Development and Experimental Validation of Computational Methods to Simulate Abnormal Thermal And Structural Environments

J. L. Moya, R. D. Skocypec, R. K. Thomas
Sandia National Laboratories
Albuquerque, NM, 87185

Introduction

Over the past 40 years, Sandia National Laboratories (SNL) has been actively engaged in research to improve the ability to accurately predict the response of engineered systems to abnormal thermal and structural environments. These engineered systems contain very hazardous materials. Assessing the degree of safety/risk afforded the public and environment by these engineered systems, therefore, is of upmost importance. The ability to accurately predict the response of these systems to accidents (to abnormal environments) is required to assess the degree of safety. Before the effect of the abnormal environment on these systems can be determined, it is necessary to ascertain the nature of the environment. Ascertaining the nature of the environment, in turn, requires the ability to physically characterize and numerically simulate the abnormal environment.

Historically, SNL has demonstrated the level of safety provided by these engineered systems by either of two approaches: (1) a purely regulatory approach, or (2) by a Probabilistic Risk Assessment (PRA). This paper will address the latter of the two approaches.

As shown in Figure 1, for a PRA analysis, the characterization of an abnormal environment for a transportation accident (a crash followed by a fire) is defined by four distinct but coupled models. The first model represents the initial environmental conditions, such as: wind speed and direction, impact velocity/orientation, amount of fuel, and definition of the terrain. For a PRA analysis, the chaotic nature of accidents is manifested in the initial conditions which are typically expressed as probabilistic distributions. The approach presented in Figure 1 processes initial environmental conditions to assess the response, and ultimately, the consequence of subjecting an engineered system to a particular environment. For a transportation accident, data is processed in the following manner: initial conditions first are passed to the crash dynamics model where an assessment is made regarding the level of damage to the system (i.e., amount of damage to fuel tanks, mechanical damage to the cargo, etc.). Initial conditions and quantification of the level of mechanical damage are in turn fed to the fuel dispersion model. The dispersion model adds to the data stream the location of the fire and the amount fuel available from burning. The fire model then uses all the information provided from the other models to create a hypothetical thermal environment to which the system is subjected. How the response of the system is quantified is presented in the

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paper entitled "Modeling the Thermal and Structural Response of Engineered Systems to Abnormal Environments."

Historically there have been two means of processing the information -- by the use of historical accident data, or expert elicitation. More recently, an effort at SNL has focused on developing deterministic models to process the information. Each technique by itself has its limitations. For example, if the deterministic model is based on overly simplified assumptions, its predicted outcome may not match real accident data because an important piece of physics may not be included. Historical data may be incomplete, or skewed due to some unknown variable, and thereby affect the results. For expert elicitation, the phenomenology may be counter-intuitive (or, the intuition of the experts can be wrong). Each technique can be used in support of the other techniques. For example, a model and/or historical data can augment the insight of the experts. Similarly, historical data and expert opinion can support a model and its development. The focus of this paper is to discuss deterministic models developed to support a PRA. For these models to be compatible with the PRA process, they must be capable of being exercised efficiently over a broad parameter space. In essence, they must be capable of resolving tens of thousands of scenarios in a realistic time frame.

Crash Dynamics Models

Mechanical environments are defined as loads and displacements imparted to an engineered system or package resulting from an accident. A typical scenario is an airplane crash, where the problem is to define the acceleration loads on a package carried in the aircraft, and the hardness or irregularity of objects such as puncture probes, that the package may impact. For convenience the mechanics phenomena are grouped into areas of crush, impact, and penetration. Thus, the abnormal environments imparted to engineered systems or packages are defined by simple loads and displacements for crush, impact, and penetration. Figure 2 illustrates an example of finite element penetration calculation of a shell structure by a probe.

Numerical simulation of a crash dynamics problem involving aircraft, railroad, and highway transportation vehicles is extremely difficult due to the complexity of the structure to be modeled, large deformations, and nonlinear behavior of the material response. Transient dynamics, finite element, computer codes are available at SNL for conducting these types of simulations. However, the time spent developing the models is very long (~6 months), the finite element models are large and cumbersome (~1-5 million degrees of freedom); and the computer run times are often prohibitively expensive (100's of hours on a supercomputer). Only a few scenarios can be realistically modeled. Abnormal mechanical environments acting on engineered systems, therefore are usually determined from full-scale and scale-model test data. Approximate analytical and numerical models can be constructed if sufficient test data is available.

