

On The Development of a Subgrid CFD Model for Fire Extinguishment

Sheldon R. Tieszen¹ & Amalia R. Lopez
Sandia National Laboratories, Albuquerque, NM 87185

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1. Corresponding Author Address:

Sandia National Laboratories
Reactive Processes Department
PO Box 5800
Albuquerque, NM, USA 87185-0836
fax: (505) 844-8251
e-mail: srtiesz@sandia.gov

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Abstract

A subgrid model is presented for use in CFD fire simulations to account for thermal suppressants and strain. The extinguishment criteria is based on the ratio of a local fluid-mechanics time-scale to a local chemical time-scale compared to an empirically-determined critical Damkohler number. Local extinction occurs if this time scale is exceeded, global fire extinguishment occurs when local extinction has occurred for all combusting cells. The fluid mechanics time scale is based on the Kolmogorov time scale and the chemical time scale is based on blowout of a perfectly stirred reactor. The input to the reactor is based on cell averaged temperatures, assumed stoichiometric fuel/air composition, and cell averaged suppressant concentrations including combustion products. A detailed chemical mechanism is employed. The chemical time-scale is precalculated and mixing rules are used to reduce the composition space that must be parameterized. Comparisons with experimental data for fire extinguishment in a flame-stabilizing, backward-facing step geometry indicates that the model is conservative for this condition.

Introduction

The purpose of this study is the development of a subgrid flame extinction model for use in CFD-based numerical simulations for fire extinguishment. Desired model attributes include compatibility with combustion models commonly used by the fire community, a balance between simplicity and fidelity, and a model that provides sufficient, but not overly, conservative results. The motivation is a desire to have a CFD based tool for fire suppression system design. While the search for a 'drop-in' replacement for Halon 1301 continues, it is prudent to examine alternative design options due to the difficult chemical challenges [1].

For reasons to be discussed, this work is limited to thermal suppressants, i.e., that primarily act by heat capacity and dilution. Due to the length scale range involved in fire extinguishment, minimum computational cell sizes will exceed flame thicknesses [2]. Therefore, a subgrid model is necessary to describe flame extinction processes. By its nature, a flame extinction subgrid model is an engineering approximation, intended to capture the dominant physical/chemical effects, which in this case are thought to be flow-induced flame-strain and the effect of injected thermal suppressants.

It is well known that non-premixed, diffusion flames can be extinguished from strain alone (cf [3,4]). From a flamelet perspective, as the inflow velocity increases, the width of the diffusion flame decreases and there is a progressive reduction in the flame temperature, and eventual extinction (cf [5]). It is reasonable to assume that this decrease in residence time most strongly affects the slowest reactions [6,7]. Numerical studies suggest that flames are more sensitive to lower frequency oscillations than to higher frequency ones [8]. The exothermic reactions that produce the high temperatures required to sustain reaction also tend to be slow reactions active in the higher

temperature regions of the flame (cf [5]). Hence, as these reactions have less time to complete, the temperature is lowered, and the specific heat release rate drops which leads to flame extinction.

Strain also affects the suppressant loading required to extinguish a flame (cf [9,10]). Suppressants can act by chemical and thermal means. Detailed numerical opposed-flow flame studies [11] show that for thermal suppressants, the location of heat absorption does not affect the ability of the agent to extinguish the flame as long as it is convected into the flame zone. Since the current study is restricted to thermal suppressants, we assume that flame extinction, from either strain or suppressant loading, or both, is not highly sensitive to structural details within the flame zone itself. To the extent that this assumption is correct, it should be possible to develop a model based on properties from the grid level, extrapolated down to the flame zone level, that has a reasonable chance of engineering utility.

Combustion models commonly employed in studies of fires are typically time-filtered (Reynolds-Averaged-Navier-Stokes, or RANS). The most common combustion models are the EDC (cf [12]) and PDF methods (cf [13]). To close a non-linear source term, the output of a combustion model consists of *mean* properties (time mean at a point for RANS, or volume mean at a given time for Large Eddy Simulation - LES) that are obtained from integrating over a (usually assumed) distribution.

The extinguishment model establishes criteria for extinguishment, thus its requirements are different than for source-term closure models. Consider a collection of flames that either pass a point (RANS) or are within a cell volume (LES). Experimental data (cf [14]) show statistical fluctuation for a given strain and suppressant loading in a turbulent flow. Typically, a 90% confidence level is chosen as representative of extinguishment. For modeling purposes, a metric of extinguishment

difficulty requires definition in terms of local strain and suppressant loading (and any other factors that may affect extinguishment difficulty). The state corresponding to 90% of the difficulty range is the desired model metric.

