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Methodology Assessment and Recommendations for the Mars Science Laboratory Launch Safety Analysis

Gregory C. Bessette, Nathan E. Bixler, John C. Hewson, David G, Robinson, Donald L. Potter, Dana A. Powers, Christopher B. Atcitty, Brian W. Dodson, Heather J. MacLean, Kurt E. Metzinger, Beverly R. Sturgis, Ronald J. Lipinski, John E. Kelly, and Kenneth D. Bergeron

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Sandia National Laboratories

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METHODOLOGY ASSESSMENT AND RECOMMENDATIONS FOR THE MARS SCIENCE LABORATORY LAUNCH SAFETY ANALYSIS

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Printed: September 2006

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Abstract

The Department of Energy has assigned to Sandia National Laboratories the responsibility of producing a Safety Analysis Report (SAR) for the plutonium-dioxide fueled Multi-Mission Radioisotope Thermoelectric Generator (MMRTG) proposed to be used in the Mars Science Laboratory (MSL) mission. The National Aeronautic and Space Administration (NASA) is anticipating a launch in fall of 2009, and the SAR will play a critical role in the launch approval process. As in past safety evaluations of MMRTG missions, a wide range of potential accident conditions differing widely in probability and severity must be considered, and the resulting risk to the public will be presented in the form of probability distribution functions of health effects in terms of latent cancer fatalities. The basic descriptions of accident cases will be provided by NASA in the MSL SAR Databook for the mission, and on the basis of these descriptions, Sandia will apply a variety of sophisticated computational simulation tools to evaluate the potential release of plutonium dioxide, its transport to human populations, and the consequent health effects. The first step in carrying out this project is to evaluate the existing computational analysis tools (computer codes) for suitability to the analysis and, when appropriate, to identify areas where modifications or improvements are warranted.

The overall calculation of health risks can be divided into three levels of analysis. Level A involves detailed simulations of the interactions of the MMRTG or its components with the broad range of insults (e.g., shrapnel, blast waves, fires) posed by the various accident environments. There are a number of candidate codes for this level; they are typically high resolution computational simulation tools that capture details of each type of interaction and that can predict damage and plutonium dioxide release for a range of choices of controlling parameters. Level B utilizes these detailed results to study many thousands of possible event sequences and to build up a statistical representation of the releases for each accident case. A code to carry out this process will have to be developed or adapted from previous MMRTG missions. Finally, Level C translates the release (or "source term") information from Level B into public risk by applying models for atmospheric transport and the health consequences of exposure to the released plutonium dioxide. A number of candidate codes for this level of analysis are available. This report surveys the range of available codes and tools for each of these levels and makes recommendations for which choices are best for the MSL mission. It also identifies areas where improvements to the codes are needed. In some cases a second tier of codes may be identified to provide supporting or clarifying insight about particular issues. The main focus of the methodology assessment is to identify a suite of computational tools that can produce a high quality SAR that can be successfully reviewed by external bodies (such as the Interagency Nuclear Safety Review Panel) on the schedule established by NASA and DOE.

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Table 1. List of Acronyms

AOC	Accident Outcome Condition
AIC	Accident Initial Condition
ATCA	Atmospheric Transport and Consequence Analysis
BCI	Bare Clad Impact
CCAFS	Cape Canaveral Air Force Station
CCDF	Complementary Cumulative Distribution Function
CDF	Cumulative Distribution Function
CFD	Computational Fluid Dynamics
CEL	Coupled Eulerian Lagrangian (code)
CMF	Cumulative Mass Fraction
CPU	Central Processor Unit
DOE	Department of Energy
EIS	Environmental Impact Statement
EOS	Equation of State
FSAR	Final Safety Analysis Report
FTS	Flight Termination System
GIS	Graphite Impact Shell
GPHS	General Purpose Heat Source
HANDI	Heating Analysis Done Interactively
INSRP	Interagency Nuclear Safety Review Panel
JPL	Jet Propulsion Laboratory
KSC	Kennedy Space Center
MC	Monte Carlo
MMRTG	Multi-Mission Radioisotope Thermoelectric Generator
MSL	Mars Science Laboratory
NARAC	National Atmospheric Release Advisory Center
NASA	National Aeronautics and Space Administration
NRC	Nuclear Regulatory Commission
PBL	Planetary Boundary Layer
PDF	Probability Distribution Function
PESA	Probabilistic Event Sequence Analysis
PLF	Payload Fairing
PNH	Pluto New Horizons
PRA	Probabilistic Risk Assessment
QA	Quality Assurance
RTG	Radioisotope Thermoelectric Generator
SAR	Safety Analysis Report
SMA	Charring Material Ablation
SMF	Sandia Fireball Model
SMYRA	Sandia Modified Young's Reconstruction Algorithm
SNL	Sandia National Laboratories
SPH	Smooth Particle Hydrodynamics
SVT	Safety Verification Test
TAOS	Trajectory Analysis and Optimization Software

1. Introduction

1.1 Purpose of This Study

The National Aeronautics and Space Administration (NASA) plans to launch the Mars Science Laboratory (MSL) mission in the fall of 2009. This mission will land a science rover on the surface of Mars for the purposes of exploration and scientific analysis. The rover is proposed to be powered by a Multi-Mission Radioisotope Thermoelectric Generator (MMRTG) (Figure 1 and Figure 2). The energy source for the MMRTG is the radioactive alpha-particle decay of approximately 4.8 kg of plutonium dioxide (using primarily ^{238}Pu) contained within General Purpose Heat Source (GPHS) modules. Space launches involving nuclear systems of this size require a special launch approval process called out in Presidential Directive / NSC-25 (Lake 1995). A key part of this process is the preparation, by the Department of Energy (DOE), of a Safety Analysis Report (SAR) addressing the nuclear risks of the launch.

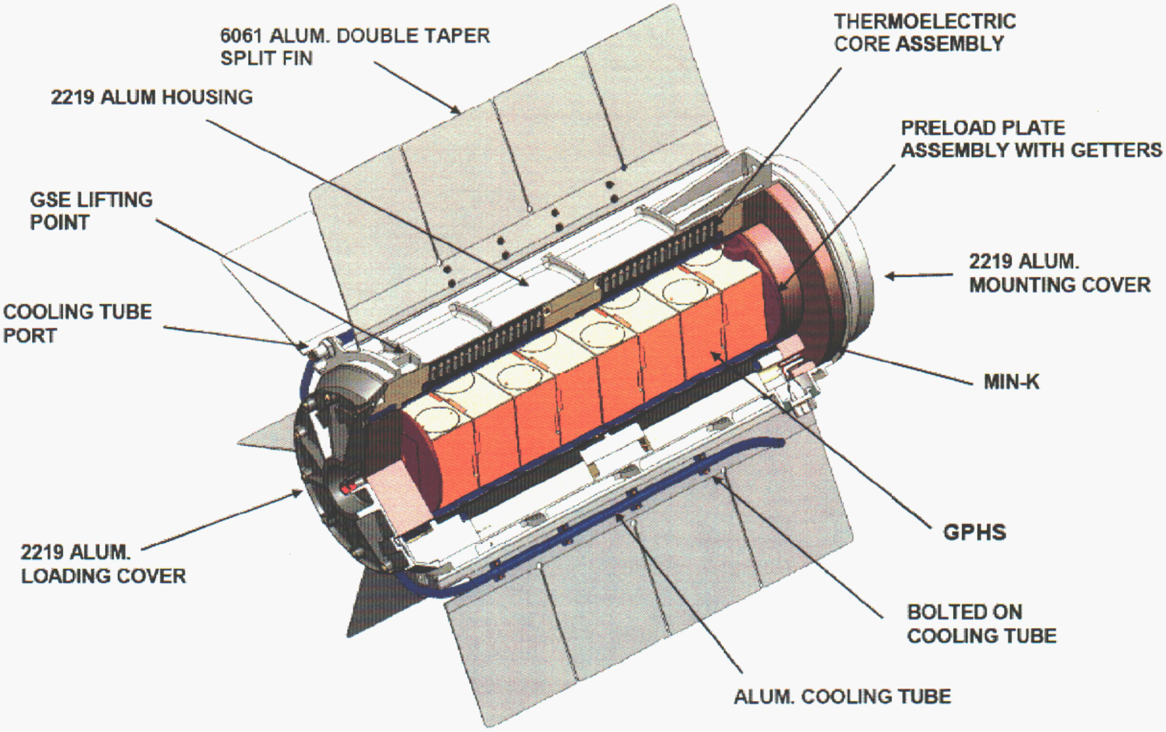

Figure 1. General Layout of Multi-Mission Radioisotope Thermoelectric Generator

The DOE has tasked Sandia National Laboratories (SNL) with preparing the SAR, and an early step towards that goal is a review of the kinds of safety calculations needed, the approaches used in earlier missions, the computational tools currently available, and the needs for additional development. This report summarizes the results of that review. The recommendations to be presented are necessarily tentative, since insights developed during the calculational stages of the program may identify more suitable methods or additional needs.

The focus of the nuclear safety work will be on the health risks to the public (U.S. and world) due to exposure to plutonium dioxide released as a result of a launch accident. As for earlier NASA missions, several quantitative measures of that risk will be calculated, including radiation dose and fatalities due to increased incidence of cancer. These risks will be estimated with Probabilistic Risk Assessment (PRA) tools, which produce probability distributions of health effects in terms of latent cancer fatalities.

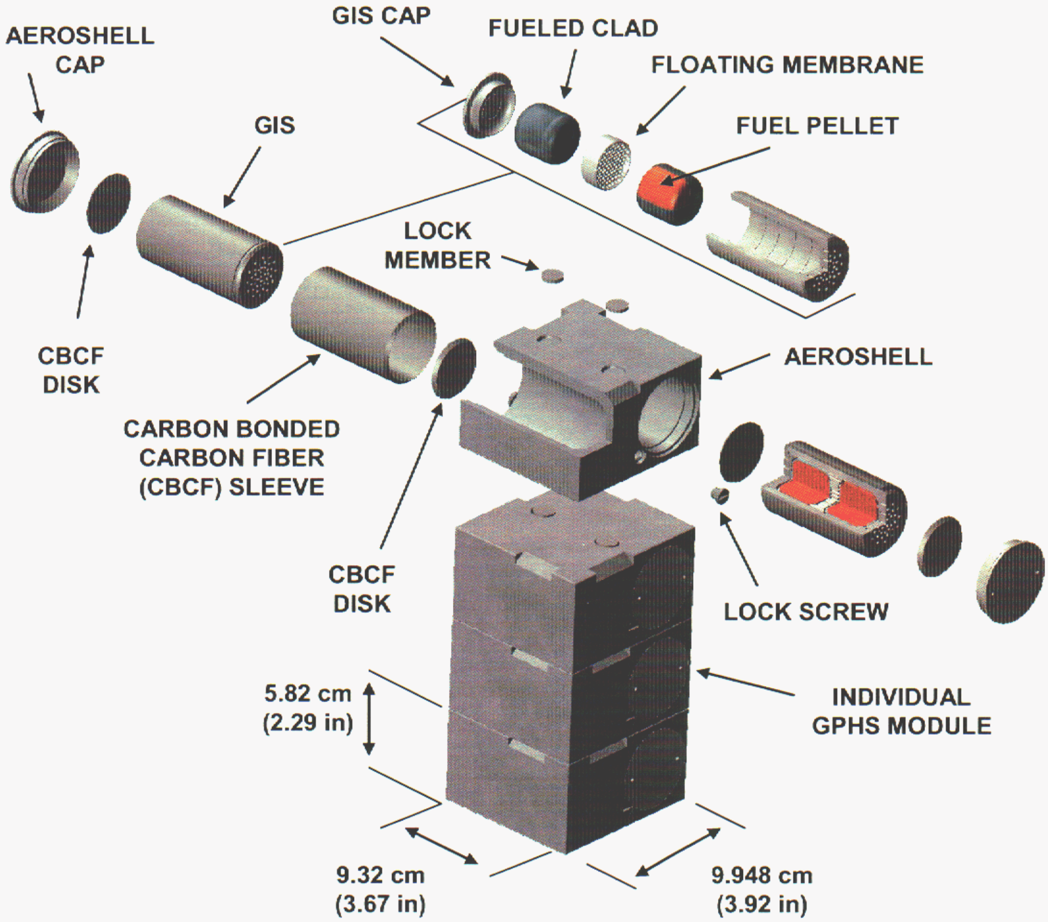

Figure 2. Components of the Step-2 General Purpose Heat Source (GPHS) Showing Location of Plutonium Dioxide Fuel

Because NASA has not yet fully defined the mission details for MSL, SNL has relied extensively on the Pluto New Horizons (PNH) Final Safety Analysis Report (FSAR) (Lockheed Martin 2005) for evaluating the calculational needs for MSL. While there are some significant differences expected in configuration details, the PNH mission, which was launched on January 19, 2006, also utilized a Radioisotope Thermoelectric Generator (RTG) for electrical power and heating of the space vehicle (although it was a GPHS-RTG rather than an MMRTG). Therefore, it is expected that SNL's overall calculational approach will be similar to that used by Lockheed Martin for PNH. However, it is also anticipated that there will be opportunities to improve on the PNH modeling and to develop new analysis approaches for safety issues that are unique to MSL.

1.2 Accident Categories and Environments

The starting point for analysis will be established by NASA in the MSL SAR Databook (hereafter referred to simply as the "Databook"), which will group all significant accidents into a set of Accident Outcome Conditions (AOC) and specify a variety of boundary conditions, initial conditions, and quantitative characterizations of the various threats that the launch vehicle and its components pose to the MMRTG. For each AOC, SNL will carry out a separate risk assessment, and also compute the risk profile of the entire mission by combining the results based on probabilities of each AOC as provided by the Databook. NASA has issued a preliminary version of the Databook that identifies nine AOCs (Table 2). When the final Databook is issued, it will include detailed delineations of the spectrum of threats that the accident environments associated with each AOC pose to the MMRTG and its components. These threats include such things as blast waves from exploding propellant, shrapnel generated by explosions, ground impacts on steel, concrete or sand surfaces, burning liquid or solid propellants, and/or reentry processes. The Databook will characterize the magnitude and probability of each of the specific threats associated with each AOC. The nuclear safety analysis will translate these threats into predictions of damage to the MMRTG and its components, the plutonium dioxide source term produced, and the radiological consequences of the releases expressed in the form of Complementary Cumulative Distribution Functions (CCDFs).

Table 2. Accident Outcome Conditions for MSL as Specified in the Draft Databook

AOC 1 ***Full Stack Intact Impact***	Events that result in the whole launch vehicle impacting the surface. Depending on the exact location of impact, the surface could be land or water. The initial failure can occur in the time interval from liftoff to t_x (after which there is no potential for MMRTG land impact).
AOC 2 ***Stage 2/SV Intact Impact***	Events that result in the space vehicle and the second stage impacting land or water together. The initial failure can occur in the time interval from liftoff to t_x.
AOC 3 ***Space Vehicle Intact Impact***	Events that results in the space vehicle impacting land or water. The initial failure can occur in the time interval from liftoff to t_x.
AOC 4 ***On Pad Explosion***	Events that result in an explosion on the launch pad. The initial failure can occur during pre-launch processing or at liftoff.
AOC 5 ***Low Altitude FTS***	Events that result in the activation of the Flight Termination System (FTS) before t_x. The initial failure can occur in the time interval from liftoff to t_x.
AOC 6 ***High Altitude FTS***	Events that result in the activation of the FTS over water. The initial failure can occur in the time interval from t_x to Payload Fairing (PLF) jettison.
AOC 7 ***Low Altitude MMRTG/Module Detachment***	Events that result in the detachment of the MMRTG from the launch vehicle at low altitude as well as any subsequent break up of the MMRTG prior to ground impact. The initial failure can occur in the time interval from liftoff to t_x.
AOC 8 ***Sub-orbital Reentry***	Events that result in a sub-orbital reentry. Reentry may be preceded by the activation of the FTS. The initial failure can occur in the time interval from liftoff to the first cut-off of the second stage engine.
AOC 9 ***Orbital Reentry***	Events that result in an orbital reentry. The initial failure can occur in the time interval from liftoff to escape. This AOC does not involve any FTS destruct action.

1.3 Past RTG Safety Analyses

The safety analysis approach for past RTG launches has developed over the past 40 years, culminating most recently with the Galileo, Ulysses, Cassini, and PNH missions. For all the RTG missions, the primary concern is the containment of the plutonium dioxide. The approach has been to use a suite of codes with different levels of detail in modeling in order to yield the bottom line, which is a calculated risk of additional latent cancer fatalities. This information is all summarized in the FSAR for each launch.

An example of the bottom line result is shown in Figure 3, taken from the Cassini FSAR Executive Summary produced by Lockheed Martin (1996).

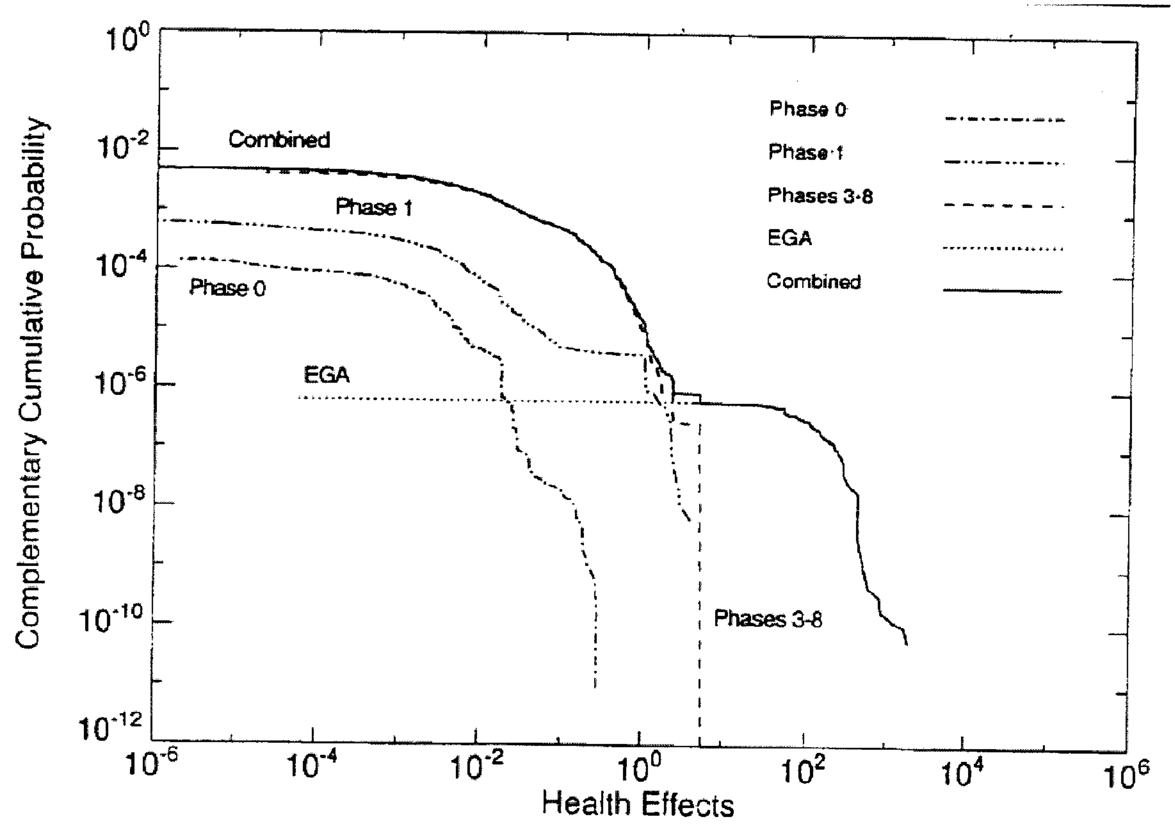

Figure 3. Probability Distribution of Incremental Cancer Fatalities for Each Phase in the Cassini Mission Profile

The portrayal of risk contained in the FSAR has many different dimensions, and the quantitative analyses show what the most important contributors are: which phases of the mission, which types of accident environment, which populations, and so forth. Results such as these allow reviewers at DOE, the Interagency Nuclear Safety Review Panel (INSRP), and the Office of Science and Technology Policy to quantitatively evaluate the risk to the public due to the mission and to provide advice regarding launch approval.

SNL's approach to creating the SAR for the MSL mission will be similar to those used in past missions, though a number of opportunities for improvement are anticipated. Insights from INSRP reviews of PNH and Cassini will be an important resource for identifying such opportunities. In addition, DOE has indicated that it would be desirable for the computational tools developed for the MSL mission to be more generic in applicability than has been the case for previous missions. In other words, missions beyond MSL would use the same family of tools without the need to create custom software for each mission. The result would be increased reliability of the software, decreased cost for each mission, and an ability to direct the saved resources to improve the quality of the overall analysis. However, the goal of achieving full cross-mission generality will not be achieved immediately, since the principal focus of the MSL MMRTG safety project will be to produce a SAR on the schedule established by NASA and DOE.

1.4 Assessment Approach

The goal of this methodology assessment is to identify a set of existing computational analysis tools that are suitable for carrying out the MSL nuclear safety studies and, in addition, to identify code improvements that would add significantly to the quality and reliability of the analyses. In some cases, one code will be identified as the primary calculational tool, but a second tier code may also be identified for possible use in special circumstances or to help verify the results of the first tier code. While the primary focus is the MSL mission, a secondary goal is to create a systematic computational approach that can be readily adapted to other missions involving MMRTG power.

The specific AOCs of the MSL mission are the principal drivers for code choices, but the absence of quantitative detail in the preliminary Databook's description of these environments necessitates that we depend considerably on reviews of the nuclear safety analyses performed for PNH. However, there are a number of significant differences between the missions that should be kept in mind in evaluating MSL's computational needs. For example:

- The PNH spacecraft and its General Purpose Heat Source RTG (GPHS-RTG) were mounted in a common payload fairing with the third stage, a STAR48B rocket motor containing approximately 2,000 kg of solid propellant. Because of the close proximity of this propellant to the RTG, the propellant plays a significant role in producing the source term in the PNH risk profile. (Lockheed Martin 2005, Appendix D, Vol. II).
- The MSL spacecraft does not have solid propellant in such close proximity (referring to the STAR-48 which was mounted below the observatory in PNH), though there are hydrazine propellant tanks containing several hundred kg in the entry vehicle and cruise stage. (Note: this is preliminary information from the Draft Databook). However, this liquid propellant is expected to play a much smaller role in producing the source term for MSL compared with any explosively-burning solid propellant fragments.
- The spacecraft components surrounding the MMRTG (e.g., the heat shield, back shell, and descent stage) could provide greater protection against blast effects emanating from any burning second stage motor propellant. However, these spacecraft components could inhibit early detachment of the MMRTG from the launch vehicle. This may or may not be beneficial to reducing risk of release.
- The GPHS-RTG protrudes with little protection from the side of the PNH spacecraft, but the MMRTG is located in a more protected situation (behind the spacecraft heat shield) in the MSL configuration (see Figure 4).

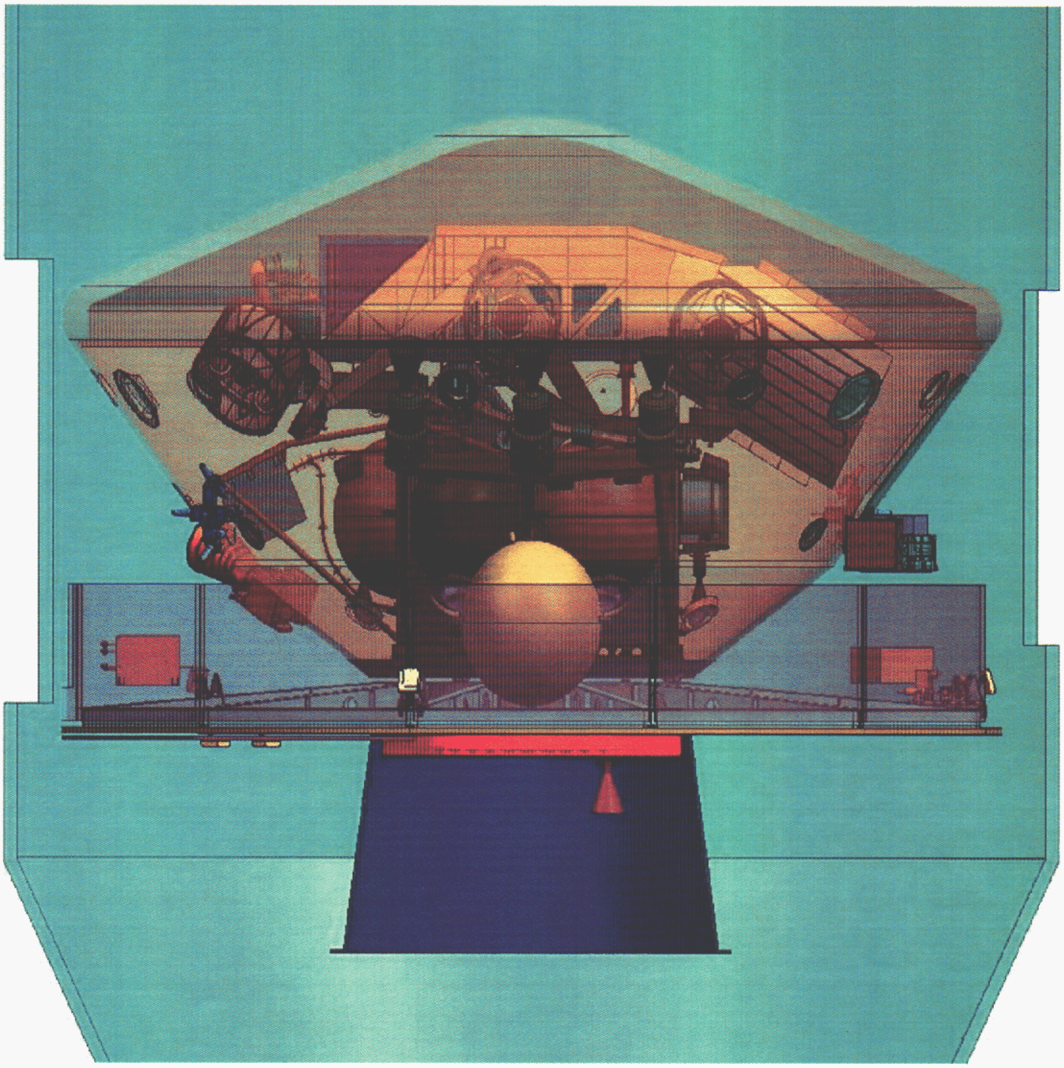

Figure 4. Integrated MSL Spacecraft Showing Location of MMRTG below Heat shield, Upper Right in Figure (Courtesy JPL)

1.5 References for Section 1

Lake, Anthony, 1995. "Revision to NSC/PD-25, dated December 14, 1977, entitled Scientific or Technological Experiments with Possible Large-Scale Adverse Environmental Effects and Launch of Nuclear Systems into Space", memo from A. Lake, Assistant to the President for National Security Affairs, Memorandum for the Vice President, dated May 17, 1995.

