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Combustion inhibition and enhancement of cup-burner flames by CF₃Br, C₂HF₅, C₂HF₃Cl₂, and C₃H₂F₃Br

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Abstract

Numerical simulations of cup-burner flames in normal Earth gravity have been performed to study the combustion inhibition and unwanted enhancement by fire-extinguishing agents CF₃Br (Halon 1301) and some potential replacements (C₂HF₅, C₂HF₃Cl₂, and C₃H₂F₃Br). A propane-ethanol-water mixture, prescribed for a Federal Aviation Administration (FAA) aerosol can explosion simulator test, was used as the fuel. The time-dependent, two-dimensional numerical code, which includes a detailed kinetic model (up to 241 species and 3918 reactions), diffusive transport, and a gray-gas radiation model, revealed unique twozone flame structure and predicted the minimum extinguishing concentration of agent when added to the air stream. Despite striking differences in the flame shape, the agent effects were similar to, but stronger than, those in microgravity flames studied previously (for two of the agents). The peak reactivity spot (i.e., reaction kernel) at the flame base stabilized a trailing flame, which was inclined inwardly by a buoyancy-induced entrainment flow. As the volume fraction of agent in the coflow (X_a) increased gradually: (1) the premixed-like reaction kernel weakened; (2) the flame base detached from the burner rim, oscillated (particularly for CF₃Br), until finally, blowoff-type extinguishment occurred; (3) the calculated maximum flame temperature remained nearly constant (≈ 1800 K) or mildly increased; and (4) the total heat release of the entire flame decreased (inhibited) for CF_3Br but increased (enhanced) for the halon replacements. In the trailing flame with C_2HF_5 , a two-zone flame structure (with two heat-release-rate peaks) developed: in the inner zone, H₂O (a product of hydrocarbon–O₂ combustion and a fuel component) was converted further to HF and CF₂O through exothermic reactions occurring in the outer zone, where exothermic reactions of the inhibitor also released heat; CO_2 was formed in-between. Thus, addition of C_2HF_5 resulted in

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unusual (non-chain branching) reactions and increased total heat release (combustion enhancement) primarily in the trailing diffusion flame.

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1. Introduction

The use of the effective fire suppressant CF_3Br (bromotrifluromethane, Halon 1301) has been discontinued because of its destruction of stratospheric ozone, with exceptions being certain critical applications such as the suppression of cargo-bay fires in aircraft. Halon replacement agents must pass a mandated Federal Aviation Administration (FAA) test [1,2], in which a simulated explosion of an aerosol can, caused by a fire, must be suppressed by the agent. Unfortunately, unlike CF_3Br , some replacement agents, when added at less than their inerting concentrations, created a higher over-pressure in the test chamber and thus failed the test.

Similar combustion enhancement by various halogenated inhibitors has been described in previous studies [3–12]. Recent work [13–15] employing thermodynamic equilibrium and perfectly stirredreactor calculations (for premixed systems) indicated that higher overpressures in the FAA aerosol can tests might be due to higher heat release from reaction of the inhibitor itself. Nonetheless, the agents should still reduce the overall reaction rate and inhibit the reaction [16,17]. For diffusion flames, however, the flame structure and inhibition or combustion enhancement processes are not yet fully understood. In a previous paper [18], the authors reported the results of comprehensive numerical simulations, based on earlier work [19–25], for zero-gravity $(0g_n)$ cup-burner flames with CF_3Br and C_2HF_5 (pentafluoroethane, HFC-125) added to the coflowing air. This paper extends the effort to normal-gravity (1gn) cupburner flames of the FAA aerosol can test [ACT] fuel mixture, and to more agents C₂HF₃Cl₂ (2, 2-dichloro-1,1,1-trifluoroethane, HCFC-123) and $C_{3}H_{2}F_{3}Br$ (2-bromo-3,3,3-trifluoropropene, 2-BTP) in addition to CF₃Br and C₂HF₅. Additional numbers of carbon and fluorine atoms in the halon-replacement-agent molecules, compared to CF₃Br, represent potential energy contributions at a fixed concentration if they burn completely to HF (and COF_2 if F/H > 1).

2. Computational method

A time-dependent, axisymmetric numerical code (UNICORN) [26,27] is used for the

simulation of coflow diffusion flames stabilized on the cup burner. The code solves the axial and radial (z and r) full Navier–Stokes momentum equations, continuity equation, and enthalpy- and speciesconservation equations on a staggered-grid system. A clustered mesh system is employed to trace the gradients in flow variables near the flame surface. The thermo-physical properties such as enthalpy, viscosity, thermal conductivity, and binary molecular diffusion of all of the species are calculated from the polynomial curve fits developed for the temperature range 300-5000 K. Mixture viscosity and thermal conductivity are then estimated using the Wilke and Kee expressions, respectively. Molecular diffusion is assumed to be of the binary-diffusion type, and the diffusion velocity of a species is calculated using Fick's law and the effective-diffusion coefficient of that species in the mixture. A simple radiation model [28] based on the optically thin-media and gray-gas assumption was incorporated into the energy equation. Radiation from CH₄, CO, CO₂, H₂O, HF, COF₂ and soot was considered in the present study. The Plank mean absorption coefficients are obtained from the literature for the first four species [28] and HF [29], or calculated for COF_2 [29] and soot [30]. The finite-difference forms of the momentum equations are obtained using an implicit QUICKEST scheme [26], and those of the species and energy equations are obtained using a hybrid scheme of upwind and central differencing.

A comprehensive reaction mechanism was assembled for the simulation of propane or ACT fuel flames with CF3Br, C2HF5, C2HF3Cl2, or $C_{3}H_{2}F_{3}Br$ added to air from four mechanisms: the four-carbon hydrocarbon mechanism of Wang and co-workers [31,32] (111 species and 1566 one-way elementary reactions), detailed reactions of ethanol (5 species and 72 reactions) of Dryer and co-workers [33–35], the bromine and chlorine parts of the mechanism of Babushok et al. [36-39] (10 additional species and 148 reactions), and a subset (51 species and 1200 reactions) of NIST HFC mechanism [40,41]. The final chemical kinetics model (187 species, 3198 reactions for CF₃Br, C₂HF₅, and C₃H₂F₃Br; or 241 species and 3918 reactions for $C_2HF_3Cl_2$) and a soot model [30] are integrated into the UNICORN code. Transport data for 139 species are available in the literature; for the remaining 38 species, data are constructed through matching these species with the nearest species (based on molecular weight) with known transport data. The fuel is the ACT fuel gas mixture (mole fractions: C_3H_8 , 0.159; C_2H_5OH , 0.454; and H_2O , 0.387), and the agent is CF₃Br, C_2HF_5 , $C_2HF_3Cl_2$, or $C_3H_2F_3Br$ added to "air" (21% O_2 in N_2).

The boundary conditions are treated in the same way as that reported in earlier papers [19–25]. The computational domain is bounded by the axis of symmetry, a chimney wall, and the inflow and outflow boundaries. The burner outer diameter is 28 mm and the chimney inner diameter is 95 mm. The burner wall (1-mm long and 1-mm thick tube) temperature is set at 600 K and the wall surface is under the no-slip velocity condition. The mean fuel velocity is 0.853 cm/s for the ACT fuel, and the mean oxidizer velocity is 10.7 cm/s at 294 K.

Validation of the code with the kinetic model was performed through the simulation of opposing-jet diffusion flames. The predicted extinction strain rates for propane–air flames (no agent) were within 7.5% of the measured values (with an error margin of 9%) by Zegers et al. [42]. The predicted extinction agent concentrations for CF₃Br and C₂HF₅ are within 4% of the measured concentrations in weakly stretched flames and within 25% in highly stretched flames. Although cup-burner data using the ACT fuel are unavailable for a direct comparison, computation with the assembled reaction mechanism should provide insights into the detailed flame structure.

3. Results and discussion

3.1. Internal flame structure

The flame-base region supported a trailing flame and controls the flame attachment, detachment, and oscillation processes [43,22]. Small variations in the agent volume fraction in the coflowing oxidizing stream (X_a) resulted in profound changes near the extinguishment limit. Figure 1 shows the calculated structure of an agent-free flame (Fig. 1a) and near-limit flames with agent added at $X_a = 0.0204$ for CF₃Br (Fig. 1b), $X_a = 0.083$ for C₂HF₅ (Fig. 1c), and $X_{\rm a} = 0.018$ for C₃H₂F₃Br (Fig. 1d). The variables include the velocity vectors (\mathbf{v}) , isotherms (T), and heat-release rate (\dot{q}) . The base of the agent-free flame (Fig. 1a) was anchored at the burner rim. In contrast to $0g_n$ flames [18], which were formed vertically, the $1g_n$ flame inclined inwardly due to the buoyancy-induced flow. The contours of the heat-release rate showed a peak reactivity spot (i.e., the *reaction kernel* [43]) at the height from the burner rim, $z_k = 0.6$ mm. The chain radical species (H, O, and OH), as well as, heat diffused back against the incoming buoyancy-induced flow at the flame base (edge), thus promoting vigorous reactions to form the reaction kernel. The values of the variables at the reaction kernel were $\dot{q}_{\rm k} = 88$ W/cm³, $|\mathbf{v}_{\rm k}| = 0.162$ m/s $T_{\rm k} = 1414$ K, $X_{\rm O22k} = 0.037$, and $-\hat{\omega}_{\rm O2}$, $_{\rm k} = 0.000236$ mol/cm³ s; where $X_{\rm O22k}$ and $-\hat{\omega}_{\rm O2}$, $_{\rm k}$ are the volume fraction and consumption rate of oxygen, respectively. For the near-limit flames (Fig. 1b-d), the flame base was pushed inward by the nearly horizontal entrainment flow. Unlike the flame with CF₃Br (Fig. 1b), the heat-release rate contours for the near-limit flame with C₂HF₅ (Fig. 1c) or C₃H₂F₃Br (Fig. 1d) showed distinct flame structure.

Figure 2 shows the radial variations of calculated temperature and the heat-release rate crossing the trailing flame with C_2HF_5 (Fig. 1c) at $z = 5.6 \text{ mm} (z_k + 5 \text{ mm})$. At this height, the flame was characterized by "two-zone" structure (inner and outer) as was evident from two heat-release rate peaks. The inner zone (7.5 mm < r < 8.5 mm)was formed by the hydrocarbon $-O_2$ combustion. Although the temperature peak (1759 K) was closer to the inner reaction zone, the larger heat-release rate peak is in the outer zone (8.5 mm < r < 10 mm) by highly exothermic agent reactions. The outer heat-release-rate peak in the trailing flame in $1g_n$ (Fig. 2) was more evident, compared to the $0g_n$ case [18], due to increased convective fluxes of reactants (i.e., the blowing effect [43]) by the buoyancy-induced incoming flow.

Figure 3 shows the radial variations of the species volume fractions (X_i) crossing the trailing flame with C₂HF₅ (added at $X_a = 0.083$) at z = 5.6 mm. Oxygen penetrated through the outer zone and a pool of chain carrier radicals (H, O, and OH) was formed in the middle of the two zones at relatively high concentrations $(X_a \approx 10^{-3})$, thus contributing to both reaction zones. The initial hydrocarbon fuel components (C₃H₈ and C_2H_5OH) diffused from the fuel side, decomposed to fragments (CH₄, C₂H₄, and C₂H₂) and reacted with the chain radicals in the inner zone. In the outer zone, the agent (C_2HF_5) from the air side decomposed and diminished, and the volume fractions of many fluorinated species (CF₂O, C₂F₆, CF₂, CHF₃, etc.) peaked, and reacted with the radicals. The final products (CO₂, HF, and CF₂O) were distributed in a wide range. Although the outer zone has a structure similar to an agent (as fuel)-air premixed flame, the fuel-lean mixture would not have been self-sustained without interactions with the inner zone. Low levels of C₂HF₅ on the fuel side and H_2 on the air side in Fig. 3 were due to leakage in the opposite directions through the quenched zone below the flame base. These species' contributions to overall reactions in the opposite zones must be insignificant. Interestingly, H₂ and H₂O (formed by hydrocarbon–O₂ reaction as well as in the original fuel mixture) were largely converted to HF and CF₂O through highly exothermic reactions.



Fig. 1. Calculated structure of propane–ethanol–water mixture (ACT fuel) flames in air with or without added agent: (a) no agent, (b) CF₃Br at $X_a = 0.0204$, (c) C₂HF₅ at $X_a = 0.083$, and (d) C₃H₂F₃Br at $X_a = 0.018$.



Fig. 2. Calculated radial variations of the temperature and heat-release rate at z = 5.6 mm in a propane– ethanol–water mixture (ACT fuel) flame in air with C₂HF₅ at $X_a = 0.083$.

Figure 4 shows the radial variations of the calculated production (+) or consumption (-) rates (Fig. 4a) and heat-release rates (Fig. 4b) of species *i* crossing the trailing flame at z = 5.6 mm. In the inner zone, H₂, CO, and the chain radicals (H, O, and OH) were formed and consumed, O₂, and CF₂O were consumed, and H₂O, HF and CO₂ were formed. In the outer zone, C₂HF₅ and O₂ were consumed, HF, CF₂O, and CO were formed. The major contributors to the overall heat-release rate (Fig. 4b) were the formation of H₂O, CO₂ and HF in the inner zone and CF₂O and HF in the outer zone. The highly exothermic reactions with the heats of reactions in "()" include:



Fig. 3. Calculated radial variations of the volume fractions at z = 5.6 mm in a propane–ethanol–water mixture (ACT fuel) flame in air with C₂HF₅ at $X_a = 0.083$.

$$\begin{split} &H_2 + OH \to H + H_2O(+61\,kJ/mol)\,(R5) \\ &CO + OH \to CO_2 + H\,(+102\,kJ/mol)\,(R61) \\ &H_2O + F \to OH + HF\,(+74\,kJ/mol)\,(R1685) \\ &H_2 + F \to H + HF\,(+135\,kJ/mol)\,(R1679) \\ &CF_2 + OH \to CF_2O + H\,(+268\,kJ/mol)\,(R1849) \\ &CF_3 + OH \to CF_2O + HF\,(+493\,kJ/mol)\,(R1669) \\ &CF_2 + O \to CFO + F\,(+150\,kJ/mol)\,(R1849) \\ &CF_3 + O \to CF_2O + F\,(+342\,kJ/mol)\,(R1663) \\ &CF_3 + H \to CF_2 + HF\,(