capable of indicating pressure and temperature within the ampoule; gas sampling capability will be integrated when available. The receiver antenna and electronics will be obtained and function verified. Individual samples will then be subjected to a thermal environment and the total ampoule pressure noted, along with any gas analysis. Then by utilizing the Chemkin software with the reaction pathways and

kinetic data which has been validated against DSC and TGA results, adjustments to conditions, e.g., constant volume instead of constant pressure, will be compared to the experimentally obtained results. By appropriately changing total pressure and partial pressure of oxidizer in ampoule and changing the heating rate, it can be determined how well the Chemkin model describes the measurements. It is anticipated that modifications may need to be made to the model to rationalize any significant discrepancies. Once individual sample tests are adequately understood, attention will be turned to simultaneous measurements for multiple samples subject to the same temperature and temperature change profile. This will validate the ability of the MEMS sensors/receivers to discriminate between information transmitted from the different samples and store the data for later retrieval and analysis.

The next step in the process will be the design and fabrication of a controlled thermal environment chamber in which a large number of specimens can be studied. This will be the design which will be flown by NASA and placed in orbit so that gravitational effects on outcome will be evident. This activity will encompass a number of issues. Its package and contents must be sufficiently robust to survive launch; this survivability will be demonstrated at the appropriate G force at the Sandia horizontal centrifuge. Attendant to this application, it will be necessary to provide for an elevated thermal environment by interfacing with the space station power supply. A thermal control system and data acquisition system which will survive both launch and orbit will also need to be demonstrated. The Sandia vertical centrifuge can provide a sinusoidally varying gravity by spinning at around 10 rpm. This will take the package through zero gravity and 2xG every 6 seconds. This package will be fully functional so that the heating and data collection system will be exercised. In addition, it is anticipated that a photo-detector will be included with the MEMS device in order to sense flare-up under variable gravity. Additionally, by examining the slope of the pressure response curve, it should be possible to determine how ignition/combustion of test materials is affected by these variable gravity conditions.

In addition to the test results, by comparing experimental data to results of a CFD calculation which includes gravitational effects, e.g., buoyancy and orientation, it will be possible to verify that commercial CFD codes are capable of modeling the observed behavior.

Equipment which is already available in the Department of Mechanical Engineering to supplement this study is an oxygen bomb calorimeter which can be used to measure the gross enthalpy of combustion for comparison to results of the DSC measurements.

Deliverables: Sharing of data collected in both the fundamental chemistry studies and the hardware development is required so that this information is available for subsequent work which is dependent on this information. Additionally, formal annual reports will be provided to Sandia National Laboratories as input to the annual report to NASA.

Effort at New Mexico Institute of Mining and Technology:

Modeling efforts will be carried out at New Mexico Institute of Mining and Technology (NMT). A faculty in the Department of Mathematics, Dr. Ranis Ibragimov is knowledgeable in a unique approach to analytic consideration of the energy diffusion

equation with internal heat generation and reactant consumption. This capability will facilitate consideration of real material response to boundary conditions which might lead to flammability. Modeling and simulation will be divided into four parts. These will be experimental data analysis, mathematical modeling of thermal ignition, use of Chemkin for chemical kinetics calculations, and CFD simulations. Chemkin and CFD calculations will be performed under the supervision of Dr. Nadir Yilmaz of the Department of Mechanical Engineering at NMT. Mathematical modeling of thermal ignition will be investigated under the supervision of Dr. Ranis N. Ibragimov, Director of *Centre RSCAMM* (Research and Support Center for Applied Mathematical Modeling) & Adjunct Professor of Mechanical Engineering at NMT. Experimental data analysis will be performed by both researchers.

Analysis of Experimental Data: Experimental data gathered using TGA and GC-MS for an extensive number of materials (i.e. 100 materials) provided by researchers at New Mexico State University will be studied using regression analysis. Curve fittings will be used to determine Arrhenius constants for the materials. In the analysis, coefficients will be obtained while assuming a first-order reaction which should be sufficient because reaction rate diminishes with depletion and rate of decomposition slows as the amount of sample disappears.