With complete knowledge of the subgrid phenomenology, this state could perhaps be defined. However, in practice, it is not possible to have sufficient information to build this statistical distribution without engineering assumptions. The relation between local strain and local concentration (much less joint with other factors) is not available. The approach used in this study is to use phenomenological reasoning and attempt to error on the side of conservatism for suppressant concentration.

SubGrid Model

The submodel extends the development in reference [12] to include suppressant chemistry. In order to maintain compatibility with a number of approaches, the output of the model is a simple, extinction/no-extinction switch that is used to shut off the combustion model. The state of the switch, on or off, is dictated by physical and chemical conditions within a computational cell. The switch can be stated as a Damkohler number (Da) as follows:

$$\begin{aligned}
 Da_{critical} < \frac{t_{flow}}{t_{chemical}} &\Rightarrow \text{Combustion Unaltered} \\
 Da_{critical} \geq \frac{t_{flow}}{t_{chemical}} &\Rightarrow \text{Combustion Terminated}
 \end{aligned} \tag{1}$$

where the characteristic flow and chemical times, t_{flow} and $t_{chemical}$, respectively, are described below. For the RANS development in this study, the critical value of the Damkohler number, $Da_{critical}$, will be assumed to be a constant and will be determined empirically. Comparison with data will determine whether or not this assumption is warranted, i.e., has sufficient accuracy to be

of engineering usefulness. A similar criteria has been recently used in LES, but $Da_{critical}$ is not assumed constant but a dynamic length scale ratio [15].

The characteristic flow time, t_{flow} will be estimated by the Kolmogorov time scale,

$$t_{flow} = \left(\frac{v}{\epsilon} \right)^{1/2} \quad (2)$$

where v is the mixture kinematic-viscosity and ϵ is the rate of kinetic energy dissipation. This isothermal estimator fails to consider a number of important effects that are known to exist in reacting flows. These include dilatation, strong viscosity gradients associated with high temperatures, and baroclinic vorticity generation. Further, as a momentum based estimator, it does not directly contain estimates of scalar gradients. Alternatives include the reciprocal of the scalar dissipation or a combination of the two (cf [15,16]). However, in the interest of compatibility and simplicity, it is used here. For our purposes, the rate of kinetic energy dissipation, ϵ , is obtained from the solution for the ϵ equation from a standard $k-\epsilon$ turbulence model. The mixture kinematic-viscosity, v , is based on the average species composition and temperature for the computational cell.

Phenomenological reasoning is used to determine what conditions are representative of a particular flame (or flame segment) which is more difficult than 90% of the other flames to suppress. The higher the strain rate, the easier a flame is to suppress. Equation 2 represents the average strain on a flame and by itself is not conservative. The reactant and suppressant species and temperature will be specified somewhat conservatively. Regardless of the species composition within a given cell, as long as there is a flame present, it is assumed that there is a stoichiometric flame in that cell that must be suppressed. Second, regardless of the source of suppressant, either from the air or fuel side, the cell averaged value for suppressant concentration will be used. This assumption is equivalent to assuming a uniformly distributed suppressant throughout the cell, thus under pre-

dicting the suppressant loading if it all comes from either the air (as usual) or the fuel side. Small scale concentration fluctuations could result in a flame not seeing any suppressant regardless of the average concentration within the cell. However, in practice, suppressants are not injected gently and small scale fluctuations are assumed to have damped by the time it reaches a flame. The temperature of the reactants will be assumed to be the cell-averaged value. This assumption is conservative in that the average reactant temperature will always be lower than the cell temperature when combustion is present, and higher-temperature reactants are more difficult to suppress.

Depending on the local strain rate, the flame structure can range from a laminar flamelet to a distributed reaction zone that in the limit becomes a perfectly stirred reactor (PSR). For pragmatic reasons, a perfect stirred reactor (PSR) [17] representation of the flame structure is chosen since it entails only point calculations and for thermal suppressants, it appears that details of location of heat absorption are not important [11]. Thus,

$$t_{chemical} = t_{PSR_{blowout}}. \quad (3)$$

The intention is to precalculate [18] the blowout times as a function of reactant composition and temperature. The condition given by Equation 1 is evaluated for each combustion cell at each time step using the precalculated values given by Equation 3 and the calculated value from Equation 2. The decision is local in time and space (to that cell for that time step). Extinction within a cell does not preclude re-ignition at a subsequent time step if the cell temperature is above an ignition criteria, conservatively taken as the auto-ignition temperature for this study. Fire extinguishment occurs when flame extinction has occurred everywhere in the domain. It is important to note that above a certain temperature, no clear blowout time exists, but the reaction temperature drops monotonically to the reactant temperature. For the calculations done here, this temperature was

around 1950 K for hydrocarbons and around 1100 K for CO/H₂. Above these temperatures it is assumed that the reaction cannot be suppressed.

