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An Adapted Flame Suppression Model for Modeling Fires

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Abstract

Suppression of flames by diluent agents is achieved through the diluents' effect on the chemical rates, thus altering the ratio of the chemical and mixing time scales. Suppressant can act as a thermal diluent or retard rates through dilution, though the former is generally found to be significant for a larger class of suppressants. Chemical scavenging of radicals can also occur, but such suppressants are not considered here. In discretized computational models, the chemical rates of reaction are not always specifically modeled. The Eddy Dissipation Concept (EDC) model is one of the more frequently used reaction models in Sierra/Fluid Mechanics module for fires, Fuego. In the EDC model, reaction rates are generally assumed to be mixing-limited so that the addition of suppressant to create a reaction-limited state needs additional modeling. We have adapted the methods of Zhang and Soteriou (2011)[1], describing the variation of global reaction rates with suppressant addition, for predicting the suppression in the context of the EDC model in Fuego. The propensity for suppression is tied to the ratio of the reaction and diffusion timescales, and therefore is calibrated to a single parameter, the critical Damköhler number. Two experimental scenarios found in the literature are evaluated to determine the fit coefficient that best replicates existing data. The scenarios include a cup burner fire and a flame stabilized behind a backward facing step.

Methods/Theory

The fire science group at Sandia uses a Fluid Mechanics capability under the SIERRA architecture. The module used for fires and other such reacting flows is the Fuego module. The SIERRA architecture is an open source framework for solving detailed engineering science problems, and contains many sub-modules for solving a variety of problem types. The EDC model is frequently used for predicting fire consequence. Because EDC is a mixing limited approximation, there is no native notion of reaction time scale, and the effects of extinction by diluent addition are generally under-predicted.

The Damköhler number relates the mixing and reaction timescales, and if those scales are known the propensity for extinction can be predicted by comparing the magnitudes. To approximate the reaction timescale, the typical model output from a perfectly stirred reactor (PSR) model is presumed applicable for the material within a computational cell.

$$Da = \tau_{mix} / \tau_{react}$$

Suppression is achieved in a perfectly stirred reactor when the rate of transport exceeds the reaction rate. Thus, solving for the extinction temperature, one can approximate the extinction time in the system.

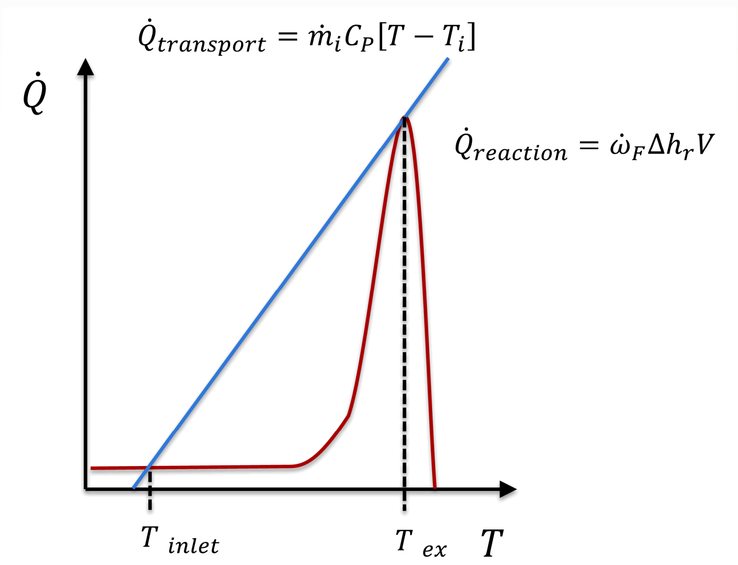

Figure 1. A schematic of the PSR approximation employed for this suppression theory.

T_{ex} occurs where the slope of the two equations is equal, which can be determined from the following relation using a Newton solver:

$$1 - \frac{T_a(T_{ex} - T_i)}{T_{ex}^2} + (n_F + n_O)\frac{1 - T_i/T_{ex}}{1 - T_{ex}/T_{ad}} = 0$$

The extinction residence time can be calculated from a model for the equality of heat rate at the extinction point and equations of state (ideal gas). A single step Arrhenius reaction model is assumed:

$$t_{res,ex} = \frac{1}{A_f \phi^{n_O}} \left(\frac{\Delta h_r \ R}{C_p p M_{mix}}\right)^{n_F+n_O-1} \frac{T_{ex} - T_i}{(T_{ad} - T_{ex})^{n_F+n_O}} T_{ex}^{n_F+n_O-1} exp(T_a/T_{ex})$$

Three temperatures are unknown for these equations, T_a (reaction activation temperature, or E_a/R), T_i (inlet temperature) and T_{ad} (adiabatic reaction temperature). T_a comes from an assumed reaction activation energy. T_i is found by walking back the stoichiometric products to an inlet temperature. T_{ad} is found by walking forward the stoichiometric reactants to completion for an adiabatic reaction temperature.

$$C_{n_C} H_{n_H} O_{n_O} N_{n_N} [Fuel] + (0.25 n_H + n_C - 0.5 n_O) O_2 -> (n_C) CO_2 + (0.5 n_H) H_2O + (0.5 n_N) N_2$$

$$C_{n_C} H_{n_H} O_{n_O} N_{n_N} [Fuel] + (0.25 n_H + n_C - 0.5 n_O) O_2 < - (n_C) CO_2 + (0.5 n_H) H_2O + (0.5 n_N) N_2$$

Excess reactant and product is a diluent in the calculation, and Cantera routines are used to extract temperatures based on the forward and reverse reactions.