Finite element models of sub-systems have been developed. For example, the wall of a trailer used to transport hazardous material was modeled using SNL transient dynamics codes to assess damage to the wall if impacted by unrestrained cargo.

It is difficult to reduce these large, nonlinear structural models to very simple models which have short computer run times and are thus compatible with the PRA process. SNL currently is pursuing "response surfaces," which is essentially computer software to interpolate between several very large, database result files from the complex three-dimensional (3-D) simulations. An advancement of this method is the use of "neural networks," in which artificial intelligent methods are employed to educate a simple model using the results from complex, 3-D finite element models.

Dispersion Model

The development of a dispersion model is underway to predict the location and amount of fuel relative to the engineered system, following an accident involving an aircraft. This model is being developed to reduce uncertainties related to the transportation of hazardous cargo by air. Given the infrequent occurrence of aircraft accidents, little data exists to characterize the duration of a thermal environment following an aircraft accident. In some instances where data is available, the data presents a somewhat unrealistic scenario. It is not uncommon, for example, for an accident file to report the duration of a fire as lasting for several days, when in fact the very definition of "fire" is in question. Accident investigators may report the duration of the fire to last until all incendiary fires (smoldering of vegetation away from cargo of interest) are extinguished. As one would expect, the use of such data would skew the results of a safety assessment.

As shown in Figure 3, the model has been formulated to have three dispersal regimes. The three dispersal regimes are defined by three corresponding fuel-tank damage regimes. The first damage regime, at low normal impact velocity, involves insignificant damage to the wing fuel tanks. In this regime, insignificant fuel leakage occurs. The second damage regime, at intermediate normal impact velocity, involves significant structural damage to the wing fuel tanks, but insufficient damage to cause complete structural failure of the fuel tanks. In this regime, fuel will leak from the damaged tank at a rate proportional to the amount of damage. The third damage regime, at high normal impact velocities, involves complete structural failure of the wing fuel tanks. In this regime, fuel will splash/disperse on impact. Specific fluid models have been developed for the intermediate and high normal-impact-velocity regimes. For the intermediate normal-impact velocity regime, the model is referred to as the "Fuel Leakage Model." For the high normal-impact velocity regime, the model is referred to as the "Splash Model." Each of these models is discussed below.

Dispersion Mode! - Fuel Leakage

The fuel leaks from the damaged wing tanks, and is dispersed as the aircraft is decelerating. The amount of fuel remaining after the aircraft comes to rest is equal to the amount of fuel at impact minus that which has leaked out. The total amount of fuel that leaks out is a function of the extent of damage to the fuel tank and the time it takes for the aircraft to come to rest. Once the aircraft comes to rest, the fuel remaining in the damaged tanks will continue to spill from the wing.

There are a number of complexities in the fuel leakage problem during deceleration. Some of these complexities are the same as those present after the aircraft comes to rest. These include damage and complex fuel tank geometry. Damage to the wing tanks can range from cracks, to the complete loss of entire sections of the fuel tank.

Two complexities are unique to the deceleration problem. The first complexity is that the aircraft deceleration, due to impact and slide-out, causes the fuel to experience a time-varying body force. Gravity also results in a body force. The sum of the two body forces changes in magnitude and direction over the deceleration phase. This time-varying body force will result in sloshing of the fuel within the tanks. Furthermore, the hydrostatic driving force for fuel leakage depends on time-varying quantities including the height of the free surface above the location of the damage, and the magnitude of the body force. The second complexity unique to a decelerating aircraft is that the total pressure (static plus dynamic) on the wing surface is a function of the aircraft velocity, which is itself a function of time. The total pressure also varies across the surface of the wing, with a maximum at the leading edge of the wing or stagnation point. Depending on the direction of the pressure gradient between the internal fuel tank pressure and the free-stream pressure, leaking fuel either will experience a driving or a retarding force. The relative magnitude between the driving force for fuel leakage induced by the pressure difference and by the hydrostatic head is not intuitively obvious.