Two kinetic sets were joined for use in this study, a high temperature and molecular weight hydrocarbon set [19] and a fluorocarbon suppressant set [20]. The hydrocarbon set has 173 species and 1169 reactions and the suppressant set has 63 species and 672 reactions. Compatibility was checked between the sets and found to be within a factor of 2 in residence time [21]. This can be taken as the uncertainty in the PSR calculations for blowout residence time for this study.

We use C₈H₁₈ as representative of aviation fuels and consider the possibility of CO and H₂ being present due to fuel rich burning that is characteristic of fires. We consider the thermal suppressants N₂, CO₂, H₂O, and C₂HF₅. Due to the presence of recirculation zones in most practical geometries, it must be considered that the combustion products, N₂, CO₂, H₂O, can act as high temperature suppressants. Short lived radicals are not considered as reactants, but the PSR assumption considers that they have infinite mobility within the reaction zone. With these considerations,

$$t_{PSR_{blowout}} = f(P, X_{C_2HF_5}, X_{CO_2}, X_{H_2O}, X_{N_2(\text{in excess of air})}, X_{CO}, X_{H_2}, X_{Fuel}, \text{Fuel Type}, T). \quad (4)$$

Thus, without some simplification, there would be 10 parameters necessary to build a table of results, corresponding to 5¹⁰ (10 million) table elements if only 5 levels for each variable was assumed. This table would be unwieldy in practice and require significant resources to build. Thus, for this study, simplifications are made. One of the largest contributors to the number of parameters is the recirculation of combustion products (i.e., N₂, CO₂, H₂O) that result in a suppressant mixture, regardless of the injected suppressant composition. A recent study [22] shows

that heat capacity effects at the extinction limit for thermal suppressants permit a mixing rule to be used for suppressant mixtures based on their pure values. The mixing rule states that

$$\frac{1}{XLIM_{suppressantmixture}} = \sum_{species} \left(\frac{X_{relative}}{XLIM_{species}} \right) \quad (5)$$

where $XLIM_{species}$ is the suppressant mole fraction that extinguishes the flame for a specific suppressant species, $X_{relative}$ is the mole fraction of that particular suppressant species divided by the total suppressant mole fraction, and $XLIM_{suppressantmixture}$ is the suppressant mole fraction for extinction for the mixture of suppressants in the specific fuel/air mixture. The rule only works for thermal suppressants and is similar to Le Chatelier's rule (cf, [23],[24]) which is used here for CO and H₂ mixtures with C₈H₁₈. Le Chatelier's rule is for premixtures; however, the same factor controlling the lean flammability limit of a premixed flame also controls the limiting concentrations of reactants for a diffusion flame [25]. These two rules significantly reduce the size of the table by only requiring pure suppressant and fuel compositions to calculate mixture compositions. Le Chatelier's rule does not apply in the pure strain limit, thus the table does not completely collapse to pure values only. From calculations, it was also found that for pressures within 25% of 1 atm the blowout times varied by less than a factor of 2, suppressant concentrations were within 12%, and that C₈H₁₈ was a good representation of low molecular weight alkanes to methane. As an implementation issue, the PSR calculations were least-squares fit with an algebraic response surface and the surface is used in the calculations.

In the interest of space, simplification and implementation details will not be given here but can be found in reference [21]. An example of the PSR calculations is shown in Fig. 1 for N₂ in C₈H₁₈. As the residence time gets shorter, the amount of N₂ in excess of air required to cause

blowout decreases until the pure strain limit is reached. With increasing reactant temperature, the amount of N_2 required for extinction increases and the residence time at the pure strain limit decreases. By approximately 1300 K, no amount of suppressant will quench the flame (provided there is fuel and oxygen present) at long residence times, and at 1950 K, no amount of suppressant will quench the flame for any residence time. All fuel and suppressant combinations show curves similar to that in Figure 1 with the exception of C_2HF_5 with CO/H_2 mixtures, in which some kinetic activity appears to exist around 900 K.