Mathematical modeling of thermal ignition: Empirically determined Arrhenius constants will be used in the mathematical model to examine cases involving thermal diffusion and capacitance effects for determination of ignitions conditions of real materials in spacecraft setting. The model will use a very unique mathematical approach known as Lie group analysis. It is anticipated to model the thermal ignition of a semi-infinite plate with depletion. Outcomes of the model will provide information about boundary conditions under which thermal ignition will happen. These boundary conditions include temperature, heat flux, conductive heating or electric element. Examination of extensive number of materials under boundary conditions relevant to spacecraft setting will be important to know for which materials smoldering and thermal run-away occurs.

In particular, Dr. Ibragimov will work on mathematical modeling of the energy conservation for symmetrically heated body.

Model: The model itself is written in terms of the following system of Partial Differential Equations relating the absolute temperature $T(x,t)$ and the mass concentration $w(x,t)$ of reactant per unit volume (see also Thomas [1]):

$$\begin{aligned} \chi \left(\frac{\partial^2 T}{\partial x^2} + \frac{j}{x} \frac{\partial T}{\partial x} \right) &= \rho c \frac{\partial T}{\partial t} + Q \frac{\partial w}{\partial t}, \\ \frac{\partial w}{\partial t} &= -f w^n \exp \left(-\frac{E}{RT} \right), \end{aligned} \tag{1}$$

where $j = 0, 1$ and 2 are for a slab, cylinder and sphere respectively. The material parameters E (activation energy), R (universal gas constant), T (absolute temperature), χ (thermal conductivity) and ρ (density) are taken as constants. Additionally, the parameter f will be determined in our work experimentally from the requirement that the effective heat transfer must be related to real surfaces to provide the results agreeable with Thomas [1]. System (1) must be solved subject to the initial conditions

$$\begin{aligned} T(x,0) &= T_{in}, \quad w(x,0) = w_{in} \\ \frac{\partial T(0,t)}{\partial x} &= 0, \quad T(L,t) = T_B, \end{aligned} \quad (2)$$

where T_{in} and w_{in} are given values from experimental data, $x = 0$ corresponds to the mid-plane for slab, center point for cylinder and sphere and $x = L$ is the boundary for slab. We will also set $x = R$ for cylinder and sphere of radius R . As it is seen from (2), the problem is complicated by discontinuity in boundary and initial conditions for T . This discontinuity appears from the following physical reason: Initial temperature is the ambient temperature assigned for the entire region. Behavior of the explosion depends on the critical temperature that is assigned at the boundary. If the boundary temperature is below the critical temperature $T = T_*$, the temperature will increase nonlinearly until it reaches the critical temperature. When T attains its critical value, energy of the system will dissipate because of the higher heat loss than general heat. In contrary, if the temperature is above the critical value, i.e., if $T(x,t) > T_*$ at the boundaries $x = 0, L$ internal heat will be generated until instability will develop because the energy will internally be generated much faster than the heat lost on the boundary.

Method: All previous analytical models in solving (1) (even with continuous boundary conditions (2)) were solved for the particular case $j = 0$, (Thomas [1]) and within the Taylor's approximation of the exponential part in the right hand side of the second equation in (1) which corresponds to a very restricted modeling in which $T - T_{in}$ is much less than T_{in} . (see e.g., Storey [2] and Adler & Enig [3]). Therefore, only approximated solutions were obtained in the previous studies.

Approach: In our mathematical modeling, the behavior of heated reactive material will be analyzed on the basis of exact solutions of the initial-value & boundary-value problem (1) – (2). The exact solutions will be obtained by the Theorem on projections of equivalence Lie algebra. This Theorem has recently been formulated and applied to several nonlinear engineering models in our previous studies in Ibragimov & Ibragimov [4]. In fact, as it is confirmed in our preliminary results, the theorem on projections proved and illustrated in [4] provides a regular method for obtaining numerous integrable approximations to the model system (1) – (4). Moreover, the results will be obtained not only for the exact form of the model (i.e., without any approximation of the exponential part in the second equation) but for all possible values of $j = 0, 1$ and 2 .