Lockheed Martin Missiles and Space, 1996. "GPHS RTGs in Support of the Cassini Mission—Final Safety Analysis Report," CDRL C.3, December 1996.

Lockheed Martin Space System Company, 2005. "General Purpose Heat Source-Radioisotope Thermoelectric Generator (GPHS-RTG) in Support of the Pluto New Horizons Mission Final Safety Analysis Report (FSAR)," LMSP-7320, February 2005.

2. Overall Calculational Approach

The purpose of the SAR is to characterize the nuclear safety aspects and risk associated with the use of the MMRTG on the MSL mission, as required by DOE directives and the launch approval process established by PD/NSC-25. At the high level, there are three types of information of interest: 1) the probability of an accident leading to a release, 2) the consequences of such releases, and 3) the associated risks. The consequences are reported in terms of radiation doses, health effects in terms of latent cancer fatalities, and land contaminated above specified levels. One way of describing the risk is through the use of a CCDF over health effects. As in past RTG safety studies, the calculation of consequences and risk metrics due to plutonium dioxide releases involves several different kinds of calculations with differing levels of physical detail (see Table 3). Each level is briefly discussed below.

Table 3. Three Levels of Analysis Required for Nuclear Safety Analysis

Level of Detail	Type of Analysis
Level A (Deterministic)	Detailed simulation of responses to the environments specified in the Databook (e.g., fragment impact on a particular MMRTG component, solid propellant fragment burning atop a fueled clad).
Level B	Incorporating simplified representations of Level A results, fast computation of many thousand event sequences controlled by numerous random variables, producing probability distributions of source term characteristics.
Level C	Probabilistic analysis of atmospheric transport of source terms from Level B and calculation of health metrics CCDFs (e.g., excess latent cancer fatalities in year 1, or by year 50, land contamination) for each AOC and for the probabilistic combination of all AOCs (mission risk profile).

2.1 Analysis Level A: Detailed Simulation of Responses to Accident Environments

The plutonium dioxide in the MMRTG is surrounded by a series of barriers that must be breached if it is to contribute to the source term. Launch accidents involve a vast range of physical processes, but the source term is, in general, produced by a number of relatively discrete violent interactions between the MMRTG or its subcomponents and the physical threats from the accident environment. These interactions can include, for example:

- A specific piece of a launch vehicle accelerated by an explosion impacts (in air) the intact MMRTG at some particular location and at a particular velocity.
- An intact Graphite Impact Shell (GIS) containing two fueled clads falls to the ground and impacts a concrete surface at a particular velocity.
- A fragment of burning solid rocket propellant falls to the ground and comes to rest adjacent to an intact fueled clad, where the propellant continues to burn for some time.

Damage to the MMRTG from such interactions can accumulate—for example, the first event listed above might eject a GIS, which subsequently impacts the concrete pad, perhaps failing one fueled clad but ejecting the second intact, and the latter clad could be exposed to the solid propellant environment described in the third event.

Such specific violent interactions are, in a sense, the building blocks of the radioactive source term, and accurate computational simulation of these is fundamental to the nuclear safety analysis. However, the interactions, while simple in comparison to the overall launch accident, require significant computational time and effort to model accurately. The most practical approach is to analyze a finite set of representative responses to accident environments, and interpolate from those results to predict what could happen in intermediate cases.

The principal insults that must be modeled in this way are blast (from exploding propellant), in-air impacts, impacts with the ground, liquid propellant fires, solid propellant fires, and reentry. For each of these threats, a variety of different configurations of the "targets" (i.e., the plutonium dioxide-containing objects) must be considered, including, for example: the intact MMRTG, an ejected GPHS module, a partly damaged but unbreached fueled clad, or a cloud of plutonium dioxide aerosol. For each such case, the goal of the calculation is to predict releases of plutonium dioxide to the atmosphere, or physical damage that can affect releases in subsequent encounters. Clearly, a variety of specialized computer simulation codes must be called upon to produce the needed calculations of the representative responses, and evaluating which codes should be used is a significant part of the current assessment effort.

2.2 Analysis Level B: Probabilistic Event Sequence Analysis

While the probability of a launch accident causing exposure of the public to plutonium dioxide is very low, the number of different event sequences that might lead to such exposure, given that a launch accident has occurred, is very large. The amount and characteristics of any plutonium dioxide release from a launch accident will depend on many random variables, such as accident initiator timing, location and timing of explosions, trajectories of fragments that might impact the MMRTG. To account for the effects of these random variables, a relatively fast-running event sequence simulation code is needed to repeatedly calculate numerous event sequences that differ primarily in the choices assigned to these random variables. For each set of values assigned to these random variables, the event sequence is tracked from the Accident Initial Condition (AIC), defined as the first system-level failure within either the launch or space vehicle that may lead to a catastrophic accident or mission failure, through all the processes and event branches that can lead to a plutonium dioxide release until no further release can occur. Such a tool, which will be called the Probabilistic Event Sequence Analysis (PESA) tool in this document, can, by running thousands of "trials", build up probability distributions of the quantitative parameters (e.g., mass released, particle size distribution) characterizing the plutonium dioxide source term for each AOC.

The software for performing PESA must incorporate, if only approximately, the results obtained at Level A. For example, it could use lookup tables that contain the results of the detailed calculations at specific points in the relevant parameter space, and interpolate linearly to estimate results for intermediate locations. More sophisticated treatments that attempt to capture non-linearities will probably be necessary, especially for processes involving known threshold effects. It is expected that close coordination between the event sequence studies and the detailed response studies will be needed, especially to "home in" on critical regions of the parameters spaces.

Another requirement of the PESA software is that it incorporates the quantitative characterizations of the accident environment threats that are specified in the Databook. In some instances it might be desirable for alternative treatments of these threats to be available (e.g., to study a more consistent analysis approach), but it is essential to be able to produce baseline results that are as faithful as possible to the Databook assumptions.

Finally, a key role for the PESA tool will be to support uncertainty studies of the nuclear safety analysis (see Section 7). Such studies will not only propagate the effect of variables that are considered to be intrinsically random (like timing), but also the quantitative effects of inaccuracies in physical models, uncertainty in material properties, or neglected phenomena. For these studies, also, close coordination with the Level A analyses will be needed.

2.3 Analysis Level C: Atmospheric Transport and Consequence Analysis

The probabilistic description of the source term produced at Level B specifies the location, magnitude, and particle size distribution of the plutonium dioxide release. To calculate health risks, the transport of the radioactive cloud through the atmosphere and to locations where the public may be exposed must be calculated. Then, information about population density, degree of sheltering or evacuation, mechanisms for exposure (ingestion, ground shine, etc.) must be brought to bear in a probabilistic analysis of health consequences. This is the role of Analysis Level C.

Details of wind patterns and precipitation are major controllers of the health risk that any particular source term poses to the public. Consequently, historical information about meteorological conditions in the vicinity of the launch site is needed to make good statistical predictions of conditions that might occur at the time of a hypothetical launch accident. Similarly, population and demographic information about the local area will be needed for the portions of the source term that are deposited in the vicinity of the launch site. For situations where the source term is spread on a global scale, coarser representations of meteorological and population statistics will be used. A number of tools and databases for this kind of analysis have been developed for nuclear safety studies of many kinds. For the MSL nuclear safety analysis, these resources will be evaluated for suitability to the particular mission, and any needed improvements will be identified. As with the other levels of analysis, uncertainty studies (i.e., the quantitative effects of model inaccuracies) will supplement the baseline studies that use nominal meteorological and population statistics.

2.4 Framework for Calculating Risk

The manner in which calculational results from the three levels of analysis discussed above will be integrated to produce CCDFs of risk metrics is illustrated in Figure 5 ("LVDB" in the figure refers to the Databook). At the heart of the analysis is, effectively, an accident simulation program marked by the letter "B," which performs the PESA.

Since a launch or reentry accident is, by nature, unpredictable, the course of events depends on a number of intrinsically random parameters, including, but not limited to:

- The time of the AIC
- The timing and location of in-flight explosions
- The trajectories and masses of fragments that might impact the MMRTG
- The size of fragments of burning solid propellant on the ground and their proximity to components of the MMRTG

Such random parameters control the amount (if any) of plutonium dioxide that is released, and while their values are not known, something is known about their probability distributions. This information is provided in the Databook. To calculate probability distribution functions (PDFs) of the released plutonium dioxide the PESA software performs repeated simulations of accident sequences that differ in the choices of the various random input parameters. Thus, the start of each "trial" is a choice (based on simple Monte Carlo sampling or more sophisticated and efficient mathematical methods) for the set of random variables that control the quantity and particle size distribution of released plutonium dioxide, or source term.

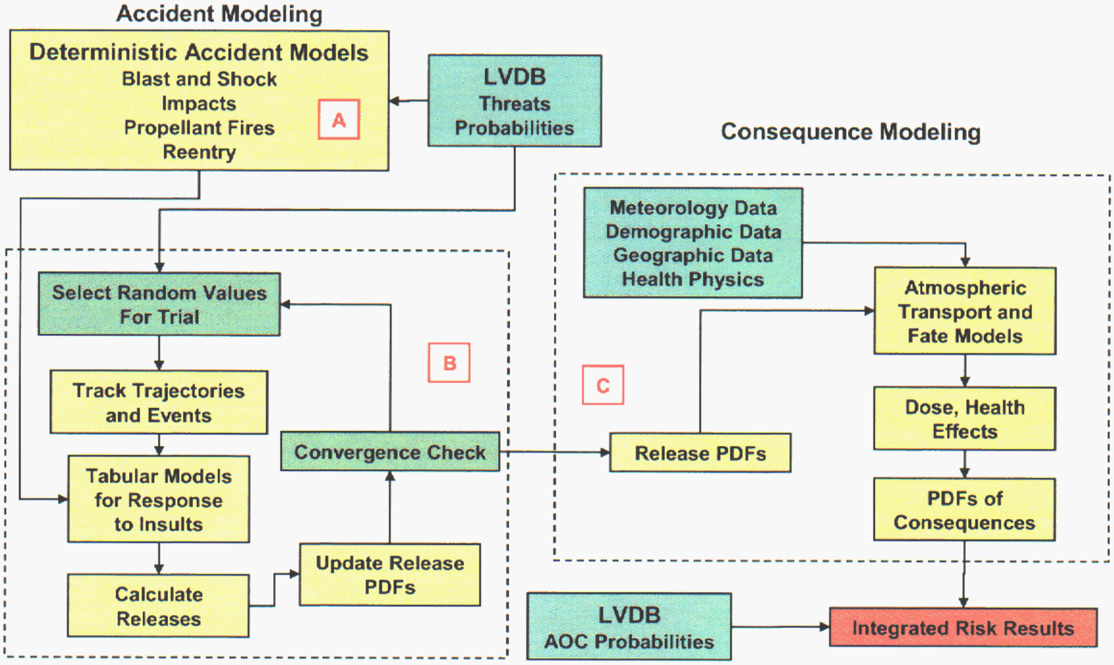

Figure 5. Simplified Information Flow for Calculating Risk

During any one trial, the accident environment may pose significant insults to the MMRTG or its components. Such insults could include fragment impacts, exposure to a sustained solid propellant ground fire, and so forth. To calculate the damage done by such insults the PESA tool employs tabular models, or lookup tables, which are distillations of numerous detailed computer simulations performed in advance by state-of-art computer codes. These calculations collectively translate accident environments into released plutonium dioxide and are represented in the box identified with the letter "A" in the figure.

It may take thousands of such trials before the PDFs of the source term are known accurately, at which time a convergence check will show that sufficient accuracy has been achieved. At this point the information about plutonium dioxide releases is saved for use by the Consequence Modeling phase of the calculations. A complete set of PDFs is created independently for each AOC.

In the box marked by the letter "C," the statistical information about the released plutonium dioxide (including size distribution characteristics, location and altitude of release, and everything else that is important to consequence analysis) is combined with another collection of statistical information: meteorological data. As in the Level B analysis, wind and precipitation information cannot be predicted in advance of an accident, but there is good scientific understanding about the statistical properties of these key variables based on historical meteorological measurements in the vicinity of the launch site or impact location. This information is combined with the source term statistics and models of how the released plutonium dioxide is transported and deposited to various locations on the earth's surface. Finally, data about population distributions and geography are used to predict (in a statistical sense) the dose to humans via various pathways and the resulting long-term health effects.

The end result of these calculations are the PDFs of various risk metrics *conditional* on each AOC occurring. When multiplied by the probability of each AOC (provided by the Databook), the results are the CCDFs such as shown previously in Figure 3. Summing the CCDFs provides the Integrated Risk Results for the mission. Substantial detail is provided in the interface between Level B and Level C (represented by the box called "Release PDFs"), so that the overall mission risk can be examined from a wide variety of perspectives. For example, Table 4 shows the median risk results for PNH for each mission phase, with and without assuming a health effects *de minimis* dose (i.e., the threshold below which it is assumed there is no discernable health effect to an individual) of 1 mrem (Lockheed Martin 2005). This kind of information is the principal product of the SAR, and is the technical basis for the launch approval process.

The preceding discussion focuses on the best-estimate calculation of risk—the truly random parameters ("variability" parameters) such as AIC time and wind velocity are treated statistically, but the values chosen for uncertain quantities about which better information could, in principle, be obtained are assigned best-estimate values. The manner in which uncertainty analysis is done for such parameters will be discussed in Section 7.

Table 4. Average Individual Risk Estimate for the Pluto New Horizons Mission

Mission Segment Description	Risk		Population at Risk	Average Individual Risk [a]	
	without De-minimis	with De-minimis		without De-minimis	with De-minimis
Pre-Launch	$9.2\text{x}10^{-8}$	$8.9\text{x}10^{-8}$	$2.83\text{x}10^{6}$	$3.2\text{x}10^{-14}$	$3.1\text{x}10^{-14}$
Early-Launch	$1.6\text{x}10^{-3}$	$1.5\text{x}10^{-3}$	$2.83\text{x}10^{6}$	$5.6\text{x}10^{-10}$	$5.3\text{x}10^{-10}$
Late-Launch	$9.6\text{x}10^{-11}$	0.0	$6.89\text{x}10^{9}$	$1.4\text{x}10^{-20}$	0.0
Sub-Orbital	$2.1\text{x}10^{-8}$	$1.1\text{x}10^{-8}$	$7.42\text{x}10^{7}$	$2.9\text{x}10^{-16}$	$1.5\text{x}10^{-16}$
Orbital	$1.5\text{x}10^{-6}$	$1.3\text{x}10^{-6}$	$3.80\text{x}10^{9}$	$4.0\text{x}10^{-16}$	$3.5\text{x}10^{-16}$
Total Mission	$1.6\text{x}10^{-3}$	$1.5\text{x}10^{-3}$	$6.89\text{x}10^{9}$	$2.3\text{x}10^{-13}$	$2.2\text{x}10^{-13}$

2.5 General Criteria for Assessment of Computational Tools

Perhaps the greatest challenge in the methodology assessment is to evaluate the needs for Detailed Response Analyses (Level A). For some types of interactions, there exist high quality test data that can be used to calibrate or validate computational tools, and in those cases the best choices are codes with a solid pedigree and a proven ability to reproduce the test results. In other cases experimental data are sparser or less precise. Such cases might require specialized tools that treat simultaneous interactions among numerous disparate phenomena, and an assessment consideration will be the ability to study modeling uncertainties. Other cases may lie at intermediate positions between these two levels.

For analysis of Event Sequences (Level B), the assessment criteria will include the flexibility to permit the risk and uncertainty analyses to be conducted at a level commensurate with the consequences of the events. The code and associated algorithms must be constructed in such a manner that rare, high consequence events are properly characterized. In addition, the uncertainty analysis algorithms embedded within the code must not be so complex as to overwhelm the accuracy of event characterization. Finally, since the computational cost of event characterization can be very high, it is desired that simulations be as computationally efficient as possible. A very desirable characteristic of the codes is that it would require a minimum number of simulations coupled with the capability to integrate simulation results collected during various stages of the risk analysis.

There are also several considerations that will enter into the selection of tools and data for Atmospheric Transport and Consequences (Level C). It should be capable of producing the types of consequence results that have been reported in previous SARs. It should be well-documented and have a proven track record in studies similar to the MSL SAR. Run times cannot be excessive, and it should be able to interface well within the larger calculational framework anticipated for this study. Finally, it must be able to deal with the relatively unusual wind patterns characteristic of Cape Canaveral.

2.6 References for Section 2

Lockheed Martin Space System Company, 2005. "General Purpose Heat Source-Radioisotope Thermoelectric Generator (GPHS-RTG) in Support of the Pluto New Horizons Mission Final Safety Analysis Report (FSAR)," LMSP-7320, February 2005.

3. Methodology Assessment for Level A: Detailed Response Analysis

3.1 Overview of Responses to Accident Environments

Analysis of launch and reentry accidents is a vastly complex undertaking, but for the space nuclear SAR there are some simplifying features that help to make the problem manageable. Since the principal quantitative output of interest is the health impact of released plutonium dioxide, numerous other aspects of these accidents can be disregarded. To a great extent the problem is one of plutonium dioxide mass accounting, and of the total plutonium dioxide inventory, the primary portion that matters is that which is (a) released from the fuel cladding, and (b) released into the atmosphere in a final form (i.e., after all accident processes are complete) as fine particles—roughly less than 50 microns.[1] To be sure, the location and fate of the rest of the plutonium dioxide inventory will be of interest (e.g., for cleanup programs or nonproliferation issues), but the overwhelming interest for the SAR is the health consequences associated with the smaller particulates. Nonetheless, we will calculate the release and effect of all particle sizes from 1 to 6000 microns to capture the full effect of release.

The purpose of the Detailed Response level of analysis is to study how the accident environments specified in the Databook can produce and release such particles. Some of the tools that will be selected are capable of evaluating many other aspects of the accident, but for this program the focus will be on the events, or sequence of events, that lead to the release of small plutonium dioxide particles (also called "fines").

Over the years, as RTG safety analysis has matured, there has been an increasing appreciation of how different processes can interact—sometimes simultaneously and sometimes sequentially—to produce the plutonium dioxide fines. For example, fragment impacts on the RTG or its components have always been known to be an important mechanism for breaching the fuel cladding, thereby releasing plutonium dioxide, but the health significance of such releases are likely to be relatively small. But when those relatively large fragments of plutonium dioxide are exposed to a fire environment, a fraction of the plutonium dioxide is converted (e.g., by means of evaporation and subsequent nucleation) into fines. Such insights have improved the accuracy of predictions for RTG accident consequences, but they also present a challenge to the computational analysts, since it becomes important to understand not only the direct consequences of a particular insult on a particular portion of the RTG system, but also the cumulative effect of multiple and varied processes.

The discussions that follow classify the responses to accident environments into several categories: Blast and Shock; Impacts; Liquid Propellant Fires; Solid Propellant Fires; and Reentry processes. Separate analyses of these phenomena are usually required because integrated computational analysis of all phenomena over the full range of possible accident conditions would require resources far beyond current capabilities. Nonetheless, the analysis approaches and the assessment criteria will explicitly factor in the way the different phenomena might interact (again, either simultaneously or sequentially) to produce the final plutonium dioxide source term.

The ultimate application of the calculations of the responses to the various types of insult is to produce a statistical profile of plutonium dioxide releases for each AOC. This calculation is done

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[1] There are various choices for the size threshold for "fines," depending on context. The 50 micron value used here is general and is on the high side of such usages.

at Level B, with the PESA tools, which capture the results of the detailed analyses in tabular models, or "lookup tables." These are created by running the detailed codes for a broad matrix of cases that populate the relevant parameter ranges sufficiently that interpolations between points not sampled will provide reasonable representations of the detailed code results. The interpolation can be linear or more sophisticated fitting methods may be used. In choosing which points in the parameter space are chosen for detailed code runs, attention must be paid to physical threshold phenomena, which cause the code results to vary more rapidly for small changes in the input parameters than in other regions. These sensitive regions in the parameter space should be populated more densely when the calculational matrices are specified.

In the remainder of this section the various types of insult and how they will be modeled will be discussed. The first two types—Blast and Shock, and Impacts and Crush—can release plutonium dioxide through mechanical pulverization of the fuel and breach of the protective barriers. The resulting release is called the mechanical source term, which is discussed in the following two subsections on the insult types. This is followed by a discussion of the thermal source term, which results when the plutonium dioxide is released into fire environments that have the ability to transform the particle size distribution from its initial form to one with more fines because of vaporization and condensation processes. Finally, releases due to reentry scenarios are discussed; these could produce either mechanical or thermal source terms.

3.2 Blast and Shock

3.2.1 Phenomenological Modeling Considerations

There are a number of AOCs that can result in a blast loading on the MMRTG. These include the destruct of the Common Core Booster, destruct of Centaur motor, and rupture of the hydrazine and pressurant tanks on board the space vehicle. The magnitude and history of the resulting pressure loading on the MMRTG can vary significantly for the different AOCs. The goal of the blast/shock analysis is to assess damage to the MMRTG when subjected to a prescribed blast loading. It does not address detachment of the MMRTG from the rover or possible ejection from the spacecraft at altitude. Any subsequent damage resulting from MMRTG detachment and/or ejection will be addressed as part of the impact analysis (Section 3.3).

The overall modeling effort is summarized as follows:

- Determine if the outer housing of the MMRTG is breached. If a breach occurs, then it will be necessary to determine if the outer housing is sufficiently intact to contain the General Purpose Heat Source (GPHS) modules. If not, then assess whether the modules can be ejected from the MMRTG prior to ground impact.
- Assess damage to the GPHS modules to determine if either the GIS or individual fueled clads can be ejected from its module.
- Assess damage to the fueled clads. Any pulverization of the plutonium dioxide could result in more fines being released as a result of additional insults to the MMRTG.
- The final outcome of the blast/shock analysis is a determination of whether the iridium clad is breached. If so, then it will be necessary to assess the amount of plutonium dioxide released. If the clad is not breached, then it will be necessary to track the amount of damage to the plutonium dioxide inside. Any pulverization could lead to additional fines being released as a result of follow-on insults, such as later time impacts against the ground.

- Depending on the magnitude of the loading, it may be necessary to determine if the MMRTG can become detached from the rover and, if so, determine its terminal velocity for follow-on analyses. These calculations will be performed on a case-by-case basis, and will largely be dependent on the definition of the blast environment provided in the MSL SAR Databook.

For the blast/shock analysis, it is assumed that the Databook will provide representative peak overpressure and impulse levels at the MMRTG location for each of the different AOCs. These values can be used to develop a loading function for a structural analysis of the MMRTG response. The structural analysis will entail detailed modeling of the MMRTG internal components, large material deformations with inter-material contact, and possible breach of the outer housing. The requirements of the structural analysis are best met with a Lagrangian finite element structural dynamics code; however, there may be some instances where detailed modeling of the shock propagation through the structure is required. This is best done using a shock physics code. Both types of analysis will need to be addressed in the code selection.

The structural analysis requires a determination of the loading on the MMRTG. This loading can be determined using either a one-way or a fully coupled approach. In a one-way coupling, an Eulerian shock physics code would be used to model the blast loading on a rigid structure having the external geometry of the MMRTG. The interface pressures would then be mapped onto a finite element mesh to assess the structural response. It is not possible to map the pressure history defined within the Databook directly onto the finite element mesh, as the Databook assumes a planar blast front impinging at the MMRTG location in the launch vehicle. One can expect the flow field about the MMRTG to be influenced by its geometry. Thus, the true geometry of the MMRTG must be taken into account in determining the loads. With a fully coupled analysis, the blast/structure interaction is implicitly taken into account over the duration of the event.