A number of comparisons were made between PSR calculations for mixtures and predictions from the response surfaces for the pure fuels combined with the mixing rules [21]. The results were good with deviations generally less than a factor of two in blowout time as long as chemical activity was not present in the suppressant. As an example, Table 1 shows the effect of recirculating product back into the fuel/air reactant mix at constant enthalpy for an initially stoichiometric mixture of C_8H_{18} :air at 1 atm. Thus, as the recirculated production mole fraction increases, the initial temperature of the product/reactant mixture increases. The products are a suppressant, but their high temperature makes the reactant mixture temperature sufficiently high that their adverse heat capacity (suppressant effect) is overcome. The mixture is increasingly more difficult to extinguish with increased product concentration as evidenced by shorter blowout times in Table 1. As has previously been noted [26], a fire in a recirculation zone with low strain rate and high product recirculation is very difficult to suppress.

The current extinguishment model was implemented as a subroutine in VULCAN which is based on the KAMELEON-Fire code (cf [27]). VULCAN uses a RANS based model suite including a $k-\epsilon$ turbulence model [28], the EDC combustion model [12], a soot model [29], and a radiation

model [30]. The conservation equations are discretized on a staggered, block-structured grid with second-order upwind differencing for the convective terms and solved using a version of the SIMPLE algorithm [31].

Constant Calibration

There are two constants in the model that require calibration. The first is the critical Damkohler number in Equation 1. This constant calibration is based on jet blowout. From experiments, it is noted that blowout occurs when the stoichiometric line reaches its maximum radial width based on isothermal jet expansion (cf [32]). Therefore, a jet mixing problem, consisting of a subsonic round-jet of ethane issuing into a quiescent atmosphere of air, was run with VULCAN and Equation 2 was calculated at the maximum radial extent of the stoichiometric ethane/air line. This value was compared to 76 μ sec, the PSR blowout time for the jet conditions. The result is $Da_{critical} = 1.367$. Grid sensitivity studies were conducted and details can be found in reference [21].

For the second constant, a practical minimum strain, or residence time needs to be defined since the $k-\epsilon$ model approach does not apply to laminar flows. It has been clearly shown that the 'flammability limits' are a function of strain level [33]. Broad flammability limits can be obtained with premixtures in carefully-controlled laminar-flow [33]. For this study, the limits of reference [10] are used based on cup-burner values for diffusion flames. The cup-burner value for N_2 extinguishment is 32-34% depending on the fuel type at 1 atm and 298 K. From Fig. 1, this corresponds to a time-scale of about 600 μ sec. For residence times longer than this value, the mole fraction to extinguish is held at the 600 μ sec value. This time scale is taken to represent an effective 'laminar' strain limit for the model and is thus applied to all mixtures.

Comparison with Experimental Data

To assess the performance of the extinction model, comparison is made with experiments on the the stabilization and extinguishment of non-premixed flames formed behind a backward-facing step. These experiments were conducted for a variety of air inlet velocities, step heights, agent concentrations, and agent injection periods [14]. Fig. 2 shows the geometry of the computational model. The grid contains 162,368 nodes, 118 axial by 32 vertical by 43 transverse. Comparison with a coarser grid solution showed minor grid sensitivities. Details on the geometry, boundary conditions, and sensitivities for the simulations can be found in [21].

Experimental details can be found in references [14, 34]. The tunnel is 0.154 m by 0.154 m by 0.87 m long with a 0.064 m high step. Behind the step is a 0.15 m by 0.15 m porous burner. For comparison with calculations in this study, conditions held constant include ambient pressure of 100kPa, a 7.6 mm/s ethane injection velocity, N_2 suppressant premixed in air, and a turbulence intensity of 6%. The walls in the experiment and simulation are hot due to the establishment of a steady-state flame prior to suppressant injection.

Three comparisons are made at two airflow rates, 9.33 m/s and 14.1 m/s, and at two suppressant injection durations (2 seconds and 0.3 seconds). An auto-ignition temperature of 745 K is used for ethane. For each comparison, the N_2 concentration is varied until the fire is extinguished. Fig. 2 shows the computational results at 25 seconds, just prior to suppressant injection for the 9.33 m/s case. The experiments showed low-frequency, large-scale flame fluctuations that are not captured by the time-averaged RANS simulation. For the long injection times, the experiments showed that 36.5% N_2 (N_2 quoted is in excess of that in air) was required for fire extinguishment for both air-flow rates. The short injection time was not tested with N_2 but earlier results [14] showed an injec-

tion time/suppressant concentration relationship for CF_3Br that predicts a ratio 1.3 for the extinguishment concentration at 0.3 seconds to 2.0 seconds.