Advantage and educational purpose of the approach: The formulation of fundamental natural laws and technological problems in the form of rigorous mathematical models is given frequently, even prevalently, in terms of non-linear differential equations. The good illustrative example is our model (1) – (2). Today engineering researchers routinely confront problems in mathematical modeling involving solution techniques for differential equations. However, very often the solutions cannot be obtained analytically by these methods, in spite of the fact that, e.g., over 400 types of integrable second-order ordinary differential equations were accumulated due to ad hoc approaches and summarized in voluminous catalogues. On the other hand, the fundamental natural laws and technological problems formulated in terms of differential equations can be successfully treated and solved by Lie group methods.

This particular model illustrates the fact that the development of group analysis provides a universal tool for tackling considerable number of differential equations even when other means of integration fails. It was a mistake for many years (including present days) to isolate the Lie Group Analysis from natural engineering applications and treat it as a branch of mathematical abstract science.

Concise list of references related to mathematical modeling

- [1] Thomas, P.H., (1961). Effect of reactant consumption on the induction period and critical condition for a thermal explosion. *Proc. Roy. Soc. A*, 262: 192-206.
- [2] Storey, P.D., (1981). Calorimetric studies of the thermal explosion properties of aromatic diazonium salts. *I. Jem. E. Symposium Series*, 68, 3/P/1-3/P/9.
- [3] Adler, J., Enig, J.W., (1964), The critical conditions on Thermal explosion theory with reactant consumption. Defense Technical Information center, Accession Number: AD0432348.
- [4] Ibragimov, N.H., Ibragimov, R.N., (2009). Invariant solutions as internal singularities of nonlinear differential equations and their use for qualitative analysis of implicit and numerical solutions. *Communications in Nonlinear Science and Numerical Simulations*, 14, 3537-3547.

Chemkin Reaction model: Using off-gas analysis and literature sources for individual reaction rate constants, global reaction mechanisms will be constructed and implemented in Chemkin. The code will be used to perform constant pressure analysis to determine ratios of oxygen to inert gas for which ignition occurs. After matching results with the constant pressure process, the model will be exercised in the constant volume mode and results will be compared to experimental data for the same materials provided by NMSU researchers.

Examination of gravity and orientation: After validating Chemkin reaction model code against TGA results and experimental data, findings from steps above will be used to examine effects of variable gravity and orientation. Buoyancy effecting energy feedback for combustion will be taken into account with gravity. Results for luminosity and pressure will be examined and gravity effects will be seen by intensity of radiation. In addition, it will be possible to test capabilities of commercial CFD codes by the observed behavior.

Software available at NMT: NMT Mechanical Engineering Department faculty posses specialized software which will be useful in modeling the experimental conditions. One relevant software package is Chemkin, which receives as input, the various chemical pathways with reaction kinetics that make up the complicated chemistry attendant to ignition. This capability will assist in interpreting results of both TGA and DSC, as well as offgas measurement which is collected during experimental work with the sealed ampoules. The other software package is Star CCM+, which is a CFD code. This code will allow for consideration of issues such as variable gravity and orientation within a gravitational field. This activity is expected to facilitate interpretation of experimental results which are to be obtained when samples are flown in the Sandia centrifuge.

Deliverables: NMT team will closely work with NMSU and Sandia researchers. NMSU will provide DSC and TGA results. NMT team will analyze the data and obtain rate constants for the sample materials. These constants will be implemented in the mathematical model to determine ignition conditions for the same materials. Chemkin reaction kinetics code will be used for constant pressure and constant volume modes.

Numerical results will be compared to experimental data obtained by the NMSU team. Finally, a commercial CFD code will be tested to examine effects of gravity and orientation. Computational results will be compared to test results of the Sandia horizontal centrifuge. A formal annual report will document results from each year's work and this will be integrated with an annual report from Sandia to NASA.