There are advantages and disadvantages to one-way versus a fully coupled approach. First, one must consider that the loading is affected by the dynamic response of the MMRTG. Any motion will result in a reduction of the interface pressures on the surface of the MMRTG. Thus, a one-way coupling can lead to an overprediction of the loading, thereby inducing excessive conservatism into the analysis. Additional problems arise if the outer housing of the MMRTG is breached during the course of being loaded. A one-way coupling cannot account for the direct loading on internal MMRTG components, since the loaded surfaces in the finite element mesh would have been removed from the calculation. One last detractor for a one-way coupling is the data handling. The mapping of data between domains is laborious and difficult to perform when complex geometries are involved. These shortcomings are generally overcome with a coupled approach. The major drawback with a coupled approach is the cost of the calculation. In general, the accuracy of the coupling is dependent on the problem resolution. The cost of the coupling combined with the need for higher fidelity can result in extremely long-running calculations. In the code selection process, accommodations will be made to address both coupling approaches, bearing in mind that a coupled solution is more appropriate for the AOCs to be encountered in the MSL SAR.

Thus far, the discussion of code expectations has focused solely on modeling the physics of the problem. Additional requirements will be levied on the code selection and are summarized as follows:

- The code must have a three-dimensional (3D) modeling capability.
- The code must have parallel processing capability.

- The structural dynamics code must support both solid and shell elements.
- The code should be mature and be verified and validated.

The AOCs are generally 3D in nature and, except in a few cases, 2D modeling fails to capture important effects. A parallel processing capability is desired (and, in practice, needed) since large problem sizes and long run times are to be expected for the blast/shock analysis. As a practical matter, the structural dynamics code used to model the MMRTG response should support both solid and shell elements. The spacecraft (and MMRTG) has numerous thin-shell structures. The use of shell elements to model these structures is almost a *de facto* requirement to avoid excessively small time steps, as would be the case if these structures were modeled using only solid elements. Code maturity is also a must. These analyses must be completed before the launch date (scheduled for the fall of 2009). Thus, the codes selected must be well established. However, there is room for some code development, primarily for model updates and improvements within an existing framework. In the code selection process, codes having a track record of use in supporting space-based applications will be given a higher precedence.

3.2.2 Interface with Launch Vehicle Databook

It is assumed that the Databook provides peak overpressure and impulse levels at the MMRTG location for each of the different AOCs. These will serve as an input for the blast/shock analysis. The load duration can be obtained from the available data by assuming a triangular pressure pulse when the pulse shape is not explicitly defined. In a coupled analysis, these will serve as a set of initial conditions for a planar blast wave impinging on the MMRTG. This is a simplification of the blast environment, which is fairly reasonable given the initial conditions specified in the Databook. It is also worth noting that this same approach was used for modeling the blast loading on the RTG for the PNH FSAR (see Bessette and Libersky 2006).

3.2.3 Generic Modeling Considerations

The MMRTG contains a variety of materials exhibiting vastly differing behaviors. Many of these materials are well defined (e.g., the behavior of the aluminum and titanium in the housing and support structures is well characterized over a range of conditions). However, there are a number of materials for which there is little constitutive data. Examples of these ill-defined materials include the iridium alloy clad and plutonium dioxide. The need for well characterized materials cannot be overstated. Material data represents a basic input to any of the analysis codes used to support the MSL SAR. A lack of well-defined data induces significant uncertainty in the safety assessment. The lack of data for the iridium and plutonium dioxide is especially problematic. The available properties for these materials are largely based on quasi-static testing, with little (if any) data applicable to the strain and strain rate regimes encountered during a launch accident. SNL is currently reviewing the available data for the various materials residing within the MMRTG to identify specific deficiencies for the modeling effort. Recommendations will be developed to assist DOE in developing an overall testing program to supplement the analysis effort.

The risk assessment will entail thousands of runs made with a probabilistic event sequence analysis code. Each run will assess the outcome from a particular initiating accident event, which can result in damage to the MMRTG from a variety of sources. The blast/shock environment is one possible source of damage. It is not possible to run a blast/shock analysis for each trial encountered in the probabilistic analysis; however, it is possible to perform a set of deterministic analyses which could populate a lookup table from which results for intermediate cases can be interpolated. This lookup table could be accessed during the course of the event sequence runs to obtain an estimate of damage to the MMRTG arising from a prescribed blast loading. Table lookup data will include a determination of breach of various MMRTG components, a determination of any rupture of the iridium clad, and the damage state of the plutonium dioxide inside each fueled clad. The latter will be used in conjunction with a release model in determining the amount of fines released from each fueled clad as a result of the blast loading. A parametric study varying the peak overpressure and impulse would be needed to fill this table. The pressure and impulse conditions would be reduced from the Databook, with excursions considered to cover the range of data needed for the risk assessment.

3.2.4 Assessment of Candidate Codes

3.2.4.1 CTH

CTH is a Eulerian shock physics code developed at SNL (McGlaun et al. 1990, 1990a; Hertel et al. 1993; Bell et al. 2006). This code is well established and has been in active use in the defense and space industries since the mid-80s. In particular, CTH has been used extensively for modeling blast effects (e.g., see Kipp, et al. 1999, Kipp and Saul 2003), as well as modeling shock propagation through solid materials (e.g., see Chhabildas et al. 2003). In addition, CTH has been used in a number of classified projects to model the pressure loading on a structure in a one-way coupling.[2] Here, we will consider CTH as a candidate for modeling the blast portion of a problem in either a one-way coupling or as part of a coupled approach. A brief overview of CTH is provided herein. Further details can be found in McGlaun et al. (1990, 1990a) and Hertel et al. (1993).

CTH is an explicit Eulerian code, falling into the category of codes commonly referred to as "wavecodes" or "hydrocodes" (this is really a misnomer since CTH includes material strength in the solution). In the underlying formulation, the computational mesh is fixed in space and the governing equations are integrated forward in time. In the explicit time integration scheme, the time step is conditionally stable and subject to the Courant condition. For a given time step, CTH utilizes a two-step solution procedure for the solution of the conservation equations. The two-step solution first involves a Lagrangian step, where the CTH mesh is allowed to deform. This deformation provides an indication of material motion through the fixed CTH reference mesh. The Lagrangian step is followed by a remap (or advection) step, which maps material quantities from the deformed Lagrangian configuration back into the fixed reference mesh. The two-step solution procedure is commonly used in explicit Eulerian solvers.

The reference mesh used by CTH is rectilinear with the mesh axes coincident with the global Cartesian coordinate system. The cells composing the mesh are rectangular parallelepipeds. Over the course of a calculation, material moves through the fixed mesh. CTH, as with most Eulerian solvers, does not explicitly track material interfaces. Instead, specialized methods have been developed to reconstruct the material interfaces. The algorithm utilized by CTH is the Sandia Modified Young's Reconstruction Algorithm (SMYRA), which is discussed in Bell (1992). With this algorithm, material interfaces are reconstructed based on the volume fraction of material in the cell of interest and its neighboring cells. The volume fractions indicate the presence or absence of materials in these cells. SMYRA provides a planar representation of the material interface within a cell, but does not ensure continuity of these planes across cells. The SMYRA algorithm has been shown to be quite robust for a range of applications.

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[2] The structural response was modeled using an explicit Lagrangian finite element code, such as Pronto3D. The focus of this discussion is on modeling the blast interaction. A detailed discussion of structural analysis codes is provided in the impact section.

CTH supports a wide range of constitutive models. For the constitutive modeling, the user must define an equation of state (EOS), a deviatoric strength model, and a fracture model. The EOS expresses a relationship between the thermodynamic pressure, density, and internal energy in a state of equilibrium. The strength model is often a plasticity model designed to capture the shear-induced response of the material. As a convenience, users can access a material library provided with the code distribution. This library provides constitutive data for a range of materials, including a number of common metal alloys, polymers, and explosives. The user also has the option to prescribe constitutive data independently or override existing data in the material library.

CTH is well suited to meet the needs of the launch safety investigation. This code is production-ready and has a track record of use in previous launch safety investigations, including shuttle launch accidents (Kipp and Saul 2003) and the PNH FSAR (Bessette et al. 2006, 2006a). In these investigations, CTH was used to model propellant initiation/detonation and the resulting blast environment on spacecraft structures as well as high velocity fragment impacts on these structures, with subsequent shock transmission through multiple materials. There is no anticipated algorithm development needed for CTH to support the MSL SAR. At present, the only anticipated needs are associated with defining material properties and other problem inputs for CTH.

3.2.4.2 Zapotec

Zapotec is a coupled Euler-Lagrange (CEL) code developed for modeling applications involving penetration and blast/structure interaction. Zapotec has been in use since the mid-90s, predominately as an internal research code at SNL. The original intent of Zapotec was to model penetration (e.g., see Silling 2000, Bessette et al. 2002, 2003); however, recent development has focused on modeling blast/structure interaction (e.g., see Bessette et al. 2003, 2003a, 2004, 2006). Recent efforts have also focused on transitioning this technology to a production environment, with the code now being used by a number of Department of Defense customers.

Zapotec links two production codes: CTH and Pronto3D. CTH, an Eulerian shock physics code, performs the Eulerian portion of the analysis, while Pronto3D, an explicit finite element code, performs the Lagrangian portion. The two codes are run concurrently with the appropriate portions of a problem solved on their respective computational domains. Zapotec handles the coupling between domains. The discussion here will focus on the coupling algorithm. CTH was discussed previously, while Pronto3D will be discussed in Section 3.3.1.4.1. Only a summary discussion of the coupling algorithm is provided here; further details can be found in Bessette et al. (2003).

Zapotec controls both the time synchronization between CTH and Pronto3D, as well as the interaction between materials on their respective domains. The time synchronization is illustrated in Figure 6. At a given time t_n, Zapotec performs the coupled treatment. Once this treatment is complete, both CTH and Pronto3D are run independently over the next Zapotec time step. In general, the Pronto3D stable time step will be smaller than that for CTH. When this occurs, Zapotec allows subcycling of Pronto3D for computational efficiency. The subcycling continues until time t_{n+1} is reached, ensuring the two codes are synchronized.

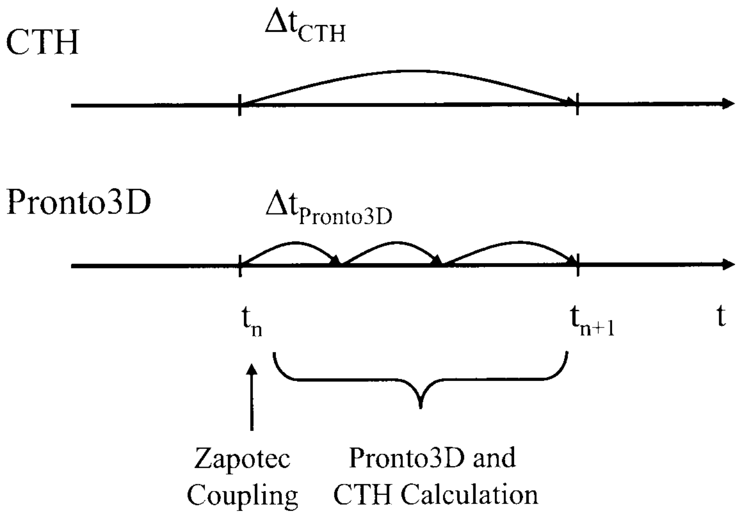

Figure 6. Time Synchronization of CTH and Pronto3D

The coupling at time t_n involves getting data from CTH and Pronto3D, working on the data, and then passing the updated data back to the two codes. Zapotec first operates on the CTH data, a process termed material insertion. This involves mapping the current configuration (and state) of a Lagrangian body onto the fixed Eulerian mesh. The insertion algorithm determines what portions of a Lagrangian body are overlapping the CTH mesh. State data from the overlapping Lagrangian body are mapped into the CTH mesh. Mapped data include the mass, momentum, stress, sound speed, and internal energy. In general, a CTH cell will be overlapped by multiple Lagrangian elements. When this occurs, the mapped element quantities are weighted by their volume overlap. The weighted quantities are accumulated for all elements overlapping a cell, after which the intrinsic value is recovered for insertion. The inserted data are then passed back to CTH as an update.

Once the material insertion is complete, the external loading on a Lagrangian material surface is determined from the stress state in the neighboring Eulerian material. Since the surface is uniquely defined, it is straight-forward to determine the external force on a Lagrangian surface element from the traction vector, element surface normal, and area. After processing each surface element, the element-centered forces are distributed to the nodes and passed back to Pronto3D as a set of external nodal forces. Once the coupled treatment is complete, both CTH and Pronto3D are run independently over the next time step with their updated data.

Zapotec can play a role in a number of the proposed accident scenarios. In particular, the coupled methodology is well suited for modeling blast/structure interaction. Zapotec has been used to assess the second stage Centaur destruct and STAR-48/Space Vehicle Intact Impact events for the PNH FSAR (Bessette and Libersky 2006). These events were quite difficult to model, requiring extensive code development to support the analysis as well as extremely long run times. The cost of the coupled calculation in conjunction with the long run times made it intractable to consider modeling an entire accident event from start to finish with Zapotec. Regardless, it is expected that Zapotec could play a role in the MSL launch safety investigation, focusing on specific events where coupled effects clearly dominate the physics of the problem. Zapotec would be used as part of a multi-step analysis, essentially handing off the results from the coupled analysis to another code for follow-on analysis. This was the approach taken in supporting the PNH FSAR.

Zapotec is relatively new to modeling blast/structure interactions and there are a number of areas where code improvements would benefit the MSL SAR. First, methods for reducing the overall cost of the coupled calculation should be investigated. This would reduce the need for a multi-step analysis. In addition, Zapotec analyses supporting the PNH FSAR encountered numerous drops in the CTH time step during the course of a calculation. This increased the need for material discard in CTH as well as additional restarts. At the time these analyses were conducted, Zapotec was linked with a pre-release of CTH Version 7.0. The standard benchmark suite for Zapotec did not indicate any major problems with the new version of CTH; however, these benchmarks were not representative of the load environments encountered with the PNH FSAR. The time step issue needs to be addressed and resolved. This also will enhance analyses supporting the MSL SAR and improve analysis turn-around times.

Another area of improvement deals with the Lagrangian solver, Pronto3D. The contact algorithm in Pronto3D is robust for hex-hex[3] contact, but has had problems evaluating hex-shell and shell-shell contacts. These difficulties are usually encountered with highly distorted meshes when element death is invoked (see Bessette and Libersky 2006). Many of these difficulties can be avoided with a properly developed mesh and modified contact tolerances; however, it would be best to address this issue and improve the overall robustness of the contact algorithm as this would simplify the mesh generation.

One last area of improvement lies with further validation of the coupling algorithm for blast on thin-shell structures. The code benefits from using two well-established production codes for solving the Eulerian and Lagrangian portions of the problem; however, there has only been limited validation of the coupling algorithm itself for modeling blast/structure interaction. Additional benchmarking for problems involving long-duration loading on thin-shell structures would provide greater confidence in the coupling algorithm.[4] In particular, the validation should focus on cases involving cylindrical geometries of thin-shell structures as well as situations where the thin structures tear. The latter is directly applicable to modeling the breach of the outer housing of the MMRTG.

3.2.4.3 Other Candidate Codes

The number of candidates available for performing the structural analysis portion in a one-way coupling is too long to list here. Generally speaking, any explicit Lagrangian finite element code will suffice. A short list of candidates includes Pronto3D developed by SNL; LS-DYNA developed by Livermore Software Technology Corporation (see Section 3.3.1.4.2); DYNA3D and ParaDyn developed by Lawrence Livermore National Laboratory; and ABAQUS/Explicit developed by Hibbitt, Karlsson, and Sorensen, Inc. These are production codes used both commercially and in the national laboratories. This "short" list contains codes thought to be most applicable for the MSL analyses. Both LS-DYNA and Pronto3D have been used in support of the PNH FSAR, making them leading candidates for use in a one-way coupling, should such an approach be taken.

There are far fewer candidates for performing a coupled analysis. Arbitrary Lagrangian-Eulerian codes can model the coupled blast/structure interaction, provided that structure deformations are moderate and that the external geometry of the structure is relatively simple to allow a conformal mesh along the interface between computational domains. These represent severe restrictions for

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[3] "Hex" refers to a hexahedral element, also know as a brick element.

[4] Thus far, benchmarks for blast loading on thin-shell structures have focused on relatively short duration loadings on flat plates where the plates deformed but did not tear.

the MSL modeling. CEL methods are better suited for the problems encountered with the MSL, largely because they support overlapping computational domains as well as an arbitrary degree of structural deformation. The list of available CEL candidates is short. To our knowledge there are only three CEL codes, in addition to Zapotec, which might meet the needs of the MSL SAR. The PISCES-2DELK, developed by Physics International, has been used to support the Cassini launch. This code has a track record of use supporting launch safety studies; however, the code is limited to 2D analyses. The availability of this code outside of Physics International is also unknown. AUTODYN, developed by Century Dynamics, is also a contender. AUTODYN has been used extensively in the defense industry for modeling blast/structure interaction. The code has a 3D capability and can run in parallel (but with shared memory only); however, it is unclear if this code has been used for similar space-based applications of interest to MSL. Furthermore, the code is proprietary, making it difficult to develop any methodology updates needed during the course of the analysis. The last candidate is Alegra-EP developed by SNL. Alegra-EP is being developed as a follow-on to Zapotec. The code is currently in development, but lacks a number of features needed to support the MSL SAR. In particular, Alegra-EP does not support shell elements with development thus far centered on modeling penetration applications.

3.2.4.4 Recommendations

Zapotec is recommended for modeling the coupled blast/structure interaction. There are areas where algorithm development or validation is needed to meet the requirements of the MSL SAR; however, the code provides a good foundation to work from with the required development/validation relatively minor.

For a one-way coupling, CTH is recommended for performing the blast portion of the analysis. CTH is also well suited for assessing plutonium dioxide damage arising from a pure shock transmission, provided that an adequate constitutive relationship can be developed for the plutonium dioxide and iridium. This type of analysis may be useful in assessing production of additional fines in the fueled clad.

Either Pronto3D or LS-DYNA is recommended for performing the structural analysis portion in a one-way coupled analysis. Both codes have a track record of use in supporting the PNH FSAR. For MSL, Pronto3D may be a better option as the source code is readily available. This is important should any model updates and/or improvements be needed during the course of the analysis.

3.3 Impacts

Fragment impacts on the RTG or its components in flight and impacts with the ground are, from a phenomenological viewpoint, quite similar. However, there are differences in scale, differences in material properties, and differences in how the outcome affects subsequent calculations in the risk analysis. Therefore they will be discussed in separate subsections below.

3.3.1 In-Air Impacts

3.3.1.1 Phenomenological Modeling Considerations

The in-air impact environment refers to the direct impact of primary and secondary fragments against the MMRTG. Primary fragments are defined as those directly generated by the failure of a particular component. Secondary fragments refer to those generated by the interaction of a primary fragment with some other intervening structure. In most cases, it will be impossible to distinguish between the two given the complexity of the launch vehicle construction. Fragment hazards can arise from a number of sources. These include the break up of the Common Core

Booster and Centaur motor, and rupture of the hydrazine and pressurant tanks on-board the space vehicle. Fragment sizes and mass can vary significantly, ranging from small scraps of hardware to large sections of the spacecraft.

The overall modeling effort is summarized as follows:

- This analysis involves modeling the impact of an arbitrary shaped fragment against a detailed model of the MMRTG. If the impact damage is isolated to a localized region, then it will only be necessary to model a small section of the MMRTG. Scenarios involving large fragments will require modeling the entire MMRTG.
- In addition to modeling single fragment impacts, it may be necessary to assess synergistic effects from multiple fragment impacts against the MMRTG.
- The final outcome of this analysis is a determination of whether the iridium clad is perforated by a fragment. If so, then it will be necessary to assess the amount of plutonium dioxide release. If the clad is not breached, then it will be necessary to track the amount of damage to the plutonium dioxide inside. Any pulverization could lead to additional fines being released as a result of follow-on insults.

The fragment velocity will dictate the method used to model its impact against the MMRTG. Low velocity impacts (<500 m/s) are best modeled using a Lagrangian method where material deformations are moderate. Impact pressures are relatively low in this velocity regime with material strength and fracture dominating the material response. In contrast, high velocity impacts (> 1000 m/s) are best modeled using an Eulerian approach. At these velocities, the impact pressures exceed the material strength. Erosion is clearly evident in the impactor and target, a consequence of plastic flow in the contact region. The velocity bounds associated with the mid-range of 500 to 1000 m/s are somewhat arbitrary, with the true bounds being dependent on the materials involved, the geometric configurations of the impactor and target, and the specific impact conditions (velocity and orientation). Thus, the stated velocity bounds are only qualitative in nature. Accidents resulting in fragments having velocities falling in this mid-range will need to be evaluated on a case-by-case basis in the modeling. For the purposes of the code selection, it will be necessary to cover all possible cases (i.e., from low to high velocity impacts).

Thus far, the discussion of code expectations has been focused solely on modeling the physics of the problem. Additional generalized requirements can be levied on the code selection, such as requiring support for 3D analyses, code maturity, etc. These general requirements were discussed in Section 3.2.1.

3.3.1.2 Interface with Launch Vehicle Databook

It is assumed that the Databook will define the fragmentation environment from the various sources. This environment is usually defined as a fragment mass and velocity distribution, which are binned based on angle from the center of detonation. If data is not available, then it will be necessary to characterize the fragmentation environment by analysis. This will entail the determination of a representative threat fragment(s) and associated impact conditions (velocity and orientation) used for the analysis.

3.3.1.3 Generic Considerations

See discussion in Section 3.2.3.

3.3.1.4 Assessment of Candidate Codes

3.3.1.4.1 Pronto3D

Pronto3D is an explicit Lagrangian, finite element code developed at SNL for modeling transient solid mechanics problems involving large deformations and contact (Taylor and Flanagan 1989, Attaway et al. 1998). Pronto3D has been in active use within SNL since the late-80s. A Smooth Particle Hydrodynamics (SPH) capability was added to Pronto3D in the early-90s to extend its capability for modeling large material deformations (Attaway et al. 1993). Pronto3D has traditionally been used to model accident analyses involving nuclear fuel storage casks (e.g., see Kalan and Ammerman 2003), low-velocity ballistic penetration (e.g., Gwinn and Metzinger, 2003), and metal forming applications (e.g., see Brown et al. 1998). Pronto3D is well suited for modeling low-velocity fragment impacts against the MMRTG. A brief overview of Pronto3D is provided herein. Further details can be found in Taylor and Flanagan (1989), and Attaway et al. (1998).

The numerical solution approach taken by Pronto3D is typical of most explicit finite element codes, and involves a discretization of the weak form of the equilibrium equations. This discretization is fairly standard and will not be discussed here (e.g., see Becker et al. 1981 for details). For this discussion, we will start from the discretized equation of motion, given by

$$\mathbf{M}\,\mathbf{a} = \mathbf{f}^{\text{ext}} - \mathbf{f}^{\text{int}} + \mathbf{f}^{\text{c}}$$

where **M** is the mass matrix, **a** is the set of nodal accelerations, and **f** is the set of assembled nodal forces. Superscripts ext, int, and c refer to the external, internal, and contact forces, respectively. The equilibrium problem is solved element-by-element, with the results assembled into the global statement above. Contributions to the external force arise from any prescribed traction boundary conditions, nodal forces, or body forces. Contributions to the internal force arise from the element stress, viscous pressure, and hourglass resistance. In the explicit finite element method, the components of the mass matrix **M** are diagonalized (or lumped). This readily permits computation of the nodal accelerations without the need for a matrix inversion.

The contact force $\mathbf{f}^{\text{c}}$ denotes a correction applied to the solution to ensure compliance between contacting bodies. Typically, a master-slave algorithm is used in the contact determination, where slave nodes are allowed to penetrate a master surface during an initial predictor step for contact. The motion associated with penetrating slave nodes and the penetrated master surface is then corrected in accordance with momentum conservation. In Pronto3D, corrections are applied to the nodal accelerations in lieu of the forces. The two are equivalent given that the mass is lumped at the nodes; however, the use of the acceleration corrections ties in well with the implementation of prescribed kinematic boundary conditions.

At the start of the time step, the deformation rates are computed, which are later used in the stress update. Constitutive behavior is evaluated with respect to the unrotated reference frame. An incremental algorithm is used to determine the rotation tensor, which is subsequently used to rotate the deformation gradient tensor to the unrotated state, allowing the material response to be evaluated in its natural unrotated state. Stresses are transformed back to the rotated state and subsequently used for the nodal force calculations. Once the material stress is updated, Pronto3D computes the internal and external nodal forces. With the nodal force and mass in hand, it is straightforward to compute the nodal accelerations (**a** = **f/m**). At this point, the nodal accelerations do not take into account inter-material contact. This is done within the contact treatment, which corrects the nodal accelerations to enforce the contact conditions at the end of the time step. Once the time step is complete, the equations of motion are integrated forward in time using a central difference scheme. One should note that the explicit time marching scheme is only conditionally stable, requiring the determination of a stable time step Δt. This time step is taken as the minimum of that computed for all elements in the problem setup.

Pronto3D accommodates several element types, including 8-node hexahedral elements, 4-node quadrilateral shells, and 2-node beams (see Attaway et al. 1998 for a description of supported element types). These elements are under-integrated and require hourglass control to eliminate the energy-less modes of deformation. Pronto3D also offers a wide range of constitutive models (see Attaway et al. 1998 for a listing), with a well documented framework for adding new ones.