Figure 3 shows a snap-shot at 2.4 seconds after injection for the 9.33 m/s case with 65% N_2 . Nitrogen concentrations for the two second injection, 9.33 m/s case were varied. It was found that 65% N_2 would completely extinguish the fire, while 60% N_2 would not. This result is quite conservative relative to the experimental value of 36.5% N_2 . For the 14.1 m/s case with two second injection, it was also found that 65% would extinguish the fire while 60% would not. For the latter case, Fig. 4 shows three variables on a vertical slice down the center axis of the channel. The first image shows the local ratio of residence time (using Equations 1 and 2 with the critical Damkohler number of 1.367 to calculate a residence time) to that required for blowout, $\tau_{\text{residence}}/\tau_{\text{extinction}}$, by purely strain. The backward facing step creates a low velocity region that results in long residence times relative to those required for extinction, even for the 14.1 m/s case. Therefore, in this velocity range with this set of experimental conditions, the model and experiments agree there is no effect of increasing velocity. For short injection times, it was found that 84.5% N_2 (i.e., 1.3 times 65%) would extinguish the flame with a 0.3 second injection but not with a 0.2 second injection in good agreement with the 1.3 ratio for the experimental data.

Discussion & Conclusions

In general, the comparisons with experimental data indicate the potential for using a subgrid flame extinction model in a CFD simulation as a design tool for fire suppression systems. The developed model was specifically designed to be compatible with common fire modeling approaches, simple, fast executing, and somewhat conservative. The trends were well predicted but the model itself is quite conservative in its present form for the conditions tested. A much broader range of

conditions requires testing to draw firm conclusions. As with fire data in general, well controlled data like that of references [34, 35] are difficult to come by and are highly valued.

Diagnostics from the model point to improvements to reduce the conservatism. From Fig. 4 it can be seen that the ratio of actual suppressant to that required for extinction is over unity except in a small region where there is high temperatures. Even at this near extinction condition, predicted temperatures are in excess of 1100 K. From Fig. 1 it can be seen that temperature plays a strong role in the amount of suppressant required. The current model is based on an 'on/off' switch. If the fire is not extinguished in a cell, then it is allowed to continue unabated, resulting in excessively high temperatures which require excessive suppression concentrations. If a 'dimmer' switch model were used, i.e., the enthalpy or reaction rate were reduced as extinction was approached, then the temperatures would drop, requiring less suppressant for extinction.

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Tables & Figures

TABLE 1 - PSR Calculations Using Hot Products Recirculated Back Into the Reactant Stream.
 Reactant Composition: stoichiometric C₈H₁₈:air. Product composition: 73.5%N₂/14.0%H₂O/
 12.5%CO₂. Reactant temperature calculated based on constant enthalpy equal to no product
 recirculation.

| Product (Suppressant) Mole Fraction | Reactant Temperature (K) | Blowout Time - PSR (μsec) | Blowout Time - Mixing rules & Response Surface (μsec) | Error in Blowout Time |
|--|--------------------------------|------------------------------|--|--------------------------|
| 0.0 | 298 | 76 | 76 | 0% |
| 0.1 | 538 | 66 | 69 | 5% |
| 0.2 | 762 | 54 | 68 | 26% |
| 0.3 | 975 | 44 | 40 | 10% |
| 0.4 | 1181 | 36 | 20 | 44% |
| 0.5 ^a | 1384 | 26 | 9 | 65% |

a. Highest value that can be suppressed due to high reactant temperatures.