Effort at Sandia National Laboratories:

Sandia is responsible for the overall management of the project, including planning, coordination of activities, reporting and assessment of test method. Other work which will be conducted at Sandia National Laboratories includes MEMS/SAWs development of a sensor which can be used to monitor offgas or oxygen depletion from the experiments, as well as monitor and report internal pressure and temperature inside the ampoule. Also, the multiple centrifuge facilities can be used to investigate the effect of alternating gravitational fields, and the survivability of a test package under launch conditions. Finally, the project planning, direction and coordination will be the responsibility of Sandia.

Project Planning, Coordination Sample Selection and Reporting:

Coordination and execution of the contract will be the responsibility of Sandia Senior Member of the Technical Staff-Dr Walter Gill. It will be his responsibility to define and redefine subtasks as information is collected. It will also be his responsibility to identify materials of interest and test conditions of interest.

As Principal Investigator (PI) he is the individual the research organization designates as having an appropriate level of authority and responsibility for the proper conduct of the research, including the appropriate use of funds and administrative requirements such as the submission of scientific progress reports to the agency. The designated PI is responsible for the quality and direction of the proposed research and for the proper use of awarded funds regardless of whether or not he/she receives support through the award. There are three identified tasks for the PI.

Point of Contact: The PI will coordinate activities by setting up the project using a work breakdown structure that can be monitored for both progress and evolving problems. Communications between participants will be facilitated through weekly teleconferences, and less often with progress review meetings. The PI will also seek out external collaboration for potential leveraging during the course of the project.

Annual Reporting and Task Book Reporting: The PI will provide an annual written report to NASA on or before the anniversary of the start of funding. This information will be used to assess the degree of progress of the project. A component of this annual report will be used for the NASA Task Book.

This information will consist primarily of:

- An abstract
- A bibliographic list of publications
- Copies of publications
- A statement of progress, including a comparison with the originally proposed work schedule

Final Report: A final report will be provided to NASA at the end of the award funding period, including a detailed listing of all peer-reviewed publications.

This information will consist primarily of:

- Statement of the specific objectives
- Significance of the work
- Background
- Overall progress during the performance period
- Narrative discussion of technical approaches including problems encountered
- Accomplishments related to approach
- An appendix with bibliography and copies of all publications and reports
- Any publications or other public materials containing data are particularly important will be included in this section.

MEMS Development:

MEMS development is ongoing at Sandia National Laboratories in support of a broad initiative to identify and integrate this technology into any appropriate military or related application. Sandia National Laboratories is home to a highly sophisticated \$500M custom MEMS manufacturing facility. The investigator who will be responsible for development of the needed sensors, along with the SAWs, antenna and interrogation/data acquisition is Kent Pfeiffer at Sandia. Because of his broad mission statement, it will not be necessary to cover Kent's manpower costs from this contract. It is anticipated that some MEMS fabrication costs, specific to the sensors which will be specific to this contract will need to be covered. So in a sense, the very valuable resource represented by Kent's expertise can be considered as "cost share". In addition to development of MEMS devices, specifically gas analysis for CO, CO₂ or O₂ depletion, and perhaps luminosity, (sensors for pressure and temperature are already available) Kent will also participate in antenna development which is compact and compatible with the ampoule geometry which is planned. Kent will also participate in specification of the antenna and data acquisition system to be used for system testing both at NMSU and the Sandia centrifuge.

Centrifuge:

Work using the centrifuge is to be managed by Ed Romero, as owner of centrifuge facility, with the data acquisition support provided by Tim Miller. Their activities in this role are now given.

Sandia National Laboratories' large centrifuge complex was developed over 5 decades ago to simulate inertial loads on components and systems as encountered in various flight environments ranging from missile launch to atmospheric reentry. Both functional and structural testing is performed on two large radius centrifuges, a 29' radius indoor centrifuge and a 35' radius outdoor centrifuge. Centrifuge capabilities cover a wide variety tests, ranging from simple structural load tests to long series of highly instrumented hardware performance tests with combined acceleration and controlled vibration. The complex has exceptional data collection and communication infrastructure. Each centrifuge has a 20 cubic foot instrumentation panel at the center of rotation with over 100 channels of slip rings. Signals may be recorded on-board or passed through a variety of slip rings including high current copper, high bandwidth copper, fiber optic or wireless. Test items can include classified, hazardous items as well as explosives.