One can expect to encounter large material deformation when modeling problems involving impact or blast. These large material deformations result in large distortions in the finite element mesh. These distortions degrade accuracy and can sometimes be severe enough to stop the calculation. For a pure finite element calculation, these large mesh distortions are handled using element death. Element death removes highly distorted elements from the calculation once some user-prescribed death criterion is met. Algorithms of this nature are used extensively throughout the penetration mechanics community for analyses conducted using explicit finite element codes and are often referred to as eroding interface algorithms. This algorithm can also be used to some degree to emulate material failure and/or fracture. The latter requires model calibration to an existing set of experimental data.

The SPH algorithm in Pronto3D provides an alternative approach for modeling materials exhibiting large deformations. It is possible to set up a problem using a mixture of both traditional finite elements and SPH. For example, consider a low-velocity ballistic penetration problem, where the penetrator undergoes very little deformation and its geometry is modeled using a standard finite element mesh. One can expect severe localized deformations in the target. In the problem development, the target is modeled using SPH elements. The SPH algorithm is capable of handling these deformations, with individual SPH elements (i.e., spherical elements in Pronto3D) able to interact with the outer surface of the penetrator via a traditional explicit transient dynamics contact algorithm (e.g., see Brown et al. 1998). SPH extends the capability of Pronto3D to model penetrating impacts at higher velocities. The upper range of applicability is problem-dependent; however, it is generally thought the method is applicable below impact velocities of 1000 m/s.

Pronto3D is well suited for modeling low velocity fragment impacts against the MMRTG for velocities in the low-to-mid range. This code has been used in several space-related accident investigations (e.g., see Metzinger, 1993, Gwinn and Metzinger, 2003) and for the PNH FSAR (Bessette and Libersky 2006). The contact algorithm is reasonably robust for hex-hex contact, but has had problems evaluating hex-shell and shell-shell contacts. These difficulties are usually encountered with highly distorted meshes when element death is invoked (see Bessette and Libersky 2006). Many of these difficulties can be avoided with a properly developed mesh and modified contact tolerances; however, it would be best to address this issue and improve the overall robustness of the contact algorithm as this would simplify the mesh generation and improve analysis turn-around times. This is an area where improvements can be made to benefit the MSL SAR.

3.3.1.4.2 LS-DYNA

LS-DYNA is an explicit finite element code developed by Livermore Software Technology Corporation (Hallquist 1998, 2001), having its roots in an earlier version developed at Lawrence Livermore National Laboratory (Hallquist 1983). LS-DYNA is a well-established commercial code that has been in active use in many industries since the early-90s. LS-DYNA is arguably the most prolific of the explicit finite element codes and is widely used to perform impact and crash simulations (e.g., see Knight et al. 2000, Marklund and Nilsson 2001). A brief overview of LS-DYNA is provided here; further details can be found in Hallquist (1998, 2001).

The general solution approach outlined for Pronto3D is typical of that used in any explicit finite element code. It is the details of the algorithm implementation that differ for these codes. Thus, we will focus our discussion on these differences. LS-DYNA offers a wider range of constitutive models and supported elements types than Pronto3D. This is not surprising since it is commercial software with a much larger customer base. Other differences include the manner in which contact is enforced. LS-DYNA applies corrections to the nodal forces instead of the accelerations as is done in Pronto3D. In addition, LS-DYNA uses a penalty enforcement as opposed to the nodal constraint approach taken by Pronto3D. With a penalty method, the contact interactions are corrected using a spring force which permits slight inter-penetrations between contacting materials. In contrast, the nodal constraint approach used by Pronto3D is essentially a "put-back-on" algorithm that does not allow any material inter-penetration. The best choice of enforcement method depends on the problem being modeled and the required accuracy in the contact treatment. Material objectivity is also treated differently, with LS-DYNA generally relying on a Jaumann rate and Pronto3D on the Green-Naghdi rate. These differences affect determination of the material response under large rotation with the Green-Naghdi rate being the more accurate (and costly) of the two. Given the differences in the algorithm implementation, one should anticipate variations in results between the two codes.

LS-DYNA is well suited for modeling low velocity fragment impacts against the MMRTG. LS-DYNA offers a wide range of constitutive models and has a very robust contact algorithm. This code has a track record was used by Rocketdyne for some of the initial MSL safety analysis work and extensively by Lockheed Martin for the PNH FSAR. A major drawback with LS-DYNA is not having access to the source code. There may be a need to develop specialized models/techniques during the course of the safety analysis. Without the source code, there will be no means to implement these models. This is an important consideration given that unexpected problems typically arise in complex analyses.

3.3.1.4.3 CTH

CTH is an Eulerian shock physics code developed at SNL. The numerical algorithm was discussed previously in Section 3.2.4.1. Here, the discussion will focus on the application of CTH for modeling ballistic impact and fragmentation. CTH has been used extensively for modeling anti-armor and hypervelocity impact applications, where impact velocities are typically greater than 1000 m/s (e.g., see Hertel 1992, Kmetyk and Yarrington 1994; Wilson et al. 1998). There has been limited extension of CTH to lower impact velocity regimes, with velocities typically greater than 300 m/s and involving only normal impacts (Silling 1992, Kmetyk and Yarrington 1994).

CTH has also been used to characterize the fragmentation environment generated by a cased charge (e.g., see Kipp et al. 1993, 1999; Wilson et al. 2001). This is a useful capability when the fragmentation environment is ill-defined. In general, it is difficult to explicitly model fragmentation, largely due to limitations in the fracture models and the mesh resolution required to accurately replicate the fragmentation process. Kipp et al. (1993) have developed post-processing techniques to overcome these difficulties, with the resulting method validated over a range of conditions (e.g., Kipp et al. 1999, Wilson et al. 2001).

CTH is well suited to model high velocity fragment impacts against the MMRTG. CTH has a track record of use in this area and has been used to support fragmentation modeling for the PNH FSAR (Bessette et al. 2006a). The fragmentation environment associated with different accident events will be provided by the Databook; however, there may be instances where data is unavailable or needs to be augmented by analysis. CTH provides a viable approach for obtaining this information when needed. There is no anticipated algorithm development needed for CTH to support the MSL SAR. At present, the only anticipated needs are associated with defining material properties and other problem inputs for CTH.

3.3.1.4.4 Other Candidate Codes

There are other codes available for modeling fragment impacts. The EPIC code, developed by Alliant Techsystems, Inc., has been used extensively within the Department of Defense community for modeling both low and high velocity impact events. EPIC is an explicit Lagrangian finite element/SPH code developed exclusively for penetration applications. EPIC is currently being modified for parallel computing. At present, this capability is not available, limiting EPIC's usefulness for the MSL SAR.

AUTODYN, developed by Century Dynamics, is another possible candidate for modeling fragment impacts. AUTODYN has been used in a number of defense-related applications involving impact and penetration. The major drawback with AUTODYN is that it is proprietary. Without the source code, it will not be possible to incorporate any model updates or improvements that may be needed during the course of the analysis.

3.3.1.5 Recommendations

The use of Pronto3D and/or LS-DYNA for modeling the low velocity impact of fragments against the MMRTG is recommended. The use of SPH within Pronto3D is particularly attractive for modeling impacts where the velocity falls into the mid-range. The use of Pronto3D is favored over LS-DYNA to maintain consistency in the modeling across a range of environments. Recall, the Zapotec code is recommended for the coupled blast/shock analysis. Zapotec links Pronto3D and CTH. LS-DYNA cannot be substituted for Pronto3D since we do not have access to the source code. Given the algorithmic differences between LS-DYNA and Pronto3D, one cannot expect the two codes to produce the same results. Thus, to maintain consistency in the overall safety study, it is recommended the fragment impact analyses be conducted with Pronto3D.

CTH is recommended for modeling high velocity fragment impacts as well as supporting any characterization of a fragmentation environment (if needed). It should be noted that any of these codes are capable of modeling synergistic effects resulting from multiple fragment impacts, with the cost of the calculation commensurate with the increased problem size.

3.3.2 Ground Impacts and Crush

3.3.2.1 Phenomenological Modeling Considerations

The ground impact and crush environment involves either the impact of the spacecraft (or possible a standalone MMRTG as well as any of its internal components) against a hard surface, or any of these components being impacted by falling heavy objects from the launch vehicle. An example of the former involves the intact impact of the MMRTG against various ground media following breakup of the launch vehicle at altitude. An example of the latter involves the full stack intact impact of the launch vehicle onto the cruise stage. Both scenarios involve impacts at relatively low velocities.

The overall modeling effort is summarized as follows:

- The ground impact portion of the analysis involves modeling the impact of the spacecraft and selected sub-components against various ground media. Ground media of interest include steel (as a worst case), concrete, sand, and water. Sub-components of interest include a standalone MMRTG and its internal components. It is necessary to consider a standalone MMRTG impact as it is possible that the MMRTG may be ejected from the cruise stage following an earlier insult (e.g., the blast from the destruct of the Centaur motor may break up the upper stage, allowing the MMRTG to become free-flying). MMRTG components to be evaluated include a standalone full-GPHS module, a half-GPHS module, the GIS, and a bare fueled clad. Variations in impact velocity and orientation will be considered.
- The crush portion of the analysis involves some portion of the launch vehicle falling on top of the intact spacecraft and/or a standalone MMRTG as it impacts the ground.
- The outcome of this analysis is a determination of whether the iridium clad is breached. If so, then it will be necessary to assess the amount of plutonium dioxide release. Any pre-damage from earlier insults will need to be taken into account for the release modeling.

The approach taken for the ground impact and crush modeling will be problem-dependent. In general, the modeling approach will be dictated by the impact velocity regime, with low velocity impacts generally modeled using a Lagrangian structural dynamics code and higher velocity impacts modeled using an Eulerian shock physics code. However, impact velocity alone is not the determining factor for choosing a modeling approach. One must also consider the materials involved and degree of deformation. The problem-dependent nature of the modeling requires some flexibility in the evaluation of candidate codes. In the ensuing discussion, we will cover a number of candidates capable of covering a range of impact and crush scenarios. The decision to choose a specific code from those recommended will be done once the impact and crush scenarios are better defined. This definition will be provided in coming drafts of the Databook.

Thus far, the discussion of code expectations has been focused solely on modeling the physics of the problem. Additional generalized requirements can be levied on the code selection, such as requiring support for 3D analyses, code maturity, etc. These general requirements were discussed in Section 3.2.1.

3.3.2.2 Interface with Launch Vehicle Databook

Specific impact scenarios will be derived from the Databook. Data derived from the Databook includes the range of impact conditions (velocity and orientation) of interest as well as the size/mass of portions of the launch vehicle landing on the cruise stage and/or a standalone MMRTG. Modeling the impact of individual MMRTG components is meant to augment other AOCs which have resulted in its separation from the launch vehicle at altitude. Ground media of interest will likely include steel (as a worst case), concrete, sand, and water.

3.3.2.3 Generic Considerations

See discussion in Section 3.2.3.

3.3.2.4 Assessment of Candidate Codes

3.3.2.4.1 Pronto3D

Pronto3D is an explicit Lagrangian, finite element code developed at SNL. The numerical algorithm has been discussed in Section 3.3.1.4.1. Here, the discussion will focus on the application of Pronto3D for modeling the ground impact and crush environment. Pronto3D has been used extensively at SNL for modeling accidents involving nuclear fuel storage casks (e.g., see Kalan et al. 2003) as well as other structural analysis applications (e.g., see Metzinger 1993, and Brown et al. 1998). Pronto3D is well suited for modeling the structural response of the MMRTG and has been used to model both the Bare Clad Impact (BCI) and Safety Verification Tests (SVT) in support of the PNH FSAR (Bessette and Libersky 2006). Furthermore, the SPH capability embedded in Pronto3D is particularly attractive for modeling impacts against soft ground media, such as sand and water. As mentioned previously, there is room for improvement in the contact algorithm for hex-shell and shell-shell contact. This is an area where improvements can be made to benefit the MSL SAR.

3.3.2.4.2 LS-DYNA

LS-DYNA is an explicit finite element code developed by Livermore Software Technology Corporation. The numerical algorithm was discussed in Section 3.3.1.4.2. LS-DYNA is well suited for modeling the ground impact and crush environment. It has been used extensively by Lockheed-Martin in support of the PNH FSAR. The only drawback to its use is not having access to the source code. There may be a need to develop specialized models/techniques during the course of the safety analysis. These techniques could not be implemented without the source code. This is an important consideration given that unexpected problems typically arise in complex analyses.

3.3.2.4.3 CTH

CTH is an Eulerian shock physics code developed at SNL. The numerical algorithm has been discussed in Section 3.2.4.1. As discussed previously, CTH has been used primarily for modeling high velocity impacts, typically greater than 1000 m/s. Recent development has focused on extending the applicability of CTH to much lower impact velocity regimes, more typical of that encountered in the ground impact and crush environment. Given its track record, CTH could play a role in modeling the ground impact and crush environments. The modeling of crushing events is a particular area where CTH would be applicable, largely due to the exceedingly large material deformations expected with this class of problem. At present, there is no anticipated algorithm development needed for CTH to support the MSL SAR.

3.3.2.4.4 Zapotec

Zapotec is a coupled Euler-Lagrange code developed at SNL. The numerical algorithm has been discussed in Section 3.2.4.2. Zapotec has been used to model low velocity impact and penetration (e.g., see Silling 2000 and Bessette et al. 2002, 2003). Zapotec could play a role in the ground impact and crush modeling, particularly for problems where the materials involved exhibit vastly differing degrees of deformation. Such might be the case with the crushing events, or impacts against soft media such as sand or water. Zapotec is a relatively new code, and there is some level of development needed to support the MSL FSAR. This was discussed in Section 3.2.4.2.

3.3.2.4.5 Other Candidates

There are other candidates for the ground impact and crush modeling. A short list includes PISCES-2DELK, DYNA3D/ParaDyn, EPIC, ABAQUS/Explicit, and AUTODYN. The merits of these codes for supporting the MSL SAR have already been discussed in Sections 3.2.4.3 and 3.3.2.4.4. In summary, each of these codes has some factor that limits its utility for the MSL analysis.

3.3.2.5 Recommendation for MSL Analysis

The codes considered for the ground impact and crush modeling fall into one of three categories: Lagrangian structural dynamics, Eulerian shock physics, and coupled. Pronto3D and LS-DYNA are examples of structural dynamics codes; CTH is an Eulerian shock physics code; and Zapotec is a coupled code. Given the problem-dependent nature of the ground impact and crush environment, it is not possible to choose any specific code or solution approach. Instead, we will make individual recommendations for each code category.

Of the structural codes, either Pronto3D or LS-DYNA are recommended for use in the ground impact and crush modeling. Both codes have a track record of use in supporting the PNH FSAR as well as application to more generalized structural analysis problems. Other structural codes are available; however, their utility is generally limited by a lack of access to the source code or not having a track record of use in launch safety studies. In keeping with this line of reasoning, we also view CTH and Zapotec as viable candidates for supporting the MSL SAR. These two codes may be applied in regimes where the structural codes are deficient.

Revisiting the selection of a structural code, we recommend the use of Pronto3D over LS-DYNA to maintain consistency in the modeling across a range of environments. Recall that the Zapotec code is recommended for the coupled blast/shock analysis. Zapotec links Pronto3D and CTH. LS-DYNA cannot be substituted for Pronto3D since we do not have access to the source code. Given the algorithmic differences between LS-DYNA and Pronto3D, one cannot expect the two codes to produce the same results. Thus, to maintain consistency in the overall safety study, the use of Pronto3D is recommended over LS-DYNA.

We should also note that Lockheed-Martin has already conducted a suite of impact calculations involving RTG sub-components for the PNH FSAR. These calculations modeled the impact of a full-GPHS module, a half-GPHS module, a GIS, and a bare fueled clad against different media at varying orientations and velocities. It may be possible to utilize the table lookup results from these calculations for the MSL SAR. This should be done with some care since the GPHS module designs vary slightly between PNH and MSL. The slightly increased thickness of the GPHS aeroshell in the Step-2 module design for MSL should afford some added protection during impact. The question then arises whether such an enhancement is sufficient to warrant generating a new set of lookup tables. This is an issue that needs to be addressed.

3.4 Mechanical Source Term

The structural and hydrodynamic response analyses discussed above are expected to do an adequate job of predicting the deformation and degradation of the mechanical barriers that contain the plutonium dioxide fuel. However, they cannot directly predict the amount and size distribution of the plutonium dioxide that may be released. There is, unfortunately, no physics-based model for such releases; all that exist are empirical curve fits to test data.

Two series of experiments have provided data on plutonium dioxide releases from fueled clads subject to mechanical disruption from impacts. The BCI tests studied the effects of fueled clads impacting solid surfaces at various velocities and angles. The Safety Verification Test (SVT) series were similar, but utilized intact GPHS modules. These tests provided information on mechanical deformation as well as a limited amount of data on released plutonium dioxide (or surrogates thereof). Both were carried out at Los Alamos in the 1980s (Pavone 1986).

3.4.1 Lockheed Martin Empirical Model

In order to develop a model for the mechanical source term for the PNH Mission, Lockheed Martin carried out an elaborate analysis of the BCI and SVT tests (Matheson 2004). The first step was to find reasonable curve fits for the plutonium dioxide particle size distribution of the fuel for each of the BCI and SVT tests (except for some tests not used because of suspected experimental problems). These curves were developed to represent the state of the plutonium dioxide after impact but before release. This was done by analyzing the BCI and SVT sieving results for post-impact analysis of the fuel that was *not* released. (Information about released fuel was not used in this stage).

The next step in the analysis was to associate each of the tests with a crushed volume fraction, a surrogate for pulverization that was expected to increase with increasing impact severity. Since crush volume was not measured in the experiments, simulations with LS-DYNA were used to predict it for each test. This allowed a curve fitting process that produced a correlation for particle size distribution that depended only on crushed volume. Comparison with the test data showed reasonably good agreement, as shown in Figure 7 which displays the Cumulative Mass Fraction (CMF) for particles smaller than the size given.

The last part of the analysis needed for a mechanical source term release model involves the dependence of the mass released on the clad rupture characteristics. The two rupture characteristics selected as controlling parameters were crack width and crack area. The first parameter was used in conjunction with the curve fits shown in Figure 7 to calculate the Escapable Mass Fraction—the cumulative mass of all particles smaller than the given crack width. What was then needed is the fraction of that limit that is actually released. For this, Lockheed Martin utilized the fifteen BCI and SVT tests in which rupture occurred. Then a five-parameter curve fit for the fractional fuel released was found for the fifteen values of release fraction as a function of the crack area.

The end result was a procedure by which the total mass released and its distribution into size bins could be calculated as a function of three parameters: crush volume, crack width, and crack area. This procedure was used for all PNH impact calculations that used LS-DYNA with a fine mesh treatment of the fueled clads (because the crack parameters could be calculated from code output only if the mesh is small compared to the crack dimensions).

For other structural response studies, a different procedure was needed for the crack areas and widths. For LS-DYNA studies involving a mesh too coarse to directly calculate the crack parameters, a correlation between crack area and maximum effective von Mises strain rate (which is available from the coarse mesh studies) was developed on the basis of numerous fine mesh LS-DYNA calculations. Another correlation mapped the area to the width.

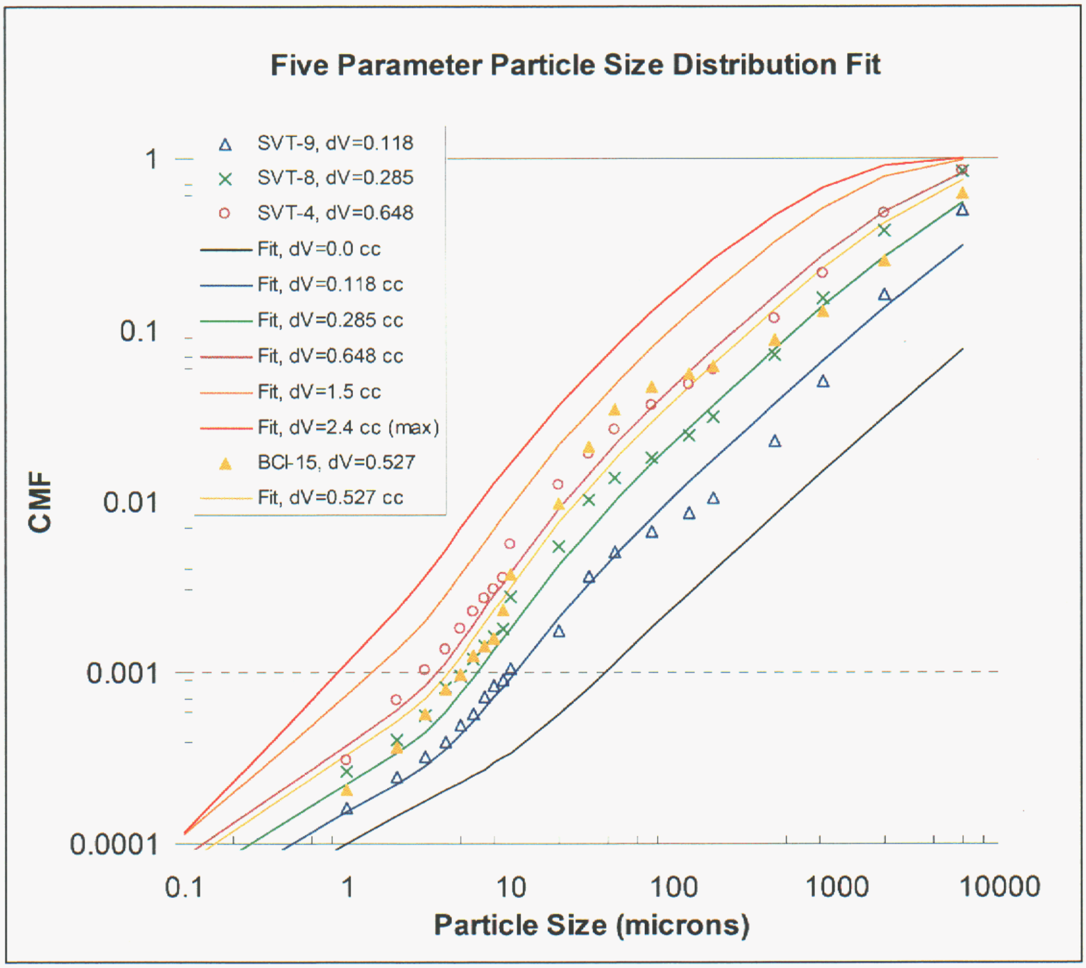

Figure 7. Lockheed Martin Empirical Model for Crushed Plutonium Dioxide Particle Size Distribution

For PNH cases in which the coupled Euler-Lagrange code, Zapotec, was used, a two-step process was used to link the code calculations to the empirical correlations developed from the BCI and SVT tests. First, since the Pronto3D part of Zapotec produced slightly different results than LS-DYNA for equivalent problems and meshing, two correlations were developed between the coarse mesh LS-DYNA results for crush volume and maximum effective strain and the corresponding values for Pronto3D. Thus, for Zapotec runs, the calculated results for crush volume and effective strain were converted to the corresponding values that LS-DYNA would (based on the Zapotec /LS-DYNA correlation) have produced. These values were then used to calculate what a fine-meshed LS-DYNA would have predicted for crack parameters (based on the fine mesh/coarse mesh correlations). Those parameters were then used to calculate the plutonium dioxide mass released and its size distribution.

Finally, for some CTH calculations involving small, highly penetrating impacts, the fraction released was assumed to be the total fraction crushed, bypassing the crack shape analysis utilized for less penetrating events.

3.4.2 Recommendations for Mechanical Source Term

The mechanical properties of the form of PuO_2 used in the MMRTG are sufficiently different from better characterized materials that there is no known credible model for pulverization and release based on the underlying phenomenology. Dependence on an empirical model based on available test data appears the only practical course for the MSL SAR work. While the methodology carried out by Lockheed Martin as described in the previous section appears to be sound, to use it directly would be unnecessarily convoluted, because of the need to translate results from, say, Pronto3D to "effective" results for LS-DYNA for direct use in their empirical model.

It is anticipated that many of the BCI and SVT tests will be utilized for the validation of the tools to be used for MSL impact analysis. Some have already been exercised in this way. It therefore seems reasonable to extend the studies of these test series for the purpose of developing an empirical model following a methodology similar to that used by Lockheed Martin for PNH. The result would be an empirical model for mass released and particle size distribution that depends directly on quantities calculated by the codes chosen for MSL analysis.

3.5 Source Terms in Thermal Environments

3.5.1 Overview of Thermal and Fire Environments

Blast, shock and impact can damage the MMRTG, the GPHS module structure, and the GIS sufficiently that fragments of the plutonium dioxide fuel are released. Some fraction of the fragments may be so small that they remain airborne and are dispersed within the environment in what is termed the mechanical source term. Other fragments may be exposed to fire environments produced by the combustion of liquid or solid propellants. Intact modules or fueled clads may also be heated by propellant combustion. If these fragments, modules, and fueled clads are heated to sufficiently high temperatures, significant amounts of plutonium dioxide will be vaporized and escape into the ambient environment. These plutonium dioxide vapors will cool and nucleate as aerosol particles, and the particles will agglomerate with other aerosols produced in the accident including soot, aluminum oxide smoke and entrained dirt to constitute the thermal source term. This thermal source term as well as the mechanical source term are inputs to the analysis of accident sequences and consequences discussed in Sections 4 and 5 of this report.