Implementation detail: The T_i extraction will occasionally fail, due to very low temperatures (below realistic thermodynamic data, due to heat loss). We model T_i in this case at the lower temperature limit defined in the code, usually 250K. Looking at the Figure 1 schematic, it is not thought to induce significant error.

1. S. Zhang, M.C. Soteriou, "An analytical model for the determination of the cup-burner minimum extinguishing concentration of inert fire suppression agents," Proc. Combust. Inst., 33, 2505-2513, 2011.

Validation & Critical Da Calibration

Extinction in the model occurs beyond a critical Damköhler, in which case no reactions are allowed by setting the EDC reaction progress variable $\gamma\chi$ to zero. Thus, a critical Damköhler number is required as a single calibration parameter for the model.

Two cases have been evaluated for calibration, a cup burner flame[2], and a flame stabilized behind a backward facing step[3-4]. The mole fraction of diluent (X) is varied in these tests, and a critical extinction of around 30% is usually reported.

Cup Burner Predictions:

The cup burner is laminar, and not the best platform to test a turbulent combustion model. But, the model should not adversely affect predictions in the laminar limit. Figure 2 shows air flame results for four critical Da's and at two mole fractions of diluent (0 and 27%)

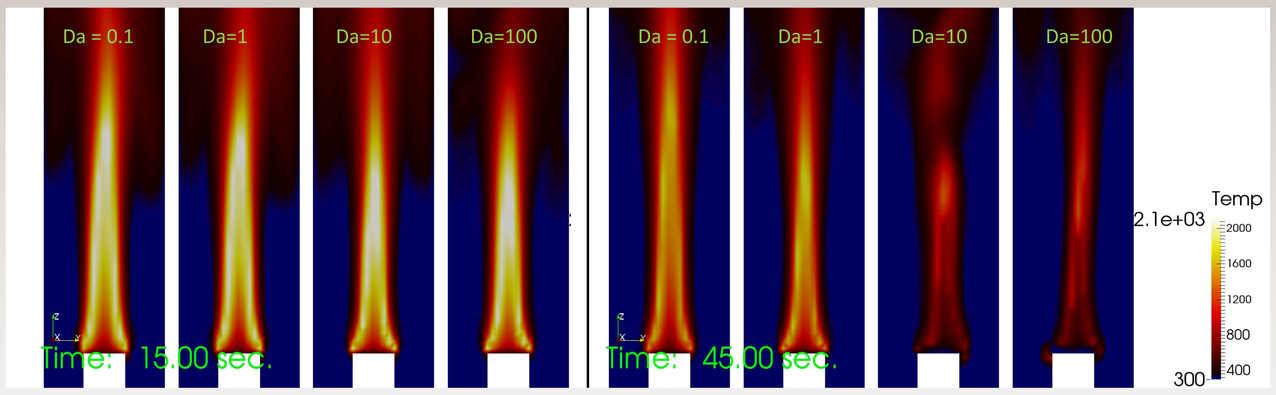

Figure 2. Cup burner predictions for four critical Damkohler numbers and two mole fractions of diluent (0 on the left and 27% on the right).

The four left cases show how the Da=100 case slightly decreases the flame height, suggesting that Da=100 may be too high. The right four cases illustrate how the suppression model decreases flame temperatures.

Backward Facing Step Predictions:

Figure 3 shows centerplane predictions for five critical Da's at 0.01 and 1.5 seconds after diluent injection (5.0 seconds) with X=32. This is the 7.1 m/s velocity condition from Takahashi et al. The first time series show how the Da=100 scenario suppresses the burning for ambient conditions (before arrival of the diluted environment). The second shows how the flame is increasingly suppressed for higher critical Da's. This helps with selecting a critical Da.