The 29-foot-radius indoor centrifuge has a load capacity of 1.6 million g-pounds, making it one of the largest in the United States. This centrifuge is housed in an underground room that is 80 feet in diameter and 12 feet high, allowing a relatively clean and temperature-controlled environment. It can accelerate a maximum payload of 16,000 pounds to 100 g's, or lighter loads to 300 g's. The maximum rotational speed of the centrifuge is 175 RPM. To more closely simulate real flight environments an innovative approach was developed at Sandia to add controlled vibration to test units under inertial loading. This "Vibrafuge" capability can provide combined acceleration + vibration environments at accelerations up to 100g with payloads up to 400lb. Further advancement for missile flight simulation has been demonstrated through the development of a "Superfuge" system. A proof of concept test rig successfully demonstrated a superfuge system capable of combining controlled acceleration, vibration and secondary axis spin at 100g, 15gmrs and 500RPM respectively. Work is underway to optimize and package the superfuge hardware into a readily available permanent test assembly.

Subtask six of this proposal includes standard centrifuge launch testing to verify the survivability and functionality of the proposed experimental package after launch. It is suggested that vibrafuge testing be performed to assure survivability in an environment that most closely matches the actual launch environment. Although none of the launch environment specifications have been provided it is expected that NASA launch environments will be similar to those typically encountered by other missile customers the centrifuge complex has worked with in the past. The current cost to prepare for and run instrumented vibrafuge tests at the SNL large centrifuge complex is attached.

Subtask six also includes the application of alternating 0g and 2g on the proposed experimental package to study gravitational effects on ignition, pressure and light emissions. This alternating acceleration can be achieved by mounting the proposed experimental package on the outer edge of a 1 meter radius disc rotating about a horizontal axis. This aspect of testing would utilize Sandia's superfuge spin motor and slip ring hardware. It would also require the fabrication and integration of a rotating disc and subsequent mounting hardware.

DATA SHARING:

Sandia has a long established history of working with higher educational facilities in New Mexico, including New Mexico State University and New Mexico Institute of Mining and Technology. In fact, three of the investigators for the current proposal have co-authored a number of papers dealing with topics that were supported by Sandia National Laboratories. And Dr Yilmaz at NMT was a doctoral study student working under the supervision of Dr Donaldson while attending NMSU. Several graduate students working in Dr Lara's analytic chemistry laboratory have been supported by Dr Donaldson, performing both Sandia research and US Army contract research for contracts with Dr Donaldson-PI. Additionally, because Sandia, NMSU and NMT are located reasonable close, it is convenient to arrange meeting with the researchers submitting this proposal. Money in the travel budget is intended to facilitate this exchange.

SCIENTIFIC/TECHNICAL/MANAGEMENT:

The graphic below shows the relationship between the various activities in fulfillment of the objectives of this proposal:

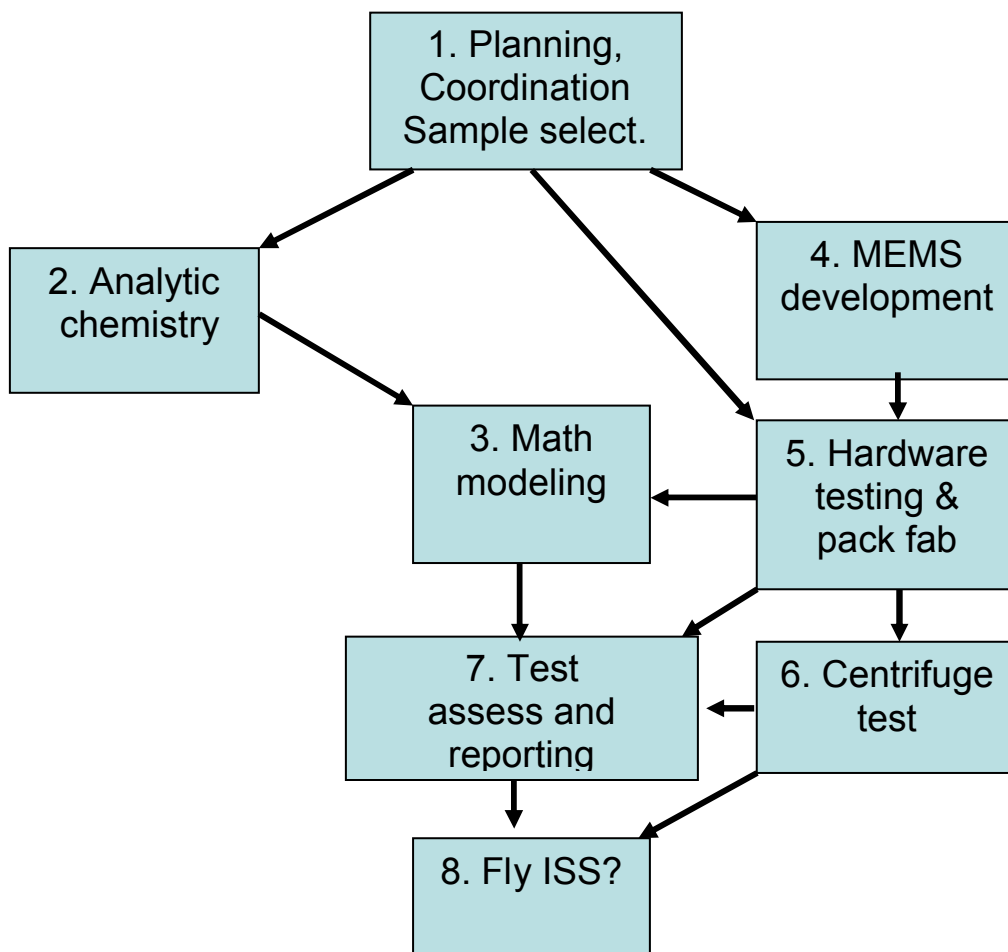


Figure 4. Relationship of activities

In this diagram, items 1, 4, 6 and 7 will be the responsibility of Sandia, items 2 and 5 will be the responsibility of NMSU and item 3 will be the responsibility of NMT. Obviously activity on items 1 and 4 will commence immediately on award of contract, followed shortly by activity on item 2. Items 3 and 4 should see significant activity during second year with CFD calculations during first half of final year, and items 6 and 7 are planned for completion during final year.

REFERENCES:

1. "Study of Flammability Limits of Gases and Vapours", Sheldon, Martin, *Fire Prevention*, p 23-31, Nov 1984
2. "Detailed Method for Estimating Mixture Flammability Limits using Chemical Equilibrium", Melhem, G.A., *Process Safety Progress*, v 16, n 4, p 203-218, Winter 1997

3. “On the Estimation of Hazard Potential for Chemical Substances” Melhem, G.A.; Shanley, E.S, Process Safety Progress, v 15, n 3, p 168-172, Fall 1996
4. “A Computational Study of Low Oxygen Flammability Limit for Thick Solid Slabs”, Kumar, Amit and Tien, James S., Combustion and Flame, v 146(1-2) p 366-378, July 2006
5. “Using Heat of Combustion Data to Estimate or Assess some Threshold Flammability Properties of Materials”, Hshieh, Fu-Yu, Hirsch, David B. and Beeson, Harold D., Fire and Materials, v 27 (6) p 267-273, November/December 2003
6. “High Throughput Flammability Characterization using Gradient Heat Flux Fields”, Gilman, Jeffery W., Davis, Rick D., Randy Shielse, J., Harris Jr. Richard H., Journal of SAME International, v 2(9), p 113-123, October 2005
7. “Flammability, Offgassing, and Compatibility Requirements and Test Procedures”, Interim NASA Technical Standard NASA-STD-(I)-6001A, National Aeronautics and Space Administration, Approved: 04-21-2008 Washington, DC 20546-0001 Expiration Date: 04-20-2009 Superseding NASA-STD-6001
8. “Pressure Effects on Oxygen Concentration Flammability Thresholds of Materials for Aerospace Applications” Hirsch1, David; Williams, Jim; and Beeson, Harold, Journal of Testing and Evaluation, October 2006