Dispersion Model -- Fuel Splash

A splash model is being developed for the high-normal-impact-velocity regime. In this regime, the wing will fragment upon impact and the fuel inside will disperse. Fragmentation is a complex process that cannot be modeled in a simple manner. For simplicity, and in keeping with the spirit of the PRA process, it is assumed the wing has no structural integrity at impact. In other words, the breakup of the wing does not influence the dispersal of the fuel. In reality, some of the impact energy will be absorbed in the fragmentation process, so the energy available for fuel dispersal is less than that considered here.

As shown in Figure 4, fuel is dispersed by its own momentum at the instant of impact. The fuel remaining in a continuous, definable "wet" spot is the fuel available to support a pool fire. The part of the splash that separates from the main flow will be assumed to be consumed as a fireball, and therefore, does not contribute to the subsequent pool fire.

An experimental program is underway to empirically quantify the amount of fuel available to support a pool fire as a function of impact angle, impact velocity, and the mass of fuel at the time of impact.

Fire Model

Quantification of the thermal insult caused by a fire to an engineered system is a necessary part of a PRA. Beginning with appropriate input parameters, a fire model will calculate the thermal environment given an object is immersed in flames. The fire model, thus, provides thermal boundary conditions for the system response model. In actuality, the thermal boundary conditions may be tightly coupled to the system response model. Given a transportation accident, modeling a pool fire is complicated by the presence of objects in the fire. The fluid flow field, turbulent structures, combustion processes, and thermal radiation fields within the fire all can be influenced significantly by the presence of objects. In addition, large, thermally-massive objects tend to cool the surrounding flames. This results in significantly lower incident heat fluxes to the object engulfed within the fire. Hence, the pool fire environment and object thermal response are coupled. This interaction must be understood and modeled to accurately predict the local heat fluxes and temperatures for an object subjected to a fire environment. Toward this end, SNL is developing a fire model that captures the object/fire coupling, and yet executes quickly enough such that it can be used as part of the PRA process.

Fire modeling to determine the thermal insult from a fire to an object immersed in flames can be performed on a variety of levels. The simplest model is to prescribe the heat flux to an object based solely on either a simple equation or experimental data. This typically is done by relating the heat flux (q) incident to an object to an effective flame temperature (T) using some variation of the equation: $q = \sigma T^4$, where σ is the Stefan-Boltzmann constant. Unfortunately, such a simple model does not include the object/fire interaction, unless the data used to determine T is from tests with objects in the fire. SNL, consequently, has made a concerted effort to develop a large database which catalogs the thermal environment conditions (fire temperature, and flame velocities) and heat transfer to different types of objects. Measurements from these large, open-pool fires have been used to illustrate the heat transfer to an object in a fire is affected by the physical size and shape of the object, as well as the thermophysical properties of the object. In addition, due to the object/ fire coupling it is essential to obtain both temperature and heat flux measurements.

Over the last two decades, advanced fire physics models have been under going development. These advanced fire physics models attempt to model all of the physics of the fire environment, including combustion, fluid hydrodynamics, turbulence, soot generation, and thermal radiation.

Since they require substantial computer resources, advanced fire physics models generally are impractical for direct use in calculating the fire environments for each of the thousands of hypothetical scenarios that must be evaluated. However, they do play a critical role in PRA fire tool development and validation, as well as in the PRA process itself.

Before discussing the role of an advanced fire physics model in the PRA process, it is necessary to first understand the capabilities of an advanced fire physics model. Since advanced fire physics models begin with the governing differential equations for energy, species, and momentum transport, they are capable of a "first principles" analysis. In other words, beginning with the fact that there is a certain object in a certain size pool of fuel, an advanced fire physics model is capable of computing the local fire temperatures, local heat fluxes to the object, local gas concentrations and velocities, and local combustion processes, with a minimal dependence on empirical factors. The word "local" refers to the fact that the quantities calculated are a function of location in 3-D space.