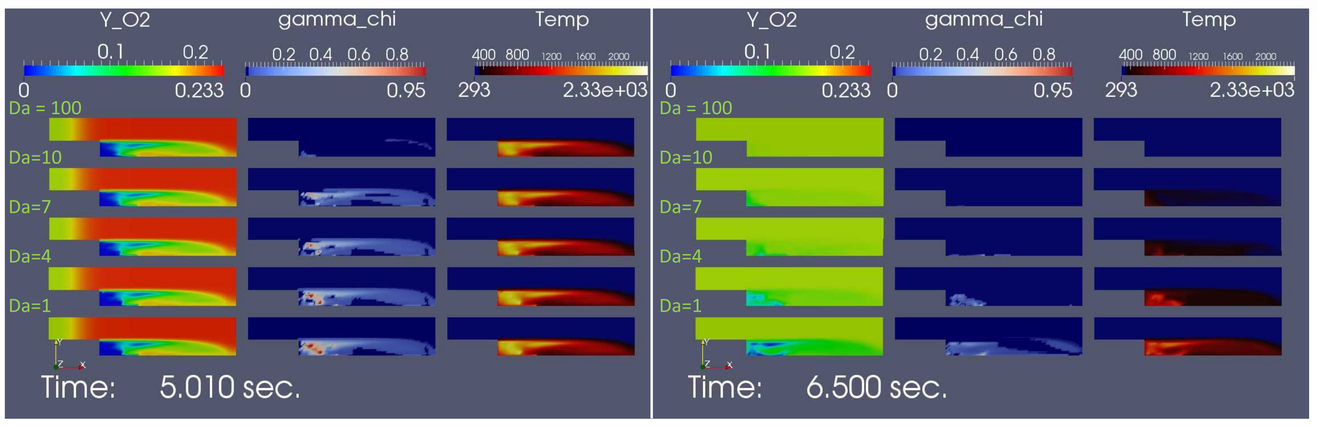

Figure 3. Predictions for five critical Da's and X=32 at two times.

This Figure 4 is similarly organized, except it shows variations in X, with the critical Da held constant at 10. This suggests the accuracy of the predictions when a critical Da of 10 is selected.

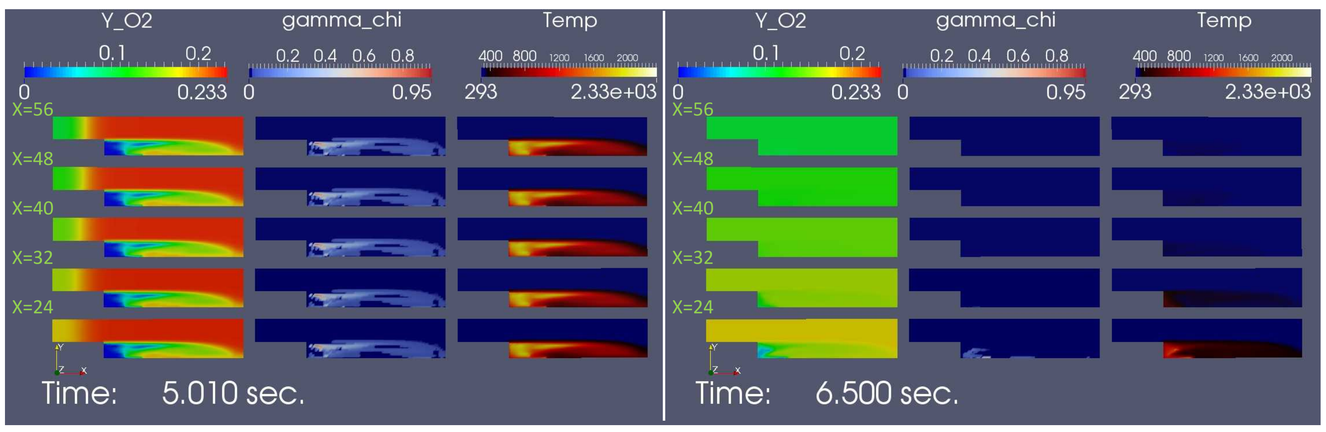

Figure 4. Predictions for five values of X, with critical Da fixed at 10 at two times.

Figure 4 suggests that extinction is found at approximately the correct molar dilution ratios, with X=32 (near the critical value) exhibiting only minor reactions at the 6.5 second point. The critical extinction molar dilution ratio from the data is X=30. This represents a significant improvement for reaction modeling in a suppressing environment.

Summary

A. We present a new method for modeling suppression with an EDC reaction model based on a PSR model.
B. A critical Damköhler number in the range of 4-10 gives respectable accuracy for this new model.
C. The suppression model represents a significant improvement for EDC model predictions of suppression, and should be useful for diluent based suppression conditions.

2. Senecal, J.A., "Flame extinguishing in the cup-burner by inert gases," Fire Safety Journal, 40, 579-591, 2005.
3. Takahashi, F., W.J. Schmoll, E.A. Strader, V.M. Belovich, "Suppression of a Nonpremixed Flame Stabilized by a Backward-Facing Step," Combustion and Flame, 122, 105-116, 2000.
4. Takahashi, F., W.J. Schmoll, E.A. Strader, V.M. Belovich, "Suppression Behavior of Obstruction-Stabilized Pool Flames," Combust. Sci. and Tech. 163, 107-130, 2001.

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