For use in consequence analysis, adequate characterization of the thermal source term requires analysis of the responses of nuclear materials either within or expelled from the MMRTG/GPHS/GIS structures when exposed to the various fire environments. The objectives of such analyses are to determine the magnitude and the nature (composition and particle size) of the thermal source term. Essential inputs to the analyses are (1) damage state of the MMRTG/GPHS/GIS determined from earlier analyses of accidents discussed in Sections 3.2 and 3.3, (2) locations and orientations of the plutonium dioxide-bearing materials relative to the burning propellants, (3) the amounts of burning propellant, and (4) the temperatures and heat fluxes produced by the propellant combustion. The Databook provides specifications of the fire environments and analyses discussed in previous sections of this report provides damage, location, and orientation information.

Analysis of the thermal source term requires treatment of the following phenomena:

- Thermal response and degradation of structures such as the GPHS module and GIS that protect the plutonium dioxide fuel
- Thermal response and vaporization of the plutonium dioxide fuel heated by the propellant

- Entrainment of plutonium dioxide fragments in the air flow created by the burning propellant
- Nucleation of and condensation on aerosol particles from the plutonium dioxide vapors
- Production of aerosols of other materials such as aluminum oxide
- Coagulation of plutonium dioxide aerosols and other aerosol materials

Because the processes leading to a thermal source term of plutonium dioxide can be energetically significant, it is useful to couple modeling of the source term processes closely with the modeling of the fire environments. Coupling between the environment and the source term modeling is also desirable because the vaporization of plutonium dioxide is not just dependent on temperature. The nonstoichiometric nature of the PuO_{2-x} system means vaporization depends on both temperature and the oxygen potential of the gas phase. For fuel exposed directly to the combustion of solid propellant sensitivity of vapor pressures to oxygen potential is not especially significant, since oxygen potentials are generally high. It is a more important consideration for fuel contained within a module where oxygen potentials are generally low (promoting vaporization) and can vary over substantial ranges, affecting vaporization significantly. It is also important within a fireball where oxygen potentials can vary spatially between very low values near the center to very high values at the perimeter where air is entrained.

Three fire environments can be considered:

- Plutonium dioxide fragments expelled into the fireball produced by combustion of liquid propellants
- Plutonium dioxide fragments or pellets dispersed in the vicinities or burning chunks of solid propellant
- Largely intact though perhaps damaged modules in the vicinities of burning solid propellants

A fourth environment can be hypothesized—clad pellets or intact modules within the fireball of burning liquid propellants. Scoping calculations show that this environment exists for too short a time to heat clad fuel or modules sufficiently to contribute to the thermal source term. This fourth environment is not considered here.

3.5.2 Fuel Fragments Exposed to the Combustion of Liquid Propellants

Combustion of liquid propellants produces a fireball that can occur either at altitude or on the ground. Temperatures within fireballs are sufficient to vaporize finely fragmented plutonium dioxide that might have been expelled from a damaged MMRTG. These vapors will nucleate as the fireball cools and the nucleated particles will agglomerate with each other and with soot formed in the fireball and dirt entrained in the fireball.

In the recent past, the Sandia Fireball Model (SFM) (Dobranich et al. 1997) has been used for the analysis of plutonium dioxide vaporization, nucleation and agglomeration in launch accidents. It has usually been found that thermal source terms from fuel fragments exposed to fireballs produced by combustion of liquid propellants are small in comparison to source terms associated with the combustion of solid propellants. However, for some individual MSL AOCs, the thermal source term may dominate if interactions with solid fuel fires are absent.

3.5.2.1 Interface with Launch Vehicle Databook

The Databook provides heat fluxes and temperature data for fireballs, but these data cannot be directly used in SFM. The essential difficulty is the rapid evolution of both temperature and chemical conditions (oxygen potential) within the fireball. Consequently, an integrated and coupled analysis of the fireball and the plutonium dioxide vaporization process is needed. This analysis is done using the masses of propellants and oxidizers prescribed in the Databook. Fireball temperatures and heat fluxes predicted with SFM are found to agree adequately with information provided in the Databook.

3.5.2.2 Code Assessment

3.5.2.2.1 Sandia Fireball Model

SFM (Dobranich et al. 1997) has been used in launch safety analyses since the Cassini launch. Figure 8 illustrates the various interactions considered. The code includes models of:

- Fireball growth and liftoff,
- Chemical speciation and thermochemical potentials within the fireball,
- Radiant and convective heat fluxes in the fireball and to the environment,
- Fuel particle vaporization rates limited by both mass transfer and heat flux,
- Vapor nucleation and condensation, and
- Aerosol agglomeration and growth.

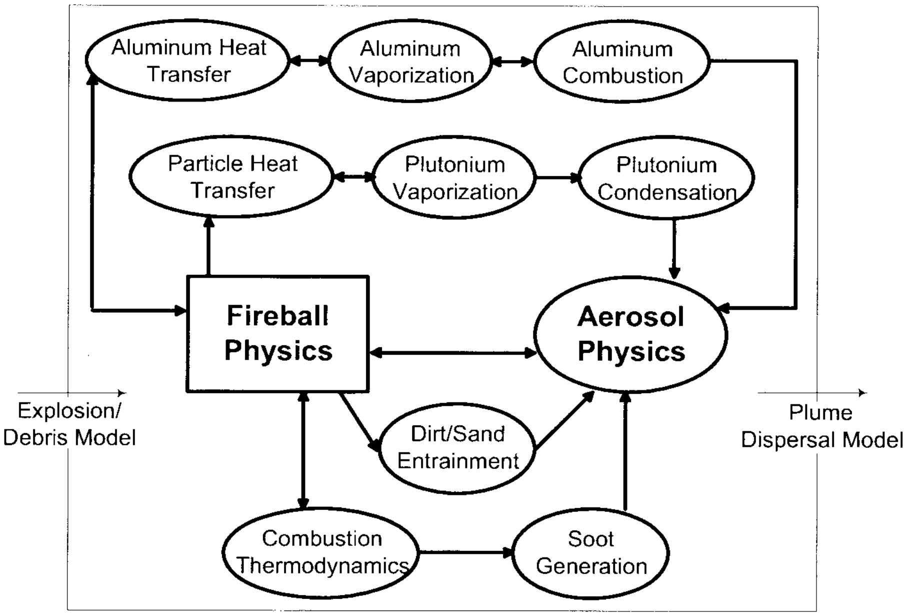

Figure 8. Phenomena and Interactions Captured in SFM

Adequate analysis of the source term produced interactions between fuel fragments and a liquid propellant fire requires that the close coupling among these phenomena be taken into account. Since a large number of computational runs must be made for the range of parameters that may occur among the various accident sequences, it is essential that, for production runs in support of a SAR, the run time of the code be kept reasonable. To achieve that goal, it is impractical at the present time to model the physics of the gas flow with computational fluid dynamics (CFD) methods. Instead, a number of simplifications of the spatial dependencies are made in the code. Such simplifications are not only motivated by the need to achieve a reasonably fast running speed, but also by the fact that there is very little experimental data for tests involving all of the interactions depicted in Figure 8.

The principal simplification made in SFM is to treat the interaction zone as a control volume, which at the time of initial combustion is (for ground-based fires) a hemisphere centered on the ground surface. As the combustion proceeds and gas temperature increases, the control volume expands and buoyancy lifts the fireball until the control volume forms a complete sphere rising above the ground. It is assumed that liquids and particles are well mixed within the fireball, and all relevant processes affecting the production and evolution of fine plutonium dioxide aerosols are modeled self-consistently within the volume. Heat transfer to aluminum structures is also modeled because of the importance of aluminum vapor condensation, chemistry, and aerosol agglomeration. A wide variety of input parameters are available to the user to study the effects of different choices on the source term.

The SFM models of the fireball including fireball growth and heat fluxes yield predictions in good accord with available data, but there is room for some improvement in the code. For one thing, as pointed out by the INSRP, there is a need to better document the validation of these models. In addition there is a need for better guidance on the user-input rates of propellant combustion.

Plutonium dioxide vaporization modeling in SFM recognizes the bivariant nature of the process. The underlying data base is no longer in accord with the best thermodynamic data now available and needs to be updated. Similarly, equilibrium thermochemical data used in SFM for the evaluation of oxygen and carbon potentials has become dated and needs to be revised to reflect best recommendations within the technical community.

The thermochemical modeling of the fireball used in SFM produces a uniform temperature and chemical environment for the vaporization of plutonium dioxide from fuel particles dispersed in the fireball. This environment is adjusted on an average basis as the fireball entrains air and loses heat. This average only approximates the spatial variation of chemical and thermal conditions within the fireball produced by air entrainment and radiation heat losses.

The thermochemical speciation modeling used in SFM is recognized to underpredict soot formation, which is important because the soot agglomerates with plutonium dioxide particles and affects the ability to disperse plutonium dioxide-bearing aerosols in the environment. SFM allows users to augment soot production by inputting soot but little guidance is provided on soot amounts. INSRP has criticized this aspect of the modeling. This is another area for improvement of the documentation.

3.5.2.2.2 Fuego/Syrinx

The Fuego/Syrinx code suite is a higher fidelity model of fluid combustion (Domino, 2005). Fuego solves the transient 3D Navier-Stokes equations for turbulent reacting flows. It tracks multiple species (fuel, oxidizer, products) and models heat release using mixing models appropriate for fire environments. In contains soot models appropriate for typical hydrocarbon fuels, although the specifics of soot formation with propellants like RP-1 and hydrazine will have to be addressed. Syrinx solves the radiative transfer equations using the discrete ordinates model.

Fuego and Syrinx are fully coupled. Absorption coefficients that are required by Syrinx are determined from the soot and gas species concentrations determined by Fuego. These parameters are employed by Syrinx to determine the radiative flux, the divergence of this being fed back as a source to the energy equation within Fuego. It has been rigorously tested in validation exercises for liquid hydrocarbon pool fires, but has not been used to predict fireballs for launch accidents.

Models of convective and radiant heat fluxes are far better developed in Fuego/Syrinx than in SFM. Fuego can be used to provide a transient simulation of the fireball evolution, and it can provide the variation of the thermochemical state with location within the fireball—for example greater oxygen partial pressures near the edge of the fireball associated with air entrainment that would occur simultaneously with lower temperatures associated with radiative heat losses.

Models of aerosol vaporization, condensation and agglomeration are being incorporated into Fuego/Syrinx as a part of separately funded and unrelated programs at SNL. Models of plutonium dioxide vaporization would have to be added to the code suite.

3.5.2.3 Recommendation for Fuel Fragments Exposed to the Combustion of Liquid Propellants

SFM is a well-established computer code for the prediction of the thermal source term from fireballs and it is recommended that SFM be used in future analyses for the MSL SAR. Refinements to the code can be made by comparisons to predictions of the Fuego/Syrinx code suite once this code suite has attained a useful level of development. Specific near-term tasks to improve the utility of SFM are:

- Provide a more comprehensive documentation of models and correlations used in SFM
- Provide documentation of the validation of SFM including comparisons of predictions with correlations used in the past
- Update thermochemical data bases used in SFM
- Introduce more mechanistic modeling of soot formation into the code
- Refine the modeling of dirt entrainment in SFM to account for new data

In the longer-term, activities to improve SFM are:

- Assess combustion rates using the more detailed Fuego code to guide SFM input parameter choices
- Compare spatial distributions of temperature and oxygen potentials in fireballs predicted with kinetic models such as Fuego with equilibrium predictions in SFM to see if revisions of the SFM modeling are warranted
- Compare air entrainment rates predicted with Fuego to those modeled by correlation in SFM to see if refinements of the correlation models are needed

3.5.3 Plutonium Dioxide Particles and Fueled Clads Exposed to Solid Propellant Combustion

In some accident sequences, bare particles of plutonium dioxide fuel as well as intact fueled clads can be dispersed in the vicinities of burning propellant on the ground. Fuel close enough to the burning propellant can be vaporized and then nucleate into fine aerosol particles. Another important process is the entrainment of small fuel fragments in the gas flow produced by the burning propellant. The thermal response of clad pellets will be only modestly delayed from that for bare fuel since the thin iridium cladding will heat quickly and may be liquefied by exothermic intermetallic reaction with aluminum metal droplets produced in the combustion process. These processes must be modeled in an integrated fashion to adequately predict the plutonium dioxide source term from fuel exposed to burning solid propellant on the ground.

3.5.3.1 Interface with the Launch Vehicle Databook

The Databook will prescribe the thermal environment imposed by accidents on the GPHS modules, GISs, fueled clads, and plutonium dioxide fuel fragments exposed to burning solid propellant. The environment description is based on results of experiments, especially one large experiment (Chang et al. 2002, Hunter et al. 2002). Results of the experiment have been used to develop a model of the combustion plume and radiant heat fluxes produced by the combustion. Particle fluxes have also been modeled based on the results of the experiments. Predictions of the model are used to prescribe temperatures at various distances from burning propellant fragments of various sizes. These temperatures are used as the boundary conditions for the predictions of the thermal responses of the plutonium dioxide.

The model that is the basis of the environmental specifications has been criticized. For example, the plume temperatures and emissivities should vary with the size of the propellant burning. It is likely that such variations will be more significant than now considered in the Databook. Also, particle deposition heat fluxes are not dependent on the orientations or temperatures of the surfaces where deposition is taking place. Higher fidelity modeling might overcome some of these criticisms.

3.5.3.2 Assessment of Candidate Codes

3.5.3.2.1 PEVACI

The PEVACI code (Haskin 2001) was developed specifically for the problem of burning solid propellant in contact with or close proximity to plutonium dioxide fuel fragments or fueled clads. The dispersal of plutonium dioxide occurs by the entrainment of smaller fuel fragments in the flow of gaseous products of propellant combustion and the vaporization of plutonium dioxide from fuel fragments too large to entrain in the gas flow. A broad range of phenomena contribute to the production of the source term under these circumstances, and PEVACI includes models for the following:

- Propellant combustion
- Heat transfer to fuel and substrate
- Vaporization, condensation, and agglomeration of plutonium dioxide
- Entrainment of gases and fuel particles below burning propellant
- Plume formation and chemistry
- Interactions between plutonium dioxide and aluminum oxide aerosols

Because a large number of calculations must be done to cover the range of propellant fragment sizes, plutonium dioxide fragment sizes and proximity, and other controlling parameters, it is essential that PEVACI run a complete case in a relatively short computational time. Therefore, as in the case of liquid propellant fire modeling, it is impractical to model gas flow with CFD methods. Simplifying assumptions are therefore made about the geometry of the combustion zone and the fuel. In particular, the burning propellant fragment is treated as a right circular cylinder and the combustion zone and condensation plume are divided into several distinct regions that are treated as control volumes. The geometrical configuration is based on a series of tests conducted by the Applied Physics Laboratory (Chang et al. 2002 and Hunter et al. 2002). As with SFM, a wide variety of input parameters are available to the user to explore their effects on the calculated source term.

PEVACI model captures the broad range of phenomena affecting the thermal source term, but there are a number of areas where improvement is needed and achievable. For example, the model for entrainment of fuel particles is based on classic studies of sand entrainment. Superior resuspension models are now available to account for continued exposure to gas flow. The entrainment modeling is applied only to positions relatively close to the burning propellant. At distances greater than two propellant fragment radii, the gas flow is assumed to be completely upward directed and incapable of entraining particulate. Vaporization is calculated with a simple univariant vapor pressure model that can no longer be considered consistent with available data on the vaporization of PuO_{2-x}. Mass transport of vapor from the fragment surface is modeled based on a plausible kinetic model that recognizes chemical and thermal diffusion across a boundary layer and the coupling to heat transfer across the same boundary layer. The PEVACI model rather simply models the nucleation of vapors and the co-agglomeration of these nuclei with aluminum oxide aerosol produced by the combustion. The agglomeration modeling for the short period between aerosol nucleation and quenching of the aerosol plume is based on the Smolochowski equation with an empirically modified interaction coefficient. This modeling has been questioned and needs to be better justified.

The PEVACI model was written before experiments had been done to well characterize the thermal environment bare fuel would suffer when exposed to the combustion of solid propellant fragments. PEVACI does not recognize the flux of particulate that will be produced by the combustion. This flux of particulate can occlude surfaces of larger fuel particles and interfere in the mass transport of vapor from the surfaces. Larger accumulations of molten aluminum oxide below and around the burning propellant can dissolve plutonium dioxide. Dissolution will substantially reduce the vapor pressure of the various plutonium dioxide vapor species. Dispersal of the molten aluminum oxide-plutonium dioxide mixture by the shear of gas flow can expand the surface area available for vaporization. All these limitations are areas for improvement in the version of PEVACI intended for the MSL mission SAR.

3.5.3.2.2 Fuego/Syrinx

The Fuego/Syrinx code suite holds the potential of providing a higher fidelity modeling of the thermal environment created by burning propellant (Domino 2005). The code suite has not been applied to the specific issues of interest here and is still under development. With focused development, it is possible that the Fuego/Syrinx code suite could be used to perform coupled analyses of both the environment produced by burning, solid propellant and the thermal source term of plutonium dioxide vapors. In particular, Fuego/Syrinx may be able to eventually predict better the flow fields around the propellant, gas temperatures and gas velocities. It may better estimate radiant heat fluxes and the effects of aluminum and aluminum oxide particles. It may be better able to predict the flow of these droplets and their impingement on fuel fragments. Substantial further development of the code would be needed to analyze the thermal source term.

3.5.3.3 Recommendation for Bare Fuel Exposed to Solid Propellant Fires

The PEVACI level of modeling appears suitable to interface with the prescription of the fire environment provided in the Databook. The PEVACI model needs to be updated. Specific improvements that are required include:

- Accounting for impingement and freezing of aluminum oxide on fuel particles
- Accounting for dissolution of plutonium dioxide in molten aluminum oxide
- Upgrading the vaporization model to better reflect current understanding of the bivariant vaporization
- Updating particle entrainment modeling especially at positions outside the perimeter of the burning propellant
- Better substantiation of the aerosol modeling
- Better documentation of the PEVACI models, their technical foundations and assessments of their validity

In the longer term, Fuego/Syrinx can be used to better describe the flow field around burning propellant and the mass transfer of vapor from the fuel surfaces exposed to combustion gases. Fuego/Syrinx may also be useful to better describe the thermal effects of impinging droplets of aluminum oxide on fuel particles.

3.5.4 GPHS Modules Exposed to Burning Solid Propellant

3.5.4.1 Overview

GPHS modules, damaged perhaps by accident events but still largely intact, can be heated by burning solid propellant to the point that plutonium dioxide fuel will vaporize to an appreciable extent. Helium within the fuel will also escape during this heating and the flow of helium will help drive plutonium dioxide vapors from the modules to contribute to the thermal source term. Calculational experience in the safety analyses for New Horizons shows that the vaporization of plutonium dioxide fuel from modules becomes most significant when temperatures are sufficient to liquefy the iridium cladding on the fuel. Once this cladding melts away (usually at the Ir-C eutectic temperature rather than at the melting point of iridium), the plutonium dioxide is exposed directly to the chemically reducing environment produced by graphite that makes up the structures of the GIS and modules. The vapor pressure of the PuO_{2-x} fuel increases with increasing deviation from the dioxide stoichiometry as well as with increasing temperature. This "threshold" behavior of the rate of plutonium dioxide vaporization places some premium on accurate prediction of the thermal response of modules in thermal environments where the ambient temperatures exceed the Ir-C eutectic.

Modeling of the contribution to the thermal source term made by fuel within modules and exposed to solid propellant combustion requires descriptions of:

- Thermal response of the module to the combustion environment,
- Bivariant vaporization of plutonium dioxide as it varies in stoichiometry,
- Helium release as a function of temperature and plutonium dioxide stoichiometry,
- Mass transport of vapors through pathways in the GIS and module,
- Nucleation of vapors that escape the module to form aerosols, and
- Agglomeration of these plutonium dioxide nuclei with aerosols in the ambient combustion environment

3.5.4.2 Interface with Launch Vehicle Databook

The Databook specifies the thermal environment to which modules are exposed at different distances from burning propellant fragments. The thermal environment is the result of convection and radiation from the burning propellant and the heat fluxes produced by the impingement of aluminum oxide droplets on the module. This thermal environment is used as input to the analysis of the thermal response of the module and the calculation of the fraction of plutonium dioxide fuel that is vaporized from the module. The input data on the environment is the same as that used for the analysis of the thermal response of fuel to burning propellant discussed in 3.5.3.1. Many of the problems associated with this input are the same as discussed there. The thermal effects associated with aluminum oxide droplets impinging on surfaces take on special importance in the analysis of module thermal response because of the above-mentioned "threshold" to extensive fuel vaporization associated with liquefaction of the iridium cladding. Experience from the New Horizons safety analysis is that the prescribed endothermic effects of droplet impingement can keep temperatures below that required to liquefy the clad.

The combustion process can heat modules to quite high temperatures. Once the modules have been heated and the combustion of propellant is completed, modules can continue to be heated by the natural convection of air to the graphite module surface where it reacts exothermically. This heat flux to the module is not addressed in the current Databook.

3.5.4.3 Assessment of Candidate Codes and Models

For the PNH FSAR, response of the GPHS, an individual GIS, or a bare fueled clad to the thermal environment of burning solid propellant was modeled primarily with a commercial thermal analysis network code, SINDA (Cullimore and Ring 2004). Although a detailed thermal model involving 1200 nodes was developed, the bulk of the calculations for the FSAR were done with a simplified model, sometimes called the "five volume model" (Lockheed Martin 2005, Vol. 2, Appendix I). While the nodalization was simple, this analysis also utilized a variety of user-supplied logic to capture the complex chemical, thermal, and flow processes that contribute to the thermal source term. The collection of these models will be called Valient for the MSL SAR program, and the combined tool SINDA/Valient.

The simple SINDA model has been benchmarked against a 3D finite element model of the thermal response of the module to the thermal environment. Valient is a lumped-node model that attempts to model the vaporization of fuel, helium release and the transport of gases and vapors from the module. The Valient model of helium release is based on models for fission gas release from reactor fuel and treats the diffusion of both atoms and micro-bubbles in fuel grains to grain boundaries. Saturation of these boundaries leads to helium release from the fuel pellet. Vapor pressures are based on a bivariant model of plutonium dioxide nonstoichiometry accounting for point defects and defect agglomerates. The chemical potential of oxygen is closely tracked in the model and includes effects of iridium vaporization observed in experiments. Mass transport through the GIS and module is considered to occur by forced flow, chemical diffusion, thermal diffusion and Knudsen diffusion. It can occur along threads in endcaps on the GIS and module, through the pore structure of the graphite bodies or through cracks and holes in these structures as determined by the blast, impact and shock analyses described earlier in this document. Vapor transport through the graphite structures depends on the permeabilities of these materials, which are not known well. The Valient model does not now handle the mass transport limitations associated with plutonium vaporization following liquefaction of the iridium cladding, nor does the model treat the nucleation of aerosol and the subsequent behavior of these nuclei in mechanistic detail.

A variety of alternatives exist for the SINDA model of thermal response to the combustion environment. A leading candidate for an alternative is CALORE (Erickson and Gill 2005). CALORE offers high-fidelity modeling of heat transfer in complex 3D structures and includes the required conduction, convection and radiation heat transfer capabilities. CALORE has been modified to account especially for the SNL heat transfer from deposited particles on the surface of a structure. It has undergone extensive verification and is an accepted code in the heat transfer community. CALORE can accept as input the environment specifications provided by the Databook or it can be coupled to a more mechanistic model of this environment such as the Fuego/Syrinx suite. Because of the high fidelity modeled by CALORE, it takes considerably more time to run a problem than Valient or SINDA. Thus it may be most appropriate for benchmarking or validating Valient or SINDA than for producing tabular values.

3.5.4.4 Recommendation for Modules Exposed to Burning Solid Propellant

It is recommended that the SINDA/Valient five volume model be used and upgraded for future analyses. Specific improvements to be made in the near term are:

- Incorporation of the kinetics of both gas phase attack on plutonium dioxide by graphite vapors and liquid phase attack on plutonium dioxide by Ir-C melts
- Modeling the post-combustion heating of the module by natural convection of air to the structure
- Modeling the nucleation and coagulation of vapors that escape the module
- Validation of the models especially the model of helium release from the fuel
- Comprehensive documentation of the Valient models that will provide the technical bases for the models and assess their validity.

In the longer term, replacement of the one-dimensional (1D) SINDA model of thermal response with the CALORE 3D model will allow assessment of natural convection effects on plutonium vapor transport.

3.6 Reentry

3.6.1 Phenomenological Modeling Considerations

Five modeling capabilities are required to adequately perform a reentry body survival evaluation and its probable impact location. They are body aerodynamics, dynamic motion, aerodynamic heating, material thermal response simulation, and impact probability modeling. The first two in this set combine to produce a reentry trajectory describing the time, altitude, and velocity history of an object as it passes through the atmosphere. The second pair work together to predict the physical response of the object to the flowfield environment encountered on its journey to impact. Information from the first four capabilities is used to determine the probable impact footprint.