Over the last several years, efforts at SNL have been devoted to the development of a set of simplified, deterministic fire heat-load models which apply first principles to the dominant physical phenomena, and rely on empirically-determined parameters to represent the remaining physics. These codes, the SNL Risk Assessment Compatible Fire Models (RACFM's), allow run times to be reduced to a level which is acceptable for a PRA analyses. These models solve the energy equation and radiative transport equation in the region of a fire near an object of interest (Figure 5). The SNL RACFM's are a suite of codes which have been developed for engulfed geometries, including a vertical flat plate, an inverted flat plate, and a cylinder in cross flow. These models have successfully illustrated the coupled responses between the object and the fire environment that have been observed in experimental data. When coupled with a conduction code to model the object thermal response, these simplified models have been used to identify a regime specified by non-dimensional parameters for which the fire can be reasonably treated as a blackbody radiant heat source. This is discussed in more detail in the paper entitled "Modeling the Thermal and Structural Response of Engineered Systems to Abnormal Environments." Each of these codes requires a set of input parameters which includes the effective gas absorption coefficient, a, and the effective volumetric energy generation rate, S'''. Flow fields are modeled using solutions from potential flow theory, and correlations are included to model convective effects. Participating media radiation heat transfer, the dominant mode of energy exchange in fire environments, is modeled in the direction normal to the surface of the object using a one-dimensional (1-D), two-flux method.

While the RACFM represents a significant advancement over using σT^4, it does have its limitations. Presently, it is only capable of modeling simplistically- shaped objects. The radiative transport model is 1-D, whereas the actual transport is 3-D. The velocity field is assumed constant and uniform, and is not coupled to the local fluid temperature or density. A constant, uniform absorption coefficient is assumed to reduce simulation times. Although the experimental data available for calibrating these models is limited, the model can be expected to yield reasonable results outside of the region of available data since the influence of the changing conditions is accounted for by modeling the dominant heat transfer mechanisms. The error associated with applying the model outside the range of available data can be decreased (at the expense of increased computational requirements) by increasing the fidelity by which the model accounts for the dominant chemical and physical processes. The use of simplified deterministic models is, therefore, a trade-off between the degree of fidelity associated with detailed models, and the computation time limitation imposed by a PRA. The methodology being followed by SNL is to use the simplified deterministic fire models to perform preliminary scenario evaluation. The detailed fire physics models are then applied to a smaller number of scenarios which have been identified from screening the results from the simplified deterministic fire models.

The RACFM's originally were developed for hydrocarbon fuel fires. Historically, scattering has been neglected for these fire environments based on particle size considerations. However, within certain areas of these fires, relatively large agglomerated particles that scatter radiant energy may be present. The addition of scattering to the models, therefore, is of interest. Furthermore, although many accident fire scenarios will involve the combustion of a hydrocarbon fuel such as JP-4, a significant number of credible scenarios exist in which the system will be exposed to burning solid propellant. The particulate matter which is present in propellant fires results in a high degree of radiative scattering. The effects of radiative scattering have been included in order to begin applying the RACFM's to propellant fire scenarios.

Opportunities for Collaboration

Experimental fire data is required to advance the development of the advanced fire physics model and RACFM's. At the present time, data is required to quantify the following distributions of physical parameters in large, open-pool fires;

- Air entrainment rates and flow velocities,
- Combustion rates,
- Soot formation rates and optical properties,
- Gas composition,
- Flame temperature, and
- Heat flux.

In addition, to further enhance SNL ability to develop crash dynamics models the following is needed:

- Damage and fracture models for structural materials, and
- Full-scale testing to help develop and validate the computational models.

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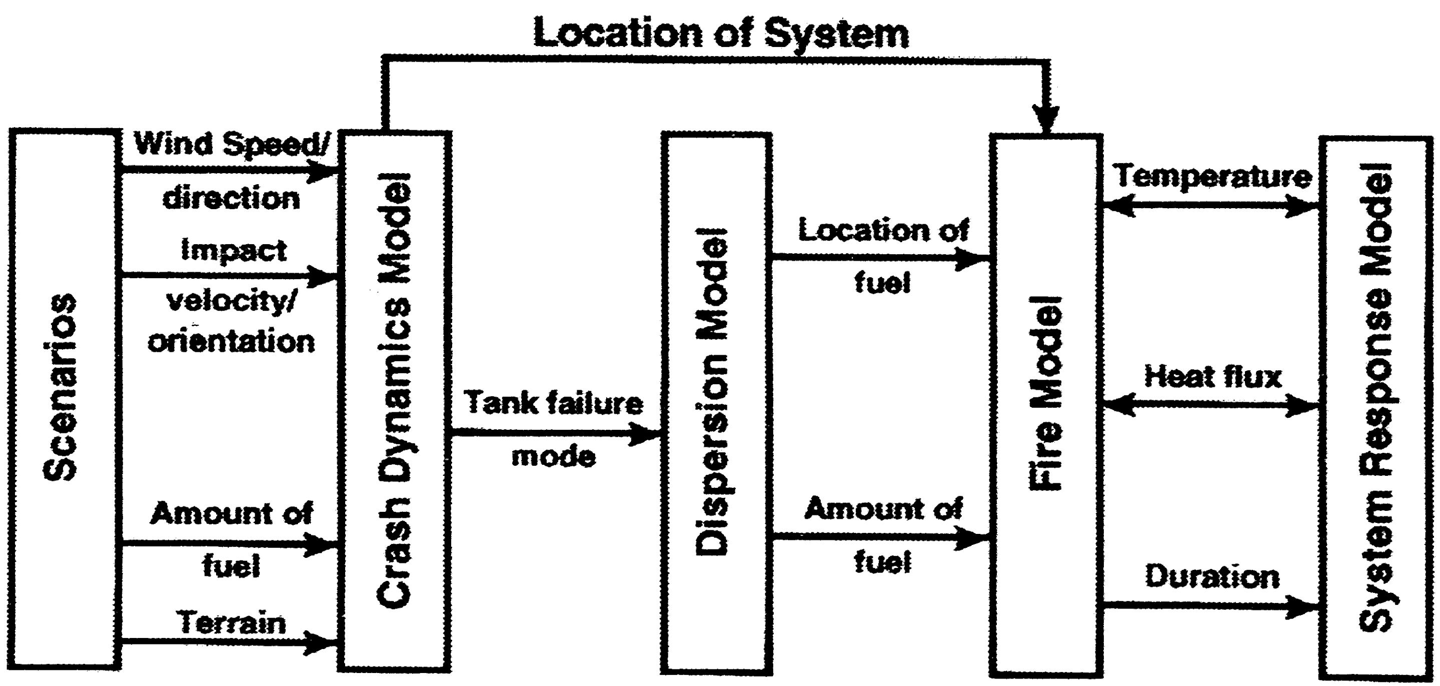

FIGURE 1. Technical Approach for Prediction of System Response to Transporation Accident Scenarios

FIGURE 2. Finite-element simulation of a penetration of a fuel vessel in a crash environment

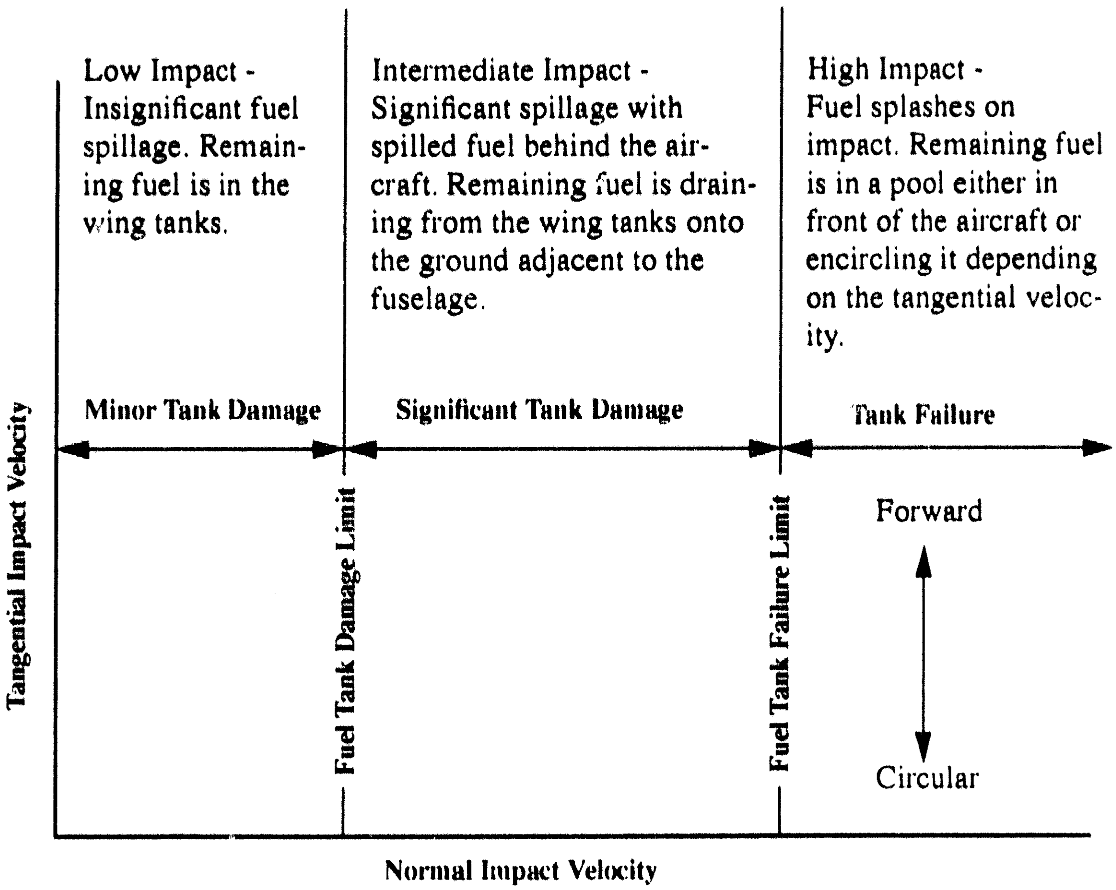

FIGURE 3. Dispersal Model. Three dispersal regimes have corresponding damage regimes. No or minor damage produces no or minor fuel leakage. Significant fuel tank damage results in fuel leaking behind the aircraft. Fuel tank failure results in fuel splashing.

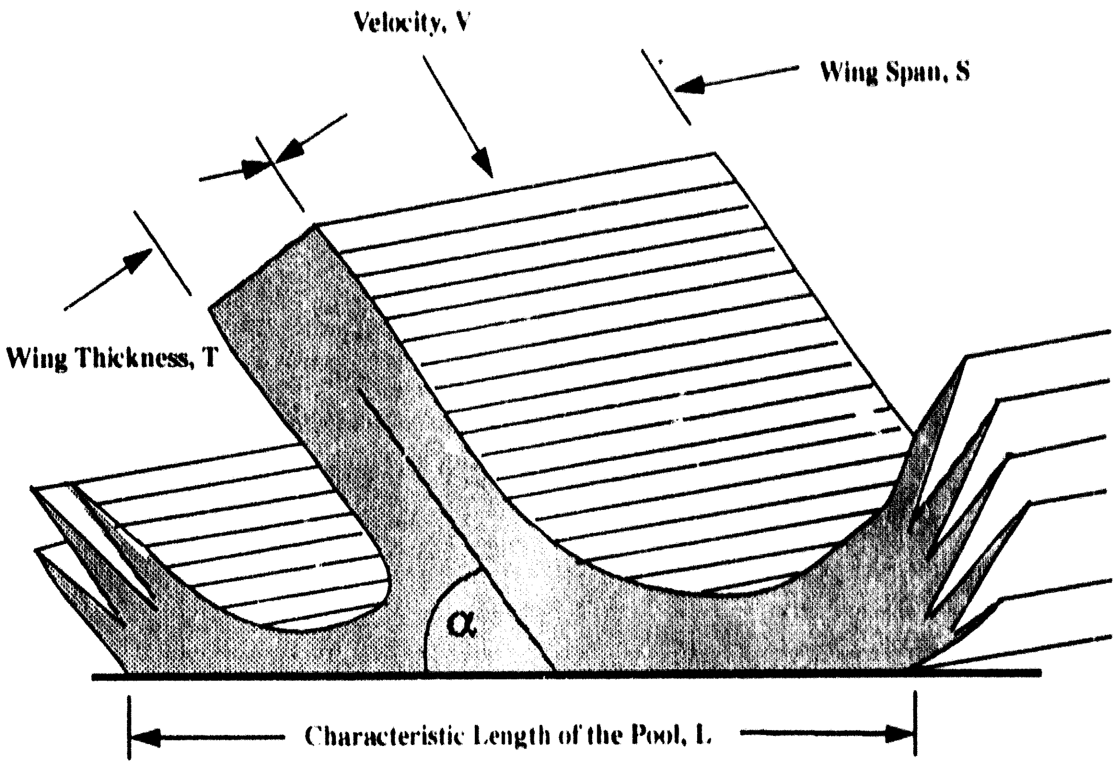

FIGURE 4. Splash Model Parameters.

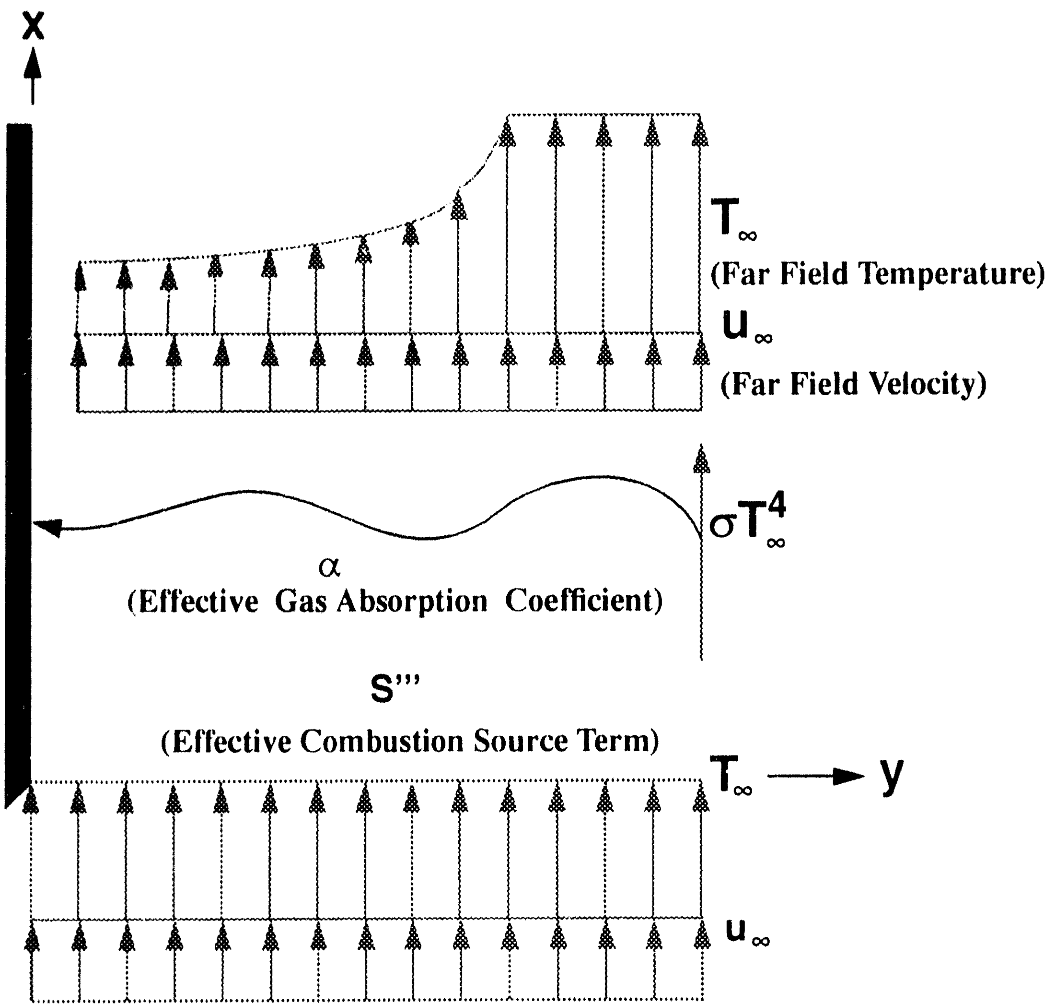

FIGURE 5. Risk Compatible Fire Model -- Flat Plate Goemetry

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