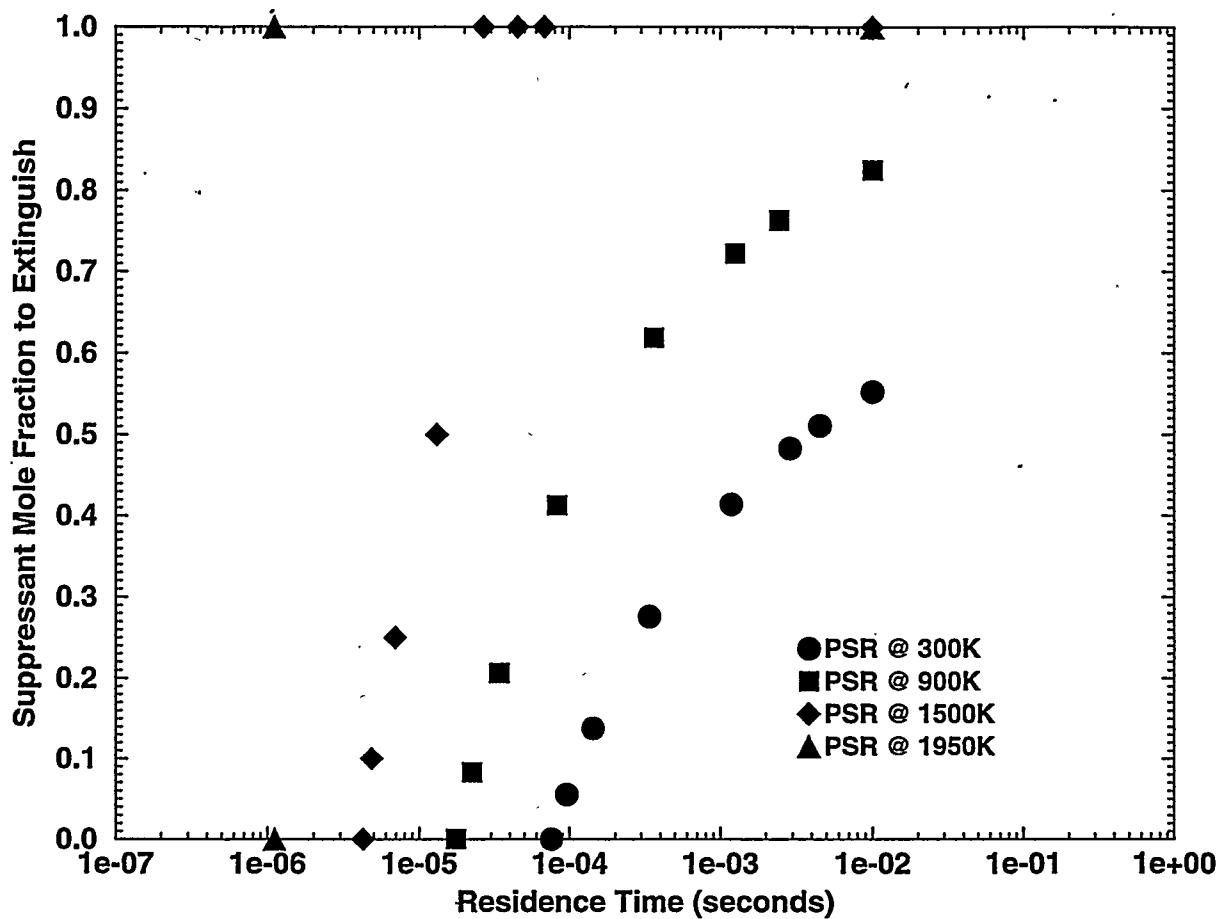


Fig. 1 - Blowout Suppressant Mole Fraction vs. Residence Time for Stoichiometric C_8H_{18}/Air

Mixtures with N_2 (in excess of air) at 1 atm Pressure.