Flowfield environment is a broad category that entails a number of quantities. Generally speaking, it is the characterization of the variables defining the environment around a flight vehicle. Characterization includes shock shape, inviscid flowfield, boundary layer, and vehicle surface parameters. The inviscid region is that part of the flowfield around a body that is not influenced by the viscous effects of the flow interaction with vehicle surface. Conversely, the boundary layer is the remaining portion of the flowfield that is influenced by the fluid friction viscous interaction with the body. The environment evaluation determines velocity, pressure, temperature, density, enthalpy, entropy, etc. distributions in the inviscid and viscous regions of the flowfield. In addition, it determines vehicle surface pressure and heating distributions. SNL uses a number of flowfield environment codes to evaluate the parameters of importance around a flight vehicle. These tools are of varying levels of model fidelity. Tool choice depends on the needs of the design and program. Four production tools are available for flowfield analysis. From simplest to most complex, they are HANDI (Potter 1996), BLUNTY (Hochrein 1969), SANDIAC/HIBLARG (Polansky 1990, Noack and Lopez 1988), and SACCARA (a derivative of PINCA (Wong 1995)). HANDI would be the appropriate choice for the number and level of heating analysis required for this program. The more complex tools would be used in a supporting role to verify the simpler approach in specific cases.

Following definition of the flowfield environment with one of the tools discussed above, a material thermal response solution is obtained using the flowfield variables as input. Material thermal response is the characterization of the material property variables of the components comprising the flight vehicle after exposure to the heat transfer rates determined in the flowfield evaluation. Material response variables of interest are ablation characteristics, surface temperature distribution, and in-depth temperature profiles. SNL uses a number of material thermal response codes to evaluate the parameters of importance to a flight vehicle. These tools are of varying levels of model fidelity. As in the flowfield evaluation, tool choice depends on the needs of the design and program. Three production tools are available for general in-depth thermal response analysis. From simplest to most complex, they are SODDIT (Blackwell et al. 1987), CMA (Blackwell and Kaestner 1970), and COYOTE (Gartling and Hogan 1994). CMA would be the choice as the primary analysis tool for this parametric evaluation.

The codes used for this purpose should be proven tools that have been examined for accuracy of their predictions and efficiency of their computational operation. SNL's tools carry that pedigree with many successful flight test designs. At the end of the reentry simulations, characterizations of the modules containing the fueled clads will be produced with the necessary certainty for the safety evaluation.

3.6.2 Interface with Launch Vehicle Databook

Reentry evaluations require initial velocity and flight path angle at a prescribed altitude to begin trajectory simulations. The Databook will provide this information in the form v-gamma maps for each category of accidental earth reentry. It will also provide the results of the analysis of whether the MMRTG impacts the Earth while still attached to other spaceccraft components, or the spacecraft breaks up and releases the MMRTG in the atmosphere. In the former case, location and velocity of the impacting structure will be specified in the Databook and the nuclear safety analysis will be accomplished by the methods described in Section 3.3.2. In the latter case, the Databook will specify the initial conditions of the MMRTG for the reentry analysis to be carried out for the SAR.

For the PNH Mission, the Databook utilized a breakup criterion based on a linear combination of integrated heatup and g-load to determine whether the MMRTG would break up before impacting the Earth. The FSAR for that mission used that criterion and an evaluation of event probabilities to determine that the only risk-significant reentry scenarios involved release of GPHS modules into the atmosphere. Heating analysis showed that the aeroshell of the GPHS module experienced little ablation during the remainder of the reentry trajectory, so the principal calculational requirement was to determine the distribution of impact locations for each accident scenario.

For the MSL mission, it is possible that other reentry outcomes will be important. Because the MMRTG is enclosed within the spacecraft and behind its heat shield, breakup of the spacecraft before earth impact may be less likely in some cases. For those cases in which the MMRTG remains attached to portions of the spacecraft until the time of earth impact, the Databook is expected to describe the conditions of the impact, and the analysis of plutonium dioxide releases due to impact will follow the approach described earlier in Section 3.3.2. On the other hand, if the MMRTG breaks free of the space vehicle, it is expected that the Databook will provide a breakup criterion governing the release of the GPHS modules similar to the one provided for PNH. The MMRTG design requirements (Rocketdyne 2003) specify that the free release of the GPHS modules shall not be inhibited by the MMRTG structures in the event of accidental reentry, so it is highly likely that if the MMRTG breaks free, the individual modules will be released. The subsequent analysis of the nuclear components will then be carried out with the tools described below.

3.6.3 Generic Considerations

All material property issues and geometry definitions must be specified for any variations of interest to the current mission.

3.6.4 Assessment of Candidate Codes

The procedure discussed in Section 3.6.1 has been accomplished in past SARs by the use of a convective stagnation point heating analysis incorporated in a trajectory code and with a 3D finite difference thermal response program. For Pluto New Horizons, trajectory and stagnation point heating analyses were performed with the Three Degree-of-Freedom Maneuvering Program. The trajectory analysis approach solves the standard three degree of freedom motion equations. Heating evaluations are the analytical/empirical approach of Lees (1956). This is contemporary and comparable to Faye and Riddell (1958).

We propose a very similar approach. However, our approach will differ from the previous efforts in some significant ways. First, the trajectory analysis will be independent of the heating analysis. This provides more flexibility to the procedure. Second, the heating analysis will examine the gas cap radiative heating issues that may be important for some of the higher reentry velocity cases. Third, the five analysis capabilities will be provided in a simple-to-execute driver program that can perform large parametric analyses over a broad design space efficiently and quickly. This tool would be a deliverable of the effort. It would be applicable to future missions by simple changes of input geometry, material properties, and reentry conditions.

All of the codes comprising this analysis suite are established standards at SNL and within the industry. They have a very long history of use for predictions of flight test and ground test experiments. They have also been used in past joint program efforts with NASA. Specific programs are listed in the discussion of the individual codes. Their ability to adequately predict the results of such tests has been thoroughly documented. The aerodynamics of the reentry shapes required would be taken from the industry standard reference book, Hoerner (1965) . Trajectory, impact probability, heating, and thermal response codes applied would be TAOS, PREDICT, HANDI, and CMA, respectively. Further information on these programs is provided below.

3.6.4.1 TAOS – Trajectory Analysis and Optimization Software

3.6.4.1.1 Typical Code Applications

TAOS is used to perform concept to launch 3-DOF and 6-DOF trajectory design and analysis for boosters, post-boost vehicles, maneuvering and ballistic reentry bodies and bombs. Multibody trajectory capability is available.

3.6.4.1.2 *Solution Approach Description*

TAOS offers many choices for earth models such as the WGS-84 datum. Gravitational terms through the second degree zonal harmonic are most often used although higher order terms may be chosen. Several choices of fixed step and variable step integrators are available to propagate the equations of motion.

TAOS is capable of using simple (e.g., drag only) to high fidelity aerodynamic models. For the MSL program, drag coefficients will be computed offline for several elementary shapes (e.g., flat rectangular plates, flat circular plates, spheres, cylinders). The drag coefficients will be computed at several total angle of attack values from 0 to 360 degrees and blended to provide an approximation of drag force for a random tumble/spin motion.

3.6.4.1.3 *Existing Validation and Verification*

Validation exists in the form of numerous successful flight test predictions. The code has been in use at SNL and in some sectors of the aerospace industry since the late-90s. Its precursors, which provided validation checks, were used for approximately 20 years.

3.6.4.1.4 *Planned Enhancements*

TAOS possesses all required physics and input/output options. No enhancements are needed for TAOS.

3.6.4.1.5 *Development Needs*

The current 6-DOF section of TAOS needs to be incorporated into the parametric analysis software suite.

3.6.4.2 PREDICT Impact Probability Code

3.6.4.2.1 *Typical Code Applications*

PREDICT (Young and Sturgis 2002) is used to perform range safety studies for SNL's launch systems. It incorporates statistical variation in several trajectory parameters (e.g., winds, ballistic coefficients, drag coefficients).

3.6.4.2.2 *Solution Approach Description*

Range safety analysis at SNL is accomplished using PREDICT, a code written at SNL that follows the Range Commanders Council (2002) 321-02 eight-step process shown below.

1. Define analysis scenarios
2. Compute pre-event conditions
3. Characterize event: breakup, destruct action, collision
4. Propagate debris
5. Develop debris statistics
6. Calculate impact probability for assets
7. Calculate expected fatalities
8. Assess overall risk

This process may be used in the MSL program to track debris through Earth's atmosphere to either an impact location on the ground or to a point in the trajectory where further breakup of the piece may occur. PREDICT does not currently include secondary breakup capability nor does it include aerothermal effects. Some of the work on the reentry section of the risk tool will involve calling the appropriate PREDICT routines from the driver code.

Most of the methodology used in PREDICT is appropriate for use in the MSL program. The identity of each piece of debris is tracked along with the piece's motion. Therefore, radioactive debris may be followed through its trajectory and identified on the ground or at any other point in its trajectory. Proximity to other pieces of interest, such as a piece of solid propellant fuel, may be determined at any point in the trajectory. Break up models from the mechanical designer of the systems may be incorporated.

Newton's second law is used to propagate the debris state vector. The gravity model includes terms through the second degree zonal harmonic. Atmosphere models are provided either by standard atmosphere information, test data for the location of the flight test and the time of year of the launch, the GRAM database, or day-of-launch weather balloon information at the launch site. The earth model is a rotating, ellipsoidal model with WGS-84 parameters.

3.6.4.2.3 Existing Validation and Verification

PREDICT has been used at SNL since the late 1990s and has been validated against RRAT, a code written by ACTA Inc. It has also been demonstrated on many flight tests.

3.6.4.2.4 Planned Enhancements

No physics is enhancements are needed for PREDICT.

3.6.4.2.5 Development Needs

Code development work is needed to incorporate PREDICT into the parametric analysis software suite.

3.6.4.3 HANDI – Heating Analysis Done Interactively

3.6.4.3.1 Typical Code Applications

HANDI is used for scoping parametric analyses of reentry bodies with simple geometries.

3.6.4.3.2 Solution Approach Description

The Heating Analysis Done Interactively program is a collection of analytical and empirical techniques (closed form and iterative) gathered into one code to solve a variety of common and not-so-common engineering problems. Its name, "HANDI", (a historical acronym relating to its original development purpose) is a play on words and somewhat of a misnomer since it provides considerably more than heat transfer solutions. HANDI's primary objective is to maximize efficiency and productivity by minimizing some of the more repetitive tasks required in many thermophysics analyses. Additionally, it is capable of approximations to problems which are otherwise unapproachable or prohibitive in time and expense by other methods. Its standard geometry convective heating options have their basis in the pioneering work done in the field by Faye, et al. (1958). Along with Lees (1956), it is the most invoked method in the industry. In fact, this approach was used by SNL in its Aerospace Nuclear Safety (ANS) program in the sixties. This work supported the launch of this nation's only nuclear reactor in space. HANDI's convective heating capabilities are a derivative of this approach. The standard geometry convective section of the code provides scoping study solutions for spheres, cylinders, fins, flaps, flat plates, antennas, concave surfaces, and reentry vehicle base geometries.

3.6.4.3.3 Existing Validation and Verification

Validation exists in the form of numerous successful flight test predictions. The code is mature and has been in use at SNL for approximately 15 years. In addition, SNL heating analysis tools have been used in joint programs with NASA in the past. Three prominent examples are the

Columbia demise investigation, Mars Sample Return Earth Entry Vehicle, and the Mars Pathfinder Mission.

3.6.4.3.4 Planned Enhancements

HANDI contains heat transfer theory comparable to the tools used for previous launch safety analyses. No aerodynamic heating software enhancements are required.

3.6.4.3.5 Development Needs

Existing heat transfer theories in HANDI are sufficient to describe the accidental reentry scenarios for MSL. However, to efficiently evaluate the parametric map sufficient for a reasonable safety analysis, HANDI needs to be incorporated into the parametric aerothermal analysis software suite.

3.6.4.4 CMA – Charring Material Ablation Program

3.6.4.4.1 Typical Code Applications

CMA is used for reentry body thermal response evaluations. These evaluations can be performed for a number of vehicle geometries. It has been used on geometries as simple as spheres and as complex as the space shuttle. The fundamental requirement for application is that temperature gradients in directions transverse to the surface normal be small in comparison to the in-depth direction. Analyses have been completed for ascent and reentry scenarios.

3.6.4.4.2 Solution Approach Description

The Charring Material Ablation (CMA) code (Lauger et al. 1973) is a 3D, implicit, finite difference, transient heat conduction thermal response code which allows for ablation at one surface and in-depth material decomposition. Although, the code is inherently 3D, it may be applied to a large class of 2D and 3D problems where transverse temperature gradients produce negligible heat transfer in off-axis directions relative to the surface normal axis energy transfer rates. This includes the class of problems containing reentry vehicles. It has been in use at SNL from its earliest form since 1966. The code currently used is a heavily modified descendant of the original version of CMA3. The code was originally written by Aerotherm of California with one of the later releases being CMA90S. Fundamental physics solved by the program have not changed since the 60's. As such, SNL has opted to continue modifying its version of CMA to suit particular requirements of our customers.

CMA provides the thermal response solution for general convective and radiative boundary condition problems. Surface phenomena are determined by a surface energy balance which employs convective film coefficients for heat and mass transfer. The actual computation of the surface energy balance involves considerations of thermochemistry. Surface thermochemical reactions are complex and an iterative procedure is required to complete their solution. In theory, the chemistry calculations could be done internal to CMA. However, it is more computationally expedient for these reactions to be evaluated externally and the results input in tabular form for CMA to access in an interpolative fashion. A thermochemistry program, ACE (Powers, 1969) produces the required input. This is the connective juncture between the heating and thermal response evaluations that requires the JANAF database reference (Dow Chemical Company).

To this point the thermal response discussion has focused on the surface phenomena. Given the complicated nature of the in-depth decomposition process and its impact on boundary layer constituents and thus plasma interaction parameters, a detailed discussion of this facet of thermal response is included. Decomposition related parameters of specific interest to the CMA thermal response program are ablator resin fraction, pyrolysis gas enthalpy, and Arrhenius decomposition rate equation constants for the material's constituents. In CMA terminology, the ablator in its original state is referred to as virgin plastic. The resin fraction of the virgin plastic is the constituent proportion of the ablator comprised of phenolic, epoxy, etc. Pyrolysis gas enthalpy represents the energy content of the gases being expelled from the material as a result of the in-depth decomposition reactions occurring in the complex ablator. They are a function of temperature and the specific binder molecular formulation being decomposed. Usually, the gas enthalpies are determined by separate runs of a chemical equilibrium program (ACE in our case) knowing the elemental mass fractions of the decomposing binder.

The most complex and difficult to define CMA material properties are the constants used in the Arrhenius reaction rate equations. In general terms, a virgin plastic ablator may be modeled as three decomposable constituents with the composite material density given by Equation 1,

$$\rho = \Gamma(\rho_A + \rho_B) + (1 - \Gamma)\rho_C \tag{1}$$

where gamma is the resin volume fraction discussed previously. The constituents are two resin components (A & B) and a single reinforcement component (C). An example of the reinforcement component would be the carbon fiber cloth in a carbon phenolic ablator. Division of the resin into two parts is the result of the experimental observation of a two stage decomposition process of phenolic resin. Decomposition rates of the three organic constituents are modeled in terms of kinetic equations of the Arrhenius form shown in Equation 2.

$$\frac{\partial\rho}{\partial\theta} = -k_i e^{-E_i/(RT)} \rho_o \left(\frac{\rho_i - \rho_{r_i}}{\rho_{o_i}} \right)^{m_i} \qquad \mathrm{i = A,\ B,\ \&\ C} \tag{2}$$

The time variable in this formulation is θ. Constants k_i, E_i/R, and m_i are the pre-exponential factor, activation energy factor, and density factor exponent, respectively, using CMA terminology. The density exponent is better known in the literature as the reaction order. Subscripts *o*, *r*, and *i* refer to the original value, char residual value, and the *i-th* component, respectively. The constants used in the above equation are determined experimentally by thermo-gravimetric analysis and differential thermal analysis. Essentially, the constants are curve fit coefficients derived from experimental results to fit the decomposition behavior of a complex ablator test sample. Normally, a sample of the composite material is subjected to a known heating environment while its weight change behavior is monitored during the process.

3.6.4.4.3 Existing Validation and Verification

Validation exists in the form of numerous successful flight test predictions. The code is mature and has been in use at SNL for approximately 40 years.

3.6.4.4.4 Planned Enhancements

CMA contains all of the necessary theory and options to perform the required material thermal response analyses. No enhancements in capability are required.

3.6.4.4.5 Development Needs

Currently, CMA is a part of the Large Analysis Parametric Software (LAPS) program. However, some development will be needed to couple HANDI solutions to CMA in an automated fashion.

3.6.4.5 Recommendations

Through the course of the discussion in the reentry section, a set of tools were defined to perform the reentry evaluations starting with an ejected RTG or other sub-components of that unit. The recommended approach for the components for which we would have responsibility is summarized here. We recommend the use of TAOS elements to evaluate reentry object trajectories, PREDICT for impact location and velocity probabilities, HANDI for flow environment and aeroheating evaluations, and CMA for material thermal response studies. No code enhancements are needed for these tools to evaluate the required physics of reentry. We further recommend that these tools be fully incorporated into an executive program to reduce the burden of the numerous parametric analyses needed to perform the required safety analysis evaluations. Development work to incorporate the recommended tools for this project would result in a highly efficient RTG reentry analysis system.

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4. Methodology Assessment for Level B: Event Sequences

As explained in the overview in Sections 1.3, the purpose of the SAR is to characterize the nuclear safety aspects and risk associated with the use of the MMRTG on the MSL mission. One way of portraying risk is with a CCDF for various launch accident consequences. One example is a plot with health effects (number of cancer deaths during the 50 years after the accident) on the horizontal axis and probability of exceeding that value on the vertical axis. This single CCDF is a display of one measure of risk for the launch and it incorporates the effects of many variable initial conditions, such as the particular type of accident, time after launch of the accident, wind direction, etc. We chose not to call the effects of these variable factors "uncertainty." Rather, we reserve the term "uncertainty" for the effects of imprecise modeling. The "uncertainty analysis" is performed after the generation of the best-estimate CCDF and is typically portrayed as a high CCDF and a low CCDF at the 5% and 95% confidence levels. The uncertainty analysis will be addressed in Section 7.

In order to determine the best-estimate CCDF, the various accident sequences must be followed along with their respective probabilities until a source term is generated. The methodology for this "Probabilistic Event Sequence Analysis" (PESA) is what is discussed in this chapter. This PESA does not result in a risk or a CCDF; rather, its output must be folded into the consequence analyses to obtain the risk or CCDF. The consequence analysis will be discussed in Section 5.

Risk analysis involves:

- Identification of potential hazards associated with both normal and abnormal operations.
- Characterization of design and operational features which preclude, minimize or mitigate the hazards.
- Evaluation of the risk associated with system operation from pre-launch through orbital escape.
- Many different types of analyses (e.g., probabilistic risk analysis, severe accident analysis, system reliability analysis, human factor safety analysis).

The level of analysis must be commensurate with the:

- Magnitude of the hazards being addressed,
- Complexity of the system begin relied on to maintain an acceptable level of risk, and
- Phases of the system life for which approval is being sought.

Risk analyses can be extremely involved and characterization of the various event sequences can be very time consuming and costly. Therefore a graded approach is typically taken. This graded approach is well accepted by NASA, DOE, the Nuclear Regulatory Commission (NRC), etc., and assures that at level of analysis is commensurate with the likelihood and consequences of an event (see Figure 9). Risk analysis simultaneously addresses the likelihood of an event and the consequences of the event. Typically, characterizing the likelihood or probability of an event is accomplished using only loose coupling with analyses of the consequences.

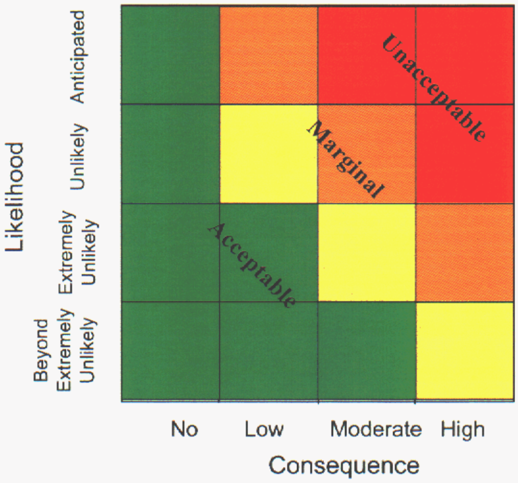

Figure 9. Graded Approach to Risk Analysis

Typically, NASA's Jet Propulsion Laboratory (JPL) provides a set of accident scenarios and environments in the Databook. Each scenario consists of a technical description of how the launch vehicle fails and a statistical distribution characterizing the conditional probability of the failure scenario given an attempted launch event. PESA algorithms are then applied to determine the conditional probability that each scenario will result in a release of radioactive material to the environment and the characteristics of the release, should one occur (altitude, mass, particle size distribution, etc.). The consequence analysis software is then applied to determine the consequences (especially health effects) that would be expected to occur in the affected population as a result of such a radiological release. The information contained in the Databook is assumed to be fixed as input and is not subject to revision during the risk evaluation.

The above risk analysis is conducted for each phase of the launch and then summarized for the entire mission.

4.1 Review of Probabilistic Event Sequence Analysis Approaches

The objective of the PESA software is to relate the accident initiating events identified in the Databook to the probability of a release event, the quantity and size distribution of the radio nuclides relinquished in a release event and the thermal environment at the time of the event. Together, these elements are characterized using probabilistic analysis. These results are then passed to the consequence analyses.

Historically, a number of approaches have been used to characterize the accident sequence probability distribution. These methods have ranged from analytical methods to full Monte Carlo (MC) simulations. As noted previously, each initiating event in the Databook results in a (potentially) large number of accident scenarios. To fully characterize each scenario, a number of computationally intensive computer codes must be exercised.

To fully characterize the event sequence probabilities, a fully integrated package of models is required involving the physics of each scenario which would be exercised for random combinations of flight conditions, time of the in-flight failure event, thermal environment that result from each event, impact conditions, etc. Hundreds of thousands of simulations would have to be investigated to adequately characterize these scenarios. Clearly, this would be computationally difficult for even the supercomputers that currently exist now or that might be developed in the foreseeable future.

Historically, a number of alternative approaches have been investigated to make the computational issues more tractable. These investigations can be classified into two broad families of event sequence analysis methods: analytical and simulation methods.

Deterministic methods are appealing since they require significantly fewer computer simulations to adequately describe the underlying probability density functions. These methods were used for some of the early event sequence analyses on such programs as the Ulysses mission FSAR. These methods have difficulty with non-linearities in the physical models and situations where random variables have significant statistical correlation.

Alternatively, there is the class of simulation-based methods; these methods have been the foundation of most event sequence analyses since Ulysses. At one end of the spectrum of simulation methods is a full MC simulation. Using a raw MC approach would require tens of thousands of computationally intensive physical simulations.

To reduce the computational cost of each simulation, approximations to the physical simulations are often employed. These approximations are typically constructed over the important regions of the physical space to be investigated. Two problems with these approximations arise. First, identifying important regions early can be difficult, and second, the approach to constructing these approximations is susceptible to error.

In addition to reducing the time for each simulation, it is possible to reduce the number of simulations required. Alternative methods for exploring the physical space (real or approximate) continue to be investigated. When using raw MC methods to characterize the likelihood of rare events, an extremely large number of computer simulations are required to assure that samples are taken that capture these rare events. To reduce the number of simulations needed various methods have been proposed, but the most common method is a variation of the Latin hypercube sampling approach (LHS).

In the most basic form, LHS is an algorithm that forces samples to be taken in the tails of the probability distributions rather than waiting for a very unlikely random generation of a sample in the rare event space. In the LHS approach, it is necessary that the number of simulations be chosen somewhat arbitrarily prior to the start of the analysis. However, even with this restriction, a significant reduction in the number of simulations results; often as much as a few orders of magnitude. The combination of physical space approximation and LHS has formed the core of both the Cassini and PNH risk analyses.

For the purpose of developing an analysis approach, SNL has had the benefit of studying two different recently developed PESA methodologies. The first involved the use of the LASEP program by Lockheed Martin, culminating in the PNH FSAR. The second methodology, which appears to have benefited greatly from the PNH work, was produced by Rocketdyne (formerly Boeing). At the present time, it has not, however, been fully implemented nor applied to a specific RTG launch mission. Since SNL's approach will draw from both methodologies it is useful to begin by summarizing the key features of each.

4.2 Lockheed Martin Analysis Approach

For the Cassini and PNH event sequence analyses, the LASEP program developed by Lockheed Martin was used. (For Cassini, SNL performed the PESA analysis using the LASEP software, while for PNH the analysis was performed by Lockheed Martin using an updated version of the LASEP software.)

The basic calculational sequence is:

1. Selection of AIC and time, t_{AIC}. The cumulative probability distributions (CDFs) for AICs are provided by NASA/JPL in the Databook. An altitude and velocity of the launch vehicle after the AIC is determined probabilistically.
2. Flight of the vehicle to the AOC at time t_{AOC}, for example:
    a) In-flight explosion
    b) In-flight fragment field
    c) In-flight fireball

   The time of AOC, along with the attitude, position and velocity of the vehicle are simulated with consideration of the meteorological conditions at launch. Meteorological conditions are sampled from a database of conditions possible at the launch pad.
3. Post-AOC reentry of MMRTG (intact or broken into parts)
4. Impact of post-AOC MMRTG or parts on the ground with the environment being some combination of:
    a) impact
    b) explosion
    c) fragment
    d) fireball or solid propellant fire

At each stage of the accident scenario, the physical state of the system is reviewed. For example, in the event of a ground impact a table of fueled clad response to the structural impact is sampled and a probability of release is developed (along with the particle size distribution of released material). In the case of a physical impact, the lookup table might be generated as a result of hundreds of deterministic computer runs of the structural response model. Each deterministic run may take hours or days on a supercomputer and characterization of the lookup table may take several hundred computer runs. In case of an in-flight fireball, characteristics of the fireball would also be estimated based on external physics models and various thermal parameters would be exchanged with the consequence model.

4.3 Rocketdyne Analysis Approach

A common approach for complex event sequence analyses is to have a computer simulation embedded within another computer simulation. In this method, the variables are divided (with some forethought) into two groups often referred to as inner and outer variables. A sample vector of values from the outer group variables is chosen at random. Using these samples as nominal values for the set of outer variables, a simulation is conducted over the sample space of inner variables. Once these simulations are complete, a new sample of outer variables is chosen and used as input to the simulation of the inner variables. Figure 10 illustrates the concept. This inner/outer simulation process continues until the required number of samples is taken. This approach is similar to that used in design-of-experiments analyses. In fact, design-of-experiment analyses are often used to initially identify the important regions on which to focus more complex analyses.

Using this approach requires a different structure than is presently in the LASEP code. The other drawback to the inner/outer approach is that it can lead to excessive computer simulations if the algorithm is not carefully established at the beginning of the analysis.

The inner/outer approach to event sequence analysis is the basis for the Rocketdyne approach proposed for the MSL risk analysis. The Rocketdyne approach to characterizing probabilistic event sequences is a fairly traditional one. It shares some characteristics with the Lockheed Martin approach in that the complex physics models are exercised off line and only approximations are used within the analysis.

In developing their approach and software, Rocketdyne effectively started from scratch. The result has both good and bad points. In general, Rocketdyne took advantage of the lessons learned by Lockheed Martin and the software appears to be better organized and better integrated than the Lockheed Martin LASEP software. The code is written heavily in C and Java, making the code more portable and more easily modified for future efforts. On the other hand, the Lockheed Martin code evolved in spurts and jumps as situations arose. (These conclusions are based on presentations made by each group and not through actual application of the software.) The event sequence analysis approach within the Rocketdyne effort seems be a very basic approach and is, therefore, very tractable.

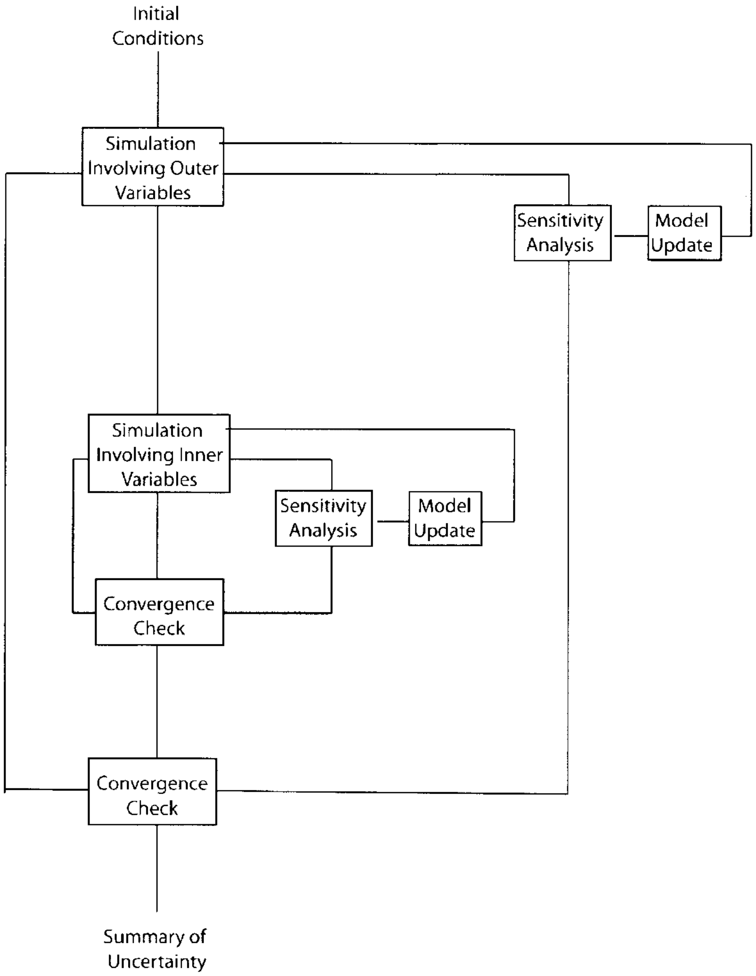

Figure 10. Proposed Approach for Probabilistic Event Sequence Analysis

The direction and intent of the Rocketdyne software seems to be clear. However, the software appears to be a work in progress. There are also some serious problems with the internal sampling algorithms. As noted previously, the Rocketdyne software uses an inner/outer loop approach to sequence probability quantification, making the approach very simple and tractable. The general idea is the each inner/outer simulation loop is exercised until some stopping criterion is met (e.g., the statistical sampling error drops below a specified level). This is a good idea, but care must be taken since this approach can run into difficulty with various methods of simulation. Unfortunately, the Rocketdyne approach employs a very traditional (raw) MC simulation method in both the inner and outer loops. The result is that rare events (including those with high consequences) that are associated with the tails of the variable probability distributions will likely not be included in the uncertainty analysis. There are some issues with how the sequences in the outer and inner simulation models are combined.

4.4 Proposed Sampling Methodology

The current approach for event sequence analysis within the LASEP program is based on a methodology developed at SNL to support the safety analysis of the Cassini Mission (Wyss 2002). In addition to the Cassini analysis, the approach was eventually embedded within the

LASEP software. The methodology depends heavily on the use of LHS-type methods. There are some opportunities for improvement. These will be implemented as schedule permits. Some of these are discussed below.

A few years ago researchers at SNL began investigating alternatives to the pseudo-random sampling technique that forms the foundation of classical MC reliability analysis methods (Robinson and Atcitty 1999, Robinson 2001). These deterministic versions of MC analysis have come to be known as quasi-Monte Carlo methods. As noted by Niederreiter (1978), these methods hold distinct advantages over pseudo-Monte Carlo in particular by being more effective and having a faster rate of convergence. Pseudo-Monte Carlo methods are generally assumed to have been developed around 1949 (Metropolis and Ulam 1949) and have since been an integral tool for reliability engineers. The interest is in statistically characterizing the response of a system, y, as a function various random parameters: $f(\mathbf{x})$. For problems involving a large number of random variables, the most viable solution approach is one based on random sampling. An essential building block to all MC methods is the generation of a sequence of uniform random deviates on the interval [0,1]. Since this sequence is not truly random, having been generated via a set of rules (e.g., classical linear congruential generators), it is often referred to as a 'pseudo-random' sequence. This sequence is then transformed into a sequence of random deviates from the requisite density functions. This sequence is then employed by any of a host of sampling techniques in structural reliability including stratified sampling (e.g., LHS) or adaptive sampling (e.g., radial importance sampling).

The difficulty with LHS-type methods is that the number of samples needed to characterize the event sequence probabilities must be chosen *a priori*. If additional sampling is required, the original samples must be discarded and a new set of samples generated; if new samples are simply added, the statistical characteristics of the observations is lost. Alternatively, the number of samples chosen as the basis for the LHS-type might be excessive in developing the event sequence probability distribution. Ideally, since the computational cost for each sample can be large, it is desired to have the minimum number of samples needed to be confident in the statistical characterization of the system response. Quasi-Monte Carlo methods provide the capability to successively add additional system simulations while maintaining statistical validity of the results.

An important point to appreciate is that the ability to start/stop the sampling process provides the opportunity to update the approximations to the structural analysis, thermal, and reentry codes embedded within the event sequence software. For example, new approximations might be developed as new regions in the analysis space are identified as being important in the accident response analysis.

As with the Rocketdyne approach, the variables are divided into two categories; no explicit intent is made to suggest there is anything unique about each group. (There is the possibility of some computational benefit to the categorization.)

4.5 Recommendations

The recommended approach for the probabilistic event sequence analysis is to start with the LASEP code that was used in the previous several launch approval processes and modify it as schedule permits. The code will draw upon external tabular models generated by the accident progression codes (Level A) described in the previous section and on simplified internal models of some of the accident phenomena where appropriate.

One of the goals for the development of this software is to move towards a more generic and flexible tool. The intent is that eventually we will have a code that is not designed specifically for one RTG launch mission, but which can be applied to future missions as well, with far less re-coding (and the attendant quality assurance (QA) burden) for specific future mission features.

4.6 References for Section 4

Metropolis, N., S. M. Ulam, 1949. "The Monte Carlo Method," *Jour. Amer. Statist.* Assoc. Vol. 44, p. 335–341.

Niederreiter, H., 1978. "Quasi-Monte Carlo Methods and Pseudo-Random Numbers," *Bull. Amer. Math. Soc.*, Vol. 84, No. 6, p. 957–1041.

Robinson, D., C. Atcitty, 1999. "Comparison of Quasi- and Pseudo-Monte Carlo Sampling for Reliability and Uncertainty Analysis," AIAA Structural Dynamics and Material Conference, St. Louis, MO, April 1999 (AIAA-99-1589).

Robinson, D., 2001. "An Iterative Monte Carlo Method for Efficient Structural Reliability and Uncertainty Analysis," 8th International Conference on Structural Safety and Reliability (ICOSSAR), Newport Beach, CA, June 2001, (SAND2001-0301C).

Wyss, G., 2002. "Uncertainty Analysis for the Cassini Space Mission," 6th International Conference on Probabilistic Safety Assessment and Management, San Juan, Puerto Rico, June, 2002 (SAND2002-2135).

5. Methodology Assessment for Level C: Atmospheric Transport and Consequences

Once the PESA software has determined the probabilities of producing radiological source terms of various quantities and size distributions, an Atmospheric Transport and Consequence Analyses (ATCA) must be performed to determine the various consequences for each of these source terms (such as latent cancer fatalities, i.e., health effects, due to exposures over a 50 year period, amount of land contaminated above specified levels, etc.) The overall probability times consequence is risk and is typically portrayed as CCDFs. This section describes and compares the codes available for ATCA.

5.1 Important Phenomena

SARs created for recent and upcoming launches involving radioactive materials (e.g., Cassini and PNH) have been based on detailed statistical sampling for each accident scenario. This is done to quantify the impact of variations in accident sequences and meteorological conditions at the time of launch. Small variations in the timing of the accident (number of seconds into the launch sequence), distribution of shrapnel caused by an explosion, or intensity of fire in the vicinity of all or part of an MMRTG can lead to very different consequences. Likewise, variations in wind directions at the time of launch can lead to very different consequences, depending on wind direction, the existence of sea breezes, atmospheric stability, etc. Since none of these things can be predicted in advance, the best way to quantify these uncertainties is to perform a probabilistic assessment to quantify the effect of the uncertain input parameters on the predicted consequences.

Because of the need to perform a probabilistic assessment of consequences, a large number of consequence analyses are needed for each AOC. For example, in its preparation of the PNH FSAR, Lockheed Martin performed about 900 consequence analyses per AOC. This translates into roughly 10^4 consequence calculations to support a typical FSAR. Moreover, this large set of calculations often needs to be repeated several times to incorporate more accurate information and to respond to questions and criticisms from INSRP and other reviewers. Thus, there is an obvious limitation on the central processing unit (CPU) time needed to perform each of the consequence calculations if this large set of calculations is to be performed in a reasonable time. This restriction eliminates the more state-of-the-art codes that are primarily intended for real-time analysis.

The Florida peninsula presents somewhat unique challenges in terms of meteorological data. The peninsula is narrow enough that it is common to have meteorological conditions that are influenced by sea breezes both on the Gulf and Atlantic sides. Because of the location of Kennedy Space Center (KSC) near the Atlantic side of the state, sea breezes from that side can be particularly influential. Neglecting sea breezes could lead to gross over- or underestimates of consequences. Thus, a consequence tool used for launches from KSC should be able to handle the complex, 3D wind fields that are common in that area.

Releases from a hypothetical accident involving a space vehicle carrying nuclear material could occur anywhere from the ground surface to the upper atmosphere. Because of this, the suite of tools needed to perform consequence analysis for a space launch must be able to cover this range.

Most of the consequence tools that have been developed are intended to analyze releases within the earth's planetary boundary layer (PBL), which extends from the surface to several km above the surface. Accidents that occur within this portion of the earth's atmosphere carry the greatest consequences and tend to dominate the overall risk from a space mission. Most of the discussion in this chapter focuses on consequence tools for releases within the PBL.

Releases above the PBL must also be analyzed and included in the SAR for completeness. The consequences from these releases tend to be global in scope and exposures occur over months or years. The dose to any individual is extremely small; however, the number of people that receive a dose is very large. The quantitative impact on risk metrics from such releases is, therefore, highly sensitive to the dose response curve for very small doses. In particular, a *de minimis* value of 1 mrem (below which health effects are assumed to be not discernable) tends to eliminate the predicted consequences from upper atmospheric releases.

5.2 Assessment Criteria

The following three major requirements will be used to evaluate each candidate code for its applicability to the consequence analyses of space vehicles:

- It should be capable of treating the relevant wind fields with enough fidelity to capture the significant features at KSC.
- It should be able to calculate consequences in a few days (CPU time) for a single AOC and within a month for the complete set of accident sequences for a space mission.
- It should be capable (possibly with relatively minor modification) of producing the types of consequence results that have been reported in previous SARs.

Additional desired features of consequence codes to be used in spacecraft SARs are:

- Users' documentation that sufficiently describes the models and input parameters
- An established track record, widespread usage, and/or verification and validation documentation to provide confidence that the code works correctly and is reliable
- Ability to integrate well within a larger framework to evaluate overall risks and uncertainties

5.3 Assessment of Candidate Codes

There are a large number of consequence codes that could be used to perform analyses of upcoming space missions involving nuclear materials. Three candidates are discussed below that represent the types of codes that are available. Other codes that could have been included in this section are similar to the ones discussed below and do not offer significant advantages. The three codes are listed in order of increasing fidelity.

The first code is MACCS2, which is simple in some regards and complex in others. WinMACCS is a user interface for MACCS2 that provides flexibility and functionality to the standard MACCS2 tool. In the following discussion, the name MACCS2 should be taken to include both MACCS2 and the WinMACCS interface. MACCS2 can be used for relatively large distance consequence analyses, but does not have capabilities (or other companion codes) for performing consequence analyses on a global scale or for high-altitude releases.

The second set of codes is the SPARRC suite, which includes SATRAP, GEOTRAP, and HIAD. This code suite was designed expressly for analyses of missions at KSC. It was used in support of the Cassini Mission and was used to support the Pluto New Horizons (PNH) Mission. Thus, it is a proven commodity for the type of application considered here. It is currently an in-house tool at Lockheed Martin, and has been transmitted to SNL.

The NARAC code suite is undoubtedly the most sophisticated and highest fidelity of those discussed here. These codes are primarily intended for real-time accident management applications in which high fidelity is required.

The three codes (or code suites) are described further in the following subsections. For a relatively short but useful overview of MACCS2, NARAC, the several other codes, see the Health Physics Society web page (http://hps.org/publicinformation/ate/q364.html).

5.3.1 MACCS2

5.3.1.1 Typical Applications

MACCS2 is primarily intended to support PRAs for the NRC and documented safety analyses for the DOE. Because it is intended to be used for PRAs, it is capable of sampling both meteorological and other input data (e.g., variations in source term induced by variations in the details of the accident sequence). It is also very fast running.

Generally, the weather sampling capabilities are used for both NRC and DOE applications; although, the NRC is usually interested in means over sampled weather, and the DOE is usually interested in 95th-percentile results.

5.3.1.2 Solution Approach

MACCS2 uses a very simple wind-field approximation, a uniform wind field corresponding to a single weather station at a single elevation (usually 10 m above ground level). Hourly meteorological data are required and provide temporal variations for a plume.

The MACCS2 dispersion model is based on the Gaussian plume approximation, which accounts separately for crosswind and vertical dispersion as a function of time or distance. A Gaussian plume always travels in a straight line; thus, temporal variations in wind direction are not treated.

MACCS2 calculates a large set of consequence measures and is currently capable of producing most of the results that have been included in previous FSARs. Some minor modifications to the code might be required to extend output capabilities.

5.3.1.3 Code Maturity and Documentation

MACCS2 is undoubtedly the most widely used consequence code in the U.S. and arguably in the world. It is used extensively for NRC PRAs, has been used to perform cost-benefit analyses, and was used in a siting study. It is used even more widely within the DOE community for documented safety analyses, including EISs and authorization basis documents, and is included in the DOE toolbox of safety analysis codes. It is also used in approximately 20 other countries. An early version (1.5) was subjected by the NRC to a meticulous line-by-line QA and verification process (Dobbe et al. 1990). The code was originally released in 1998 and has been used extensively since that date. Thus, MACCS2 is a very mature code.

The MACCS2 code is accompanied by a set of documents (Chanin et al. 1998, Jow et al. 1990) that describe the underlying models, input parameters, and other details for using the code.

There are several documents that provide verification of the code. The first documented verification was performed at the University of New Mexico. Unfortunately, this document was never published; it exists only in draft form. A second document (Molenkamp et al. 2004) compares MACCS2 dispersion and deposition results with two other codes: ADAPT/LODI from the NARAC suite and RASCAL, the

NRC's emergency management code. Finally, SNL maintains a software QA file that satisfies NRC requirements for configuration control, acceptance testing, regression testing, etc.

5.3.1.4 Planned Enhancements

There is one planned enhancement (NRC funded) that could potentially benefit this program. This is the addition of a nighttime mixing height in the treatment of dispersion. MACCS2 currently uses a single mixing height for each season of the year, which can lead to low estimates of concentrations at ground level.

5.3.1.5 Additional Development Needed for the MSL Analysis

If MACCS2 were used to support the MSL mission, some minor additional output enhancements would be required. However, MACCS2 could not easily be upgraded to include a higher fidelity model of dispersion in a 3D wind field.

5.3.2 SPARRC Code Suite

5.3.2.1 Typical Applications

The SPARRC code suite, including SATRAP, GEOTRAP, and HIAD, was specifically developed to be used for safety analyses of space launches involving nuclear materials. This code suite was used in support of the Cassini Mission and is currently being used in support of the PNH Mission. It requires considerably more CPU time to run than MACCS2, but it runs sufficiently quickly for SAR applications.

5.3.2.2 Solution Approach

SATRAP uses multi-weather-station, multi-elevation wind data to create a quasi-3D wind field. Interpolation between meteorological stations is done on either an inverse distance or distance squared basis—usually the latter. Currently, wind vectors do not include a vertical velocity component. Thus, they are less than fully 3D.

SATRAP is able to take advantage of the quasi-3D wind field with its Gaussian puff model. The Gaussian puff model approximates a plume as a set of overlapping puffs that are each represented by a central point and three dispersion values that represent the size of the puff in each dimension. Usually, dispersion is treated identically in the crosswind and downwind dimensions but differently in the vertical dimension to account for the level of thermal stability in the PBL. Thus, each puff has the shape of an ellipsoid where the axis of revolution is vertical.

SATRAP generally approximates the release from a hypothetical accident as instantaneous, so only a single puff is needed for each particle size bin and each release location. These puffs are then followed through the quasi-3D wind field to determine exposures to human receptors and to calculate ground contamination levels. The Gaussian puff model moves the entire puff at the wind velocity at central point plus a downward velocity to account for gravitational settling. This treatment is simpler than the particle tracking method used in the NARAC codes, which follows a large set of individual particles.

GEOTRAP is used similarly to SATRAP, but for cases where dispersion is larger scale. GEOTRAP uses a lower resolution wind field, but on a global scale to calculate doses over long distances.

HIAD is used for very high-altitude releases. It uses a simple compartment approach to model particle residence times within layers of the atmosphere. It accounts for the latitude dependence of exposures from releases at specified elevations and latitudes.

Because the SPARRC code suite was developed specifically for safety analyses of space missions, it reports all of the consequences that are typically needed in a SAR.

5.3.2.3 Code Maturity and Documentation

The SPARRC code suite is significantly less mature than the MACCS2 code. However, it does have the advantage that it will soon have been through at least two complete FSAR cycles, including review and comment by INSRP. Most of the documentation for the SPARRC code suite is contained in the FSARs for which it has been used. The lack of complete user documentation will present a challenge for future use of the code and will necessitate significant interactions with the code developers.

5.3.2.4 Planned Enhancements

There are no planned enhancements that would benefit this program.

5.3.2.5 Additional Development Needed for the MSL Analysis

Previous applications of the SPARRC code suite used quasi-3D wind fields as the basis for atmospheric transport and dispersion, as described above. However, high elevation 3D wind-field data are available from the Cape Canaveral Air Force Station (CCAFS) and should be used in future SARs. Converting to fully 3D wind fields will allow higher-fidelity treatment of land and sea breezes. This will place a greater demand on the development of wind-field data and may require some development of the SATRAP software before the MSL mission.

5.3.3 NARAC Code Suite

5.3.3.1 Typical Applications

The NARAC (National Atmospheric Release Advisory Center located at Lawrence Livermore National Laboratory) code suite was developed to be state-of-the-art software for real-time accident management. It is the highest fidelity of the software listed in this section, but is also the slowest running.

The NARAC codes were used, for example, to follow and forecast wind data in Salt Lake City during the 2002 Winter Olympics. If an accidental or terrorist-related release of material into the atmosphere had occurred, these codes would have been used to forecast the plume motion to support emergency management and response.

5.3.3.2 Solution Approach

The NARAC software is intended primarily to treat releases within the PBL, similarly to MACCS2 and SATRAP. However, the NARAC software is higher fidelity than either MACCS2 or SATRAP. The wind-field treatment is fully 3D. Rather than using simple spatial interpolation of weather station data, like SATRAP, the wind-field representation can be calculated to enforce mass consistency. Atmospheric transport and dispersion are usually treated by tracking individual particles through the 3D wind field.

NARAC is not specifically designed for releases of radiation, so it does not report all of the consequence measures that would be required for a SAR. This method is more precise than the Gaussian puff method described above. The advantage of particle tracking is that it fully accounts for the 3D wind field because particles at different elevations experience different wind velocities; with the Gaussian puff method, the entire puff moves at the same velocity even though the puff may extend kilometers in the vertical dimension.

Using the particle tracking method, concentration fields are constructed from a large set of particles—usually on the order of 100,000. The computational effort required to construct the wind field and to perform the particle tracking is considerable.

The NARAC codes are not specifically designed for releases of radiation, so they do not report many of the consequence measures that would be required for a SAR.

5.3.3.3 Code Maturity and Documentation

The NARAC software is well established and has undergone considerable scrutiny and assessment. It is used for real-time analysis of actual and potential atmospheric releases of regional or national significance. The level of QA is high.

5.3.3.4 Planned Enhancements

The NARAC codes are under continual development. No specific improvements that would enhance capabilities for the MSL mission are known at this time.

5.3.3.5 Additional Development Needed for the MSL Analysis

The NARAC models focus on atmospheric transport and dispersion and are somewhat lacking in the area of consequence assessment. For example, modeling capabilities include calculation of airborne and surface concentrations and resulting doses. The models do not treat health effects, such as latent cancer fatalities. Some extension of the modeling capabilities would be needed to predict the consequences that are required for the MSL SAR.

5.4 Recommendations

Table 5 summarizes the modeling capabilities of each of the three codes described in the previous subsection. It is obvious that there is a tradeoff between fidelity and the CPU time required to perform the consequence analyses. The optimum choice in terms of this tradeoff is the SPARRC code suit, which is fast enough to perform the required calculations while at the same time retaining enough fidelity to adequately treat the land and sea breezes that are common at KSC. The SPARRC suite also calculates all of the consequence data that have been reported in recent FSARs; MACCS2 and the NARAC suite would require at least some minor development to be able to report the full set of consequence results.

The primary recommendation for the MSL mission is to continue performing consequence analyses with the SPARRC code suite, which has been used to support at least two FSARs and has been reviewed and accepted by INSRP. Because of the successful use of this code for previous launch safety analyses it should work well for the MSL analyses, provided that the technology is successfully transferred from Lockheed Martin to SNL. The major deficiency of the SPARRC code suite is that the level of documentation is less than desirable.

A secondary recommendation is to use the MACCS2 code for the consequence analyses. This strategy would require some additional development to be able to report additional some consequence results and to create interfaces with other existing codes that are used to perform the probabilistic analyses. While there is a good likelihood that this strategy would be successful, it would produce lower-fidelity results and might receive criticism from INSRP. The advantage of the MACCS2 code is the strength of its documentation and its reputation within the DOE and NRC communities.

Table 5. Comparison of Code Uses

Code	Sampling Capabilities	CPU Requirements for Single Sequence	Wind Field Approximation	Dispersion Approximation
MACCS2	Excellent	Very Fast (minutes)	Single weather station Uniform wind field	Gaussian plume
SPARRC Suite	Excellent	Adequate (days)	Multiple weather station Quasi-3D wind field	Gaussian puff
NARAC Suite	None	Very slow (weeks or months)	Multiple weather station Fully 3D wind field	Gaussian puff or individual particle tracking

While the MACCS2 code is not recommended as the primary tool for consequence analysis in support of the MSL mission, it could be used to perform a credibility check on the SATRAP results.

The NARAC suite is probably too slow running to be a serious contender for the MSL mission or other future space missions. However, it is the industry standard for atmospheric transport and dispersion analyses. In Lockheed Martin's current work for the PNH FSAR, the NARAC codes are being used to calibrate the accuracy of the SATRAP results. This calibration should be considered in future SARs as well.

5.5 References for Section 5

Chanin, D., et al, 1998. "Code Manual for MACCS2," NUREG/CR-6613, SAND97-0594, Sandia National Laboratories, Albuquerque, NM.

Dobbe, C.A., et al, 1990. "Quality Assurance and Verification of the MACCS Code, Version 1.5," NUREG/CR-5376, EGG-2566, Idaho National Engineering Laboratory, Idaho Falls, ID.

Jow, H-N, et al., 1990. "MELCOR Accident Consequence Code System (MACCS): Model Description," NUREG/CR-4691, SAND86-1562 Vol. 2, Sandia National Laboratories, Albuquerque, NM.

Molenkamp, C. R., et al, 2004. "Comparison of Average Transport and Dispersion Among a Gaussian, a Two-Dimensional, and a Three-Dimensional Model," NUREG/CR-6853, Lawrence Livermore National Laboratory, Livermore, CA.

6. Quality Assurance and Validation and Verification

6.1.1 Quality Assurance

QA of the software and input data used to perform launch safety analysis is an important feature of the MSL project. SNL recommends establishing a systematic QA program appropriate to the activities and goals of the MSL nuclear launch safety analysis program. It is expected that some existing processes at SNL will be suitable for incorporation, while in other cases new procedures and processes will have to be developed.

A key aspect of the QA program will be management of quality records. These are documents that track the various stages in the development of work products or that establish the source of data or information. When fully implemented, quality records will be managed in a manner consistent with an appropriate national standard.

All activities in the MSL nuclear safety analysis program will be categorized by their impacts on the work products, and procedures will be developed for each of these activities. The set of procedures will be collected into a Quality Assurance Program Plan, as well as Qualification Plans for the various codes used. Examples of the processes that are expected to be subject to QA procedures are:

- Qualification and acceptance of software from outside the program
- Change control of software modifications
- Configuration management of software development and documentation
- Configuration management of interfaces between codes (files written by code X, read by code Y)
- Development and review of calculational input decks
- Peer review of technical reports and analyses
- Quality records management
- Internal and external audits

6.1.2 Validation and Verification

Although QA of the software used is important for assessing the integrity of the models and codes used in the MSL launch safety project, of even greater importance is the validation and verification of the tools. For the codes to be used for Detailed Response Analysis (Level A, as will be discussed later), the primary means for demonstrating that the underlying models, coding, and data are adequate is to compare code predictions against experimental data. The ideal experiment or test for code validation would capture the same phenomena at the same scale and with the same materials as the accident environment in question. This ideal is generally impossible to achieve, so the challenge is to find test data that comes as close as possible. Over the decades that RTG safety has been under study, a wide variety of tests have been performed, ranging widely in data completeness and relevance to accident conditions. As part of the MSL SAR program, these test descriptions and measurements will be collected and evaluated for their usefulness in validating the Detailed Response codes. For the best test cases, the codes selected for SAR work will be used to predict test results. These validation exercises can serve the purpose either of evaluating the accuracy of the codes for such problems, or to adjust uncertain parameters to obtain the best fit.

In addition to tests performed specifically for RTG safety analysis over the years, there are many well-instrumented and well-documented experiments and tests that have been carried out for other programs. In those cases where the data is available to SNL and the range of phenomena and scales are in general a good fit to the RTG accident scenario, it may be worthwhile to run code predictions for these tests to provide an understanding of the predictive accuracy of the SAR codes. In many cases the validation work has already been carried out for other programs.) All such validation exercises will be collected into a series of reports that will be available for subsequent review by DOE, INSRP, or other oversight body.

For the codes to be used in Level B (Event Sequence Analysis) and Level C (Atmospheric Transport and Health Consequences) there is no practical way to validate against test data. Some submodels might be validated against real test data, but these codes are inherently statistical in their predictions so there is no way to validate their performance at the system level. The best way to evaluate the appropriateness and integrity of such codes is to carry out verification exercises. These often involve comparing results of test cases between two different codes that have overlapping capabilities. Another way is to set up idealized test problems that have known solutions and determine if the risk codes reproduce those solutions with the appropriate input decks. Less precisely, some problems could be set up that show that the risk codes produce the correct trends in results as parameters are varied. While these approaches to evaluating the validity of the risk codes are less satisfying than validation against test data, they appear to be the best that can be done. Ultimately, comprehensive reviews of SAR results and methods by external review committees will provide an additional degree of confidence. For that reason, all verification studies will be thoroughly documented in the course of the program.

7. Uncertainty Analysis

One approach to defining the launch risk might have been to define a single best estimate of the number of latent cancer fatalities over 50 years. Then the uncertainty in this number could have been a single lower bound number (e.g., 5% confidence level) and a single upper bound number (e.g., a 95% confidence level). These bounds would have to include all sources of variability and uncertainty, such as variations in the type of accident or meteorological conditions, as well as uncertainty in knowing the effect of a given radiation dose on an average individual. However, past FSARs have chosen to go beyond this simple answer. In addition, they have defined the launch risk in terms of a CCDF or probability distribution. This makes the definition of uncertainty a bit more complicated and in the past has resulted in the separation of uncertainty into two different types.

Past RTG launch FSARs have included a separate "uncertainty analysis" in which the uncertainty was defined as the potential range in the CCDF due to inaccuracies or lack of precise knowledge in the modeling of certain phenomena. This type of uncertainty has sometimes been called "epistemic" and refers to a lack of information that could, in principle, be obtained. Examples include the fracture threshold in iridium at a given strain rate, the probability of a lung cancer fatality in an average person for a specified dose, or the average amount of material resuspended in air in one year in Florida. In the Cassini and PNH risk analyses, this type of "uncertainty" was distinguished from "variability." Variability (sometimes referred to as "aleatory" data) was considered to be a somewhat stochastic quality of nature or events that could not be controlled, such as the particular type of accident, time after launch of the accident, wind direction, etc. In past RTG launch FSARs, it has been assumed, in essence, that there is only one actual and true CCDF for the launch, and that all variations in possible initial conditions and intrinsically random parameters are included in that probability distribution. Then "uncertainty" reflects the inability of mortal man with limited budgets to determine that probability distribution with good accuracy. Identifying which model parameters reflect uncertainty and which reflect variability is sometimes arbitrary, but the approach described is what we will aspire to. Figure 11 shows an example of the desired result taken from the Cassini Mission (Lockheed Martin 1996). The curve labeled "variability only" is the result of the calculations when all epistemic parameters are set at their best estimate values (corresponding to Figure 3 for the PNH Mission).

The first step in this type of uncertainty analysis is to decide which input parameters to the codes reflect "variability" and which reflect "uncertainty." Some examples of "variability" parameters are:

- Type of accident
- Height of accident
- Blast impulse
- Impact velocity
- Debris impact location
- Reentry velocity vector
- Wind direction
- Wind speed
- Source term

Some examples of "uncertainty" parameters are:

- plutonium dioxide mass released for a given crack size
- Aerosol deposition velocity
- Ground impact effective release height
- Inhalation dose conversion factor
- Inhalation sheltering factor
- Resuspension factor

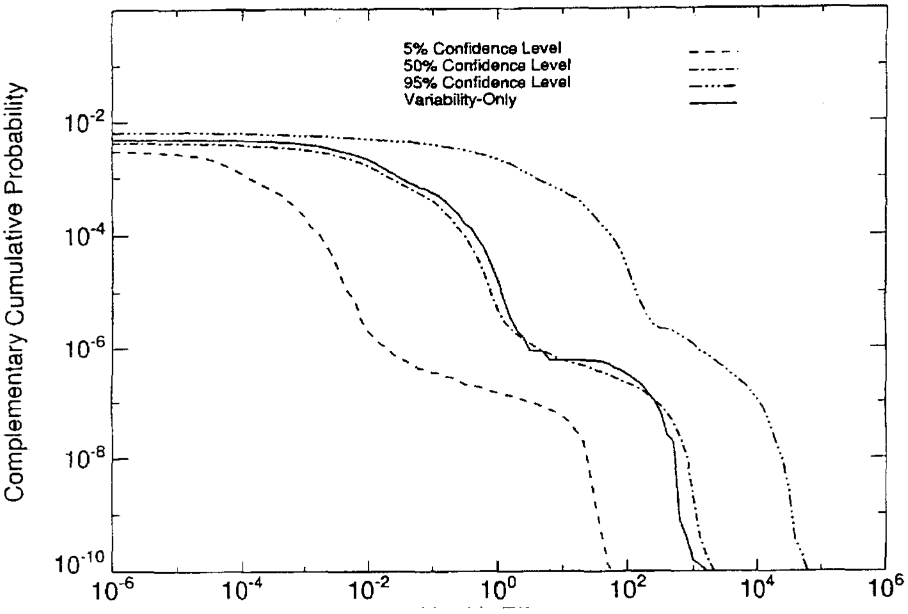

Figure 11. Uncertainty Analysis of Total Mission 50 year Health Effects for Cassini Mission

The overall approach for the uncertainty analysis in the Cassini FSAR followed the steps recommended by the National Council on Radiation Protection and Measurements (1996).

- Define the assessment endpoint.
- List all potential important uncertain parameters.
- Specify the maximum conceivable range of possibly applicable values for uncertainty parameters with respect to the endpoint of the assessment.
- For this range, specify a probability distribution that quantitatively expresses the state of knowledge about alternative values for the parameter.
- Determine and account for dependencies that are suspected to exist among parameters.
- Using either analytical or numerical procedures, propagate the uncertainty in the model parameters to produce a probability distribution of model predictions.

- Identify the parameters according to their relative contribution to the overall uncertainty in the model prediction.
- Present and interpret the results of the analysis.

7.1 Uncertainty Analysis for the New Horizons Mission

In essence, the uncertainty analysis involves creating the CCDFs all over again, but with different models or modeling assumptions. Deciding what constitutes a 5% or 95% confidence band on a single model based on various expert opinions is a challenge in itself. Then, to combine all these modeling bands and achieve the determination of 5% and 95% confidence bands could be very computationally intensive. Lockheed Martin attempted to determine the 5% and 95% confidence bands on the CCDF without excessive computational effort by employing a deconvolution technique. In essence, the change in health effect for a reduced set of accident sequences was determined for different modeling assumptions (uncertainty variations), and then this factor was applied to a broader range of similar sequences. The mathematics is somewhat involved; Figure 12 and Figure 13 show the computational flow.

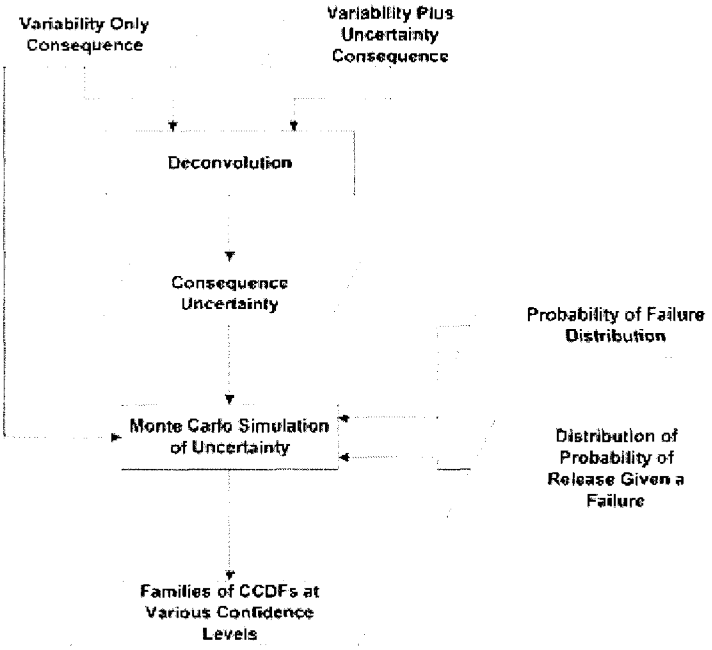

Figure 12. Overall Process for Calculation of Families of CCDFs for the PNH Mission

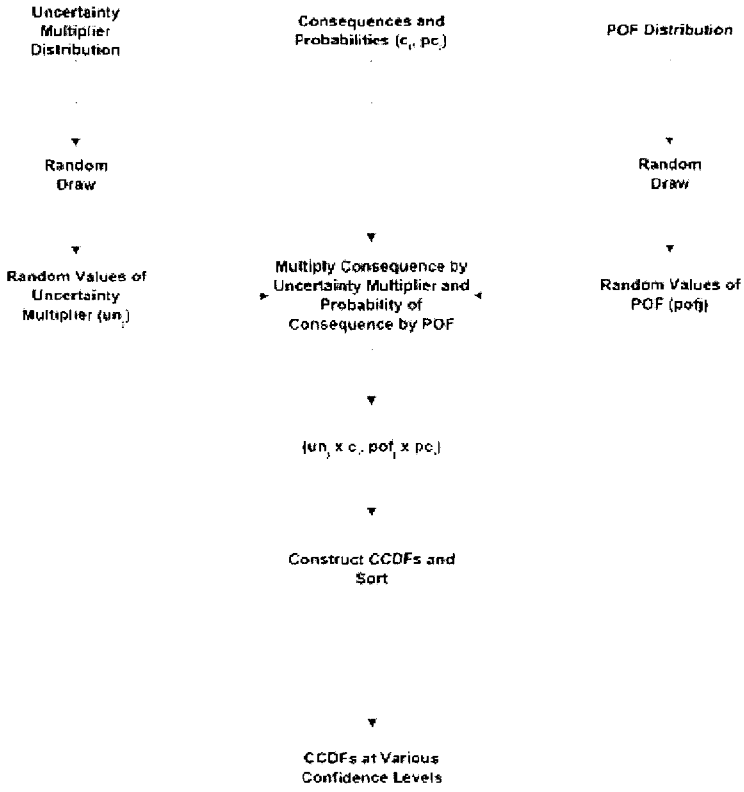

Figure 13. Monte Carlo Simulation of Uncertainty for PNH

7.2 Recommendations for MSL Analysis

The uncertainty analyses performed for the Cassini and PNH Missions were based on a convolution-deconvolution approach. We will attempt to modify the use of LASEP and SPARRC codes so that the uncertainty can be generated simultaneously with the generation of the baseline risk curve. The distinction between "variability" and "uncertainty" parameters will be retained in this analysis and will be displayed in graphs as they were in the previous mission analyses.

7.3 References for Section 7

Lockheed Martin Missiles and Space, 1996. "GPHS RTGs in Support of the Cassini Mission—Final Safety Analysis Report," CDRL C.3, December 1996.

National Council on Radiation Protection and Measurements, 1996. "A Guide for Uncertainty Analysis in Dose and Risk Assessments Related to Environmental Contamination," NCRP Commentary No. 14, Bethesda, MD, p. 6, 10.

8. Recommendations Summary

This assessment has identified the principal calculational needs for the MSL SAR program. For each category of calculation, the candidate codes or models have been evaluated and compared, and a principal recommendation has been made. In some cases it has been found that improvements to the codes will be needed. For some areas, one or more second tier codes have been identified for possible use in special circumstances, or to shed light on the results obtained with the primary code. All codes used for SAR analysis will undergo validation against key experimental results, or when that is not possible, comparison against other codes or known mathematical trends. Results will be formally documented in a series of validation and/or verification reports.

Figure 14 attempts to capture the set of recommended codes and their interactions. The analysis levels A, B, and C are grouped into separate sections, and the quantitative transfers of information are shown. Second tier codes are indicated by parentheses. Specific code recommendations are discussed following the figure.

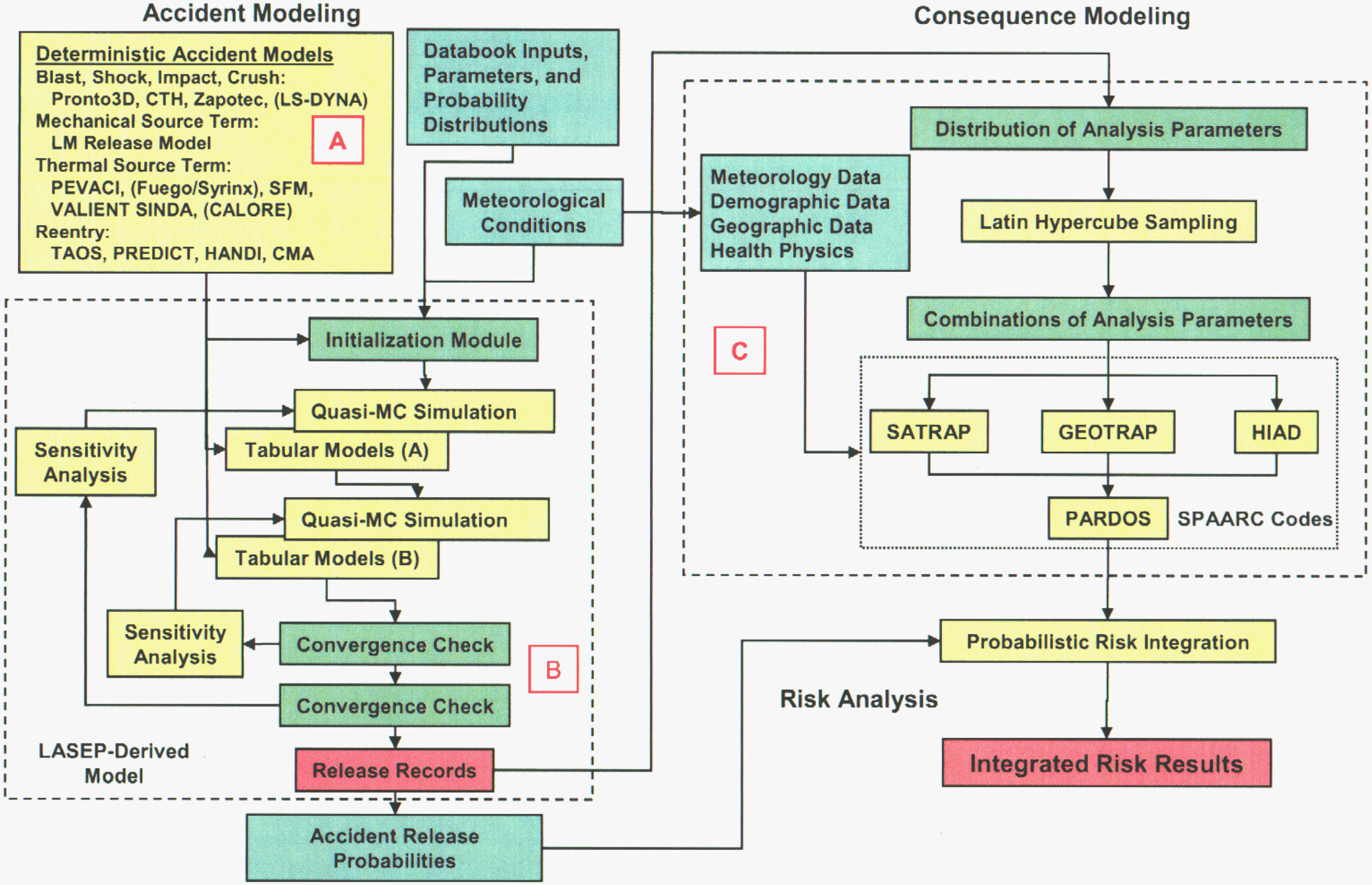

Figure 14. Proposed Code Suite for MSL Analysis

8.1 Recommendations for Analysis Level A: Detailed Simulation of Responses to Accident Environments

The explicit Lagrangian Pronto3D code is recommended for a wide variety of calculations involving structural response of the MMRTG and its components to deforming forces when shock physics and phase change in the solid structures are not important. This includes:

- The structural response part of blast/structure interactions (part of the Eulerian-Lagrangian combination Zapotec)
- In-air fragment impacts for velocities roughly below 500 m/s
- Ground impacts and crush scenarios

Because LS-DYNA has been used extensively for PNH, and the module/GIS properties for that mission are similar (but not identical) to those for the MSL mission, it may be possible to use some of the computational results from the PNH work to support the MSL SAR, thereby reducing the number of new Pronto3D calculations needed. For that reason it has been identified as a second tier code. It remains to be seen whether the differences between the codes and/or the hardware will create significant problems for this role.

Another part of the Pronto3D work will be the development of a new empirical model for the mechanical source term, based on the BCI and SVT test programs.

It is believed that Pronto3D is, in its current form, substantially ready for these MSL calculations, but a modest amount of development work is foreseen to improve run time and stability, particularly in the contact algorithm involving shell elements. Some work on the coupling in Zapotec may be justified in order to achieve faster run times for coupled Euler-Lagrange problems.

The Eulerian shock physics code CTH is recommended for:

- The gas shock portion of blast/structure interactions (as part of Zapotec), and
- In-air impacts of high velocity (roughly >500 m/s) on the MMRTG or its components.

No development of CTH for this program is foreseen, except for obtaining suitable models for material properties. In this regard, the need to obtain better characterization of material properties of the iridium alloy and plutonium dioxide substances used in the MMRTG cannot be overemphasized.

For the thermal source term (produced when fire creates plutonium dioxide fines by vaporization and condensation) the primary recommendation for production calculations are the SFM code (for liquid propellant fires) and the PEVACI code (for fuel in the proximity of or in contact with burning solid propellant). The use of a control volume approach in these codes is necessitated by the need to treat a broad range of complex interacting processes, including chemistry, vaporization, condensation, aerosol agglomeration, heat transfer, and fluid flow. Experience in the use of these codes for prior missions has revealed a number of areas for improvement of these two codes, and a practical program for producing improved versions for the MSL mission has been laid out.

Because of the high degree of user control in these two codes, a supporting role for the higher definition Fuego/Syrinx code has been identified: to provide guidance on specific aspects of the flow and thermal environment around the burning propellant fragment. In the longer run the suite has the potential of performing coupled analysis of the phenomena treated in the lumped parameter codes, but with a CFD treatment of the gas flow.

In the special case of a GIS or GPHS module exposed to a burning solid propellant fragment, it is recommended that the SINDA/Valient five volume model (which was the basis for the PNH studies) be used and upgraded for MSL analyses. In the longer term, the CALORE 3D model will be able to shed light on specific phenomenological issues and improve the way that the more simplistic treatment is used.

For reentry analysis, a suite of four well-established and well-validated codes are proposed. They are:

- TAOS, for trajectory analysis;
- PREDICT, to characterize breakup and to track debris to impact;
- HANDI, to calculated heat up of reentry objects; and
- CMA, to calculate thermal response of reentry objects.

Because of the large number of parametric possibilities, the total number of cases to be studied will be very high. Therefore, it is proposed that the needed portions of each of these codes be organized under a controlling code that will automatically handle the information transfer from one to the other. No other improvements to the codes are envisioned for this program.

8.2 Recommendations for Analysis Level B: Probabilistic Event Sequence Analysis

The recommended approach for the probabilistic event sequence analysis is to start with the LASEP code that was used in the previous several launch approval processes and modify it as schedule permits. The code will draw upon external tabular models generated by the accident progression codes (Level A) described in the previous section and on simplified internal models of some of the accident phenomena, where appropriate.

One of the goals for the development of this software is to move towards a more generic and flexible tool. The intent is that eventually we will have a code that is not designed specifically for one RTG launch mission, but which can be applied to future missions as well, with far less re-coding (and the attendant QA burden) for specific future mission features.

8.3 Recommendations for Analysis Level C: Atmospheric Transport and Consequences

The SPARRC code suite, which was developed specifically for RTG space launch safety analysis, and which has been used for two previous mission SARs, is recommended as the primary set of tools for atmospheric transport and consequence analysis. This suite consists of:

- SATRAP, for transport over relatively local regions;
- GEOTRAP, for transport on a more global scale; and
- HIAD, for transport of very high altitude releases.

It may be desirable to modify SPARRC to use a true 3D wind field, in view of the availability of 3D data from CCAFS. The MACCS2 code could play a second tier role by performing some credibility check on the SATRAP results. It is a much more mature consequence analysis code than SATRAP, its documentation is stronger, and it has a broader reputation within the larger DOE and NRC communities.

8.4 Recommendations for Risk and Uncertainty Analysis

The final calculational stage shown in Figure 14 is to combine the information about event probabilities, release probabilities, release characteristics, and health consequences to produce CCDFs of the key risk metrics (excess cancer fatalities, land contamination, etc.). These results will be provided for each AOC, and integrated results for the entire mission will also be produced. Additional insights will be developed by analyzing the detailed results for risk-dominant event sequences, phenomena, and pathways. The main focus of the risk analyses will be the best-estimate CCDFs, or the "variability only" results. In addition, a thorough analysis of how modeling and data uncertainties might affect the results will be performed in an uncertainty analysis. It is anticipated that the calculational tools used for these two levels of analysis will be better integrated and more transparent than has been the case in previous RTG missions.

The uncertainty analyses performed for the Cassini and PNH Missions were based on a convolution-deconvolution approach. We will attempt to modify the use of LASEP and SPARRC codes so that the uncertainty can be generated simultaneously with the generation of the baseline risk curve. The distinction between "variability" and "uncertainty" parameters will be retained in this analysis and will be displayed in graphs as they were in the previous mission analyses.

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