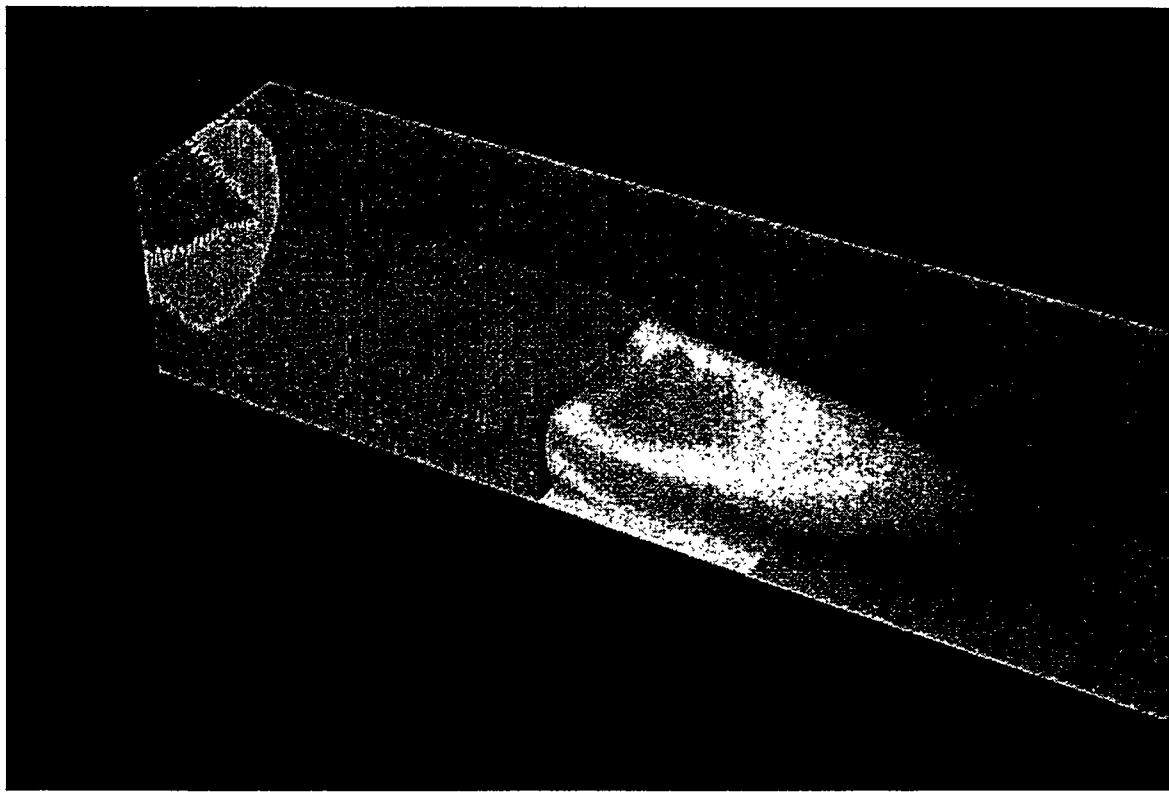


Fig. 2 - Three-Dimensional View of Steady Fire Behind the Step at Steady State Just Prior to Sup-
pressant Injection. Ethane Injection is at Base of Backward Facing Step. Temperature is Imaged.

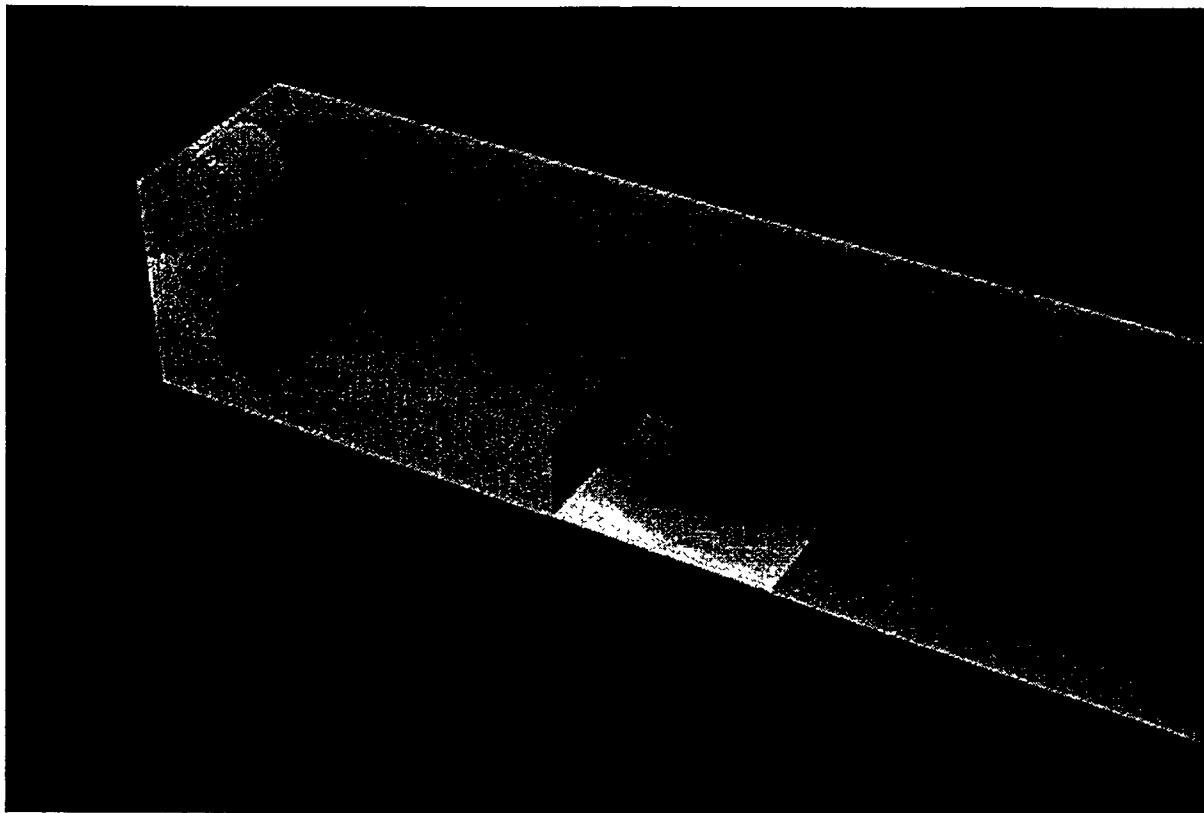


Fig. 3 - Temperature Image at 2.4 Seconds After Injection of 65% N₂ Just Prior To Complete Fire Extinguishment for the 9.33 m/s inlet velocity and 2 second injection case.

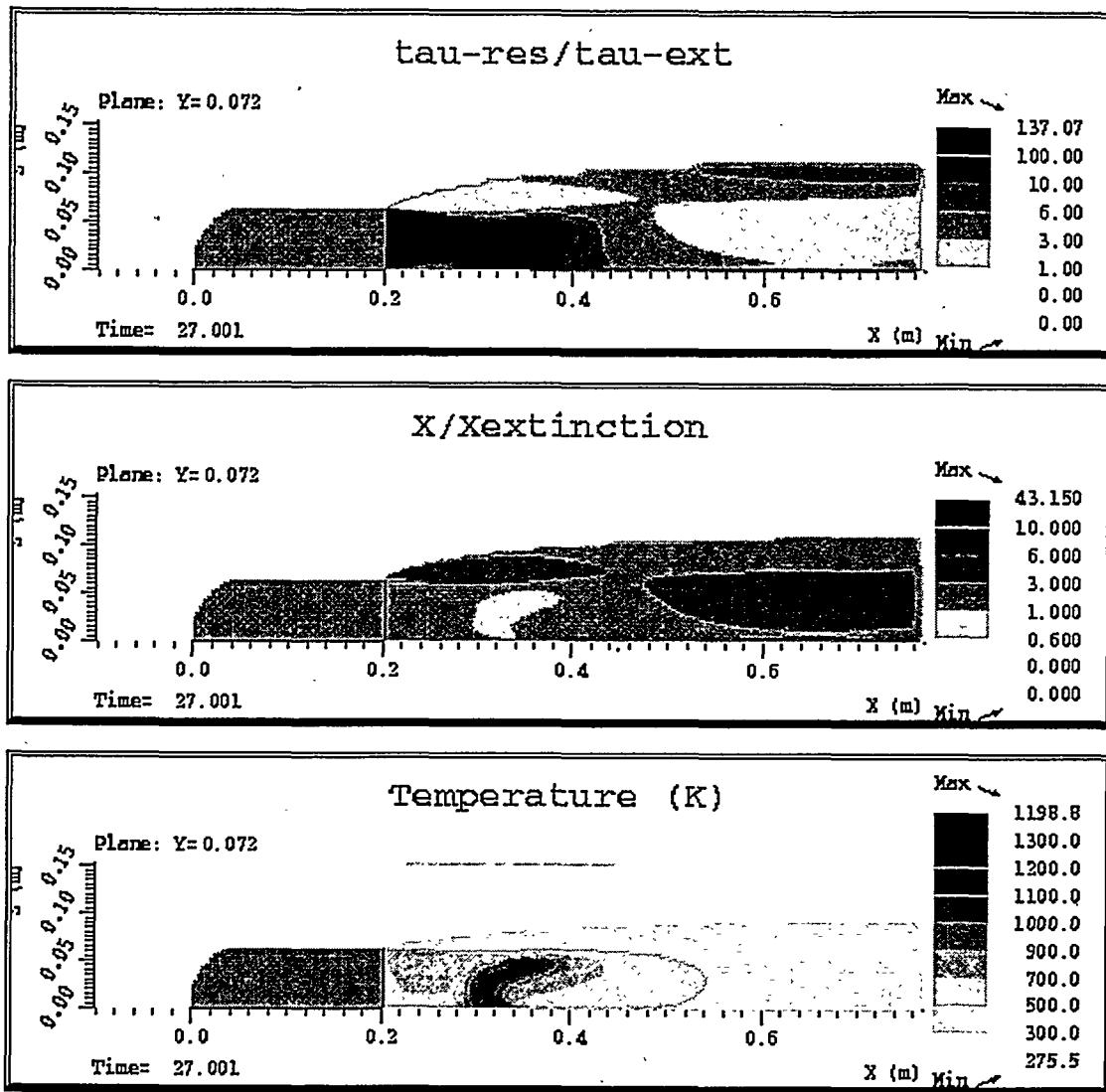


Fig. 4 - Center Channel Cross-sections Showing Local a) Residence-Time/Extinction Time, b) Suppressant Mole Fraction/Extinction Mole Fraction, and c) Temperature for the case with 60% N₂, 14.1 m/s, with a 2 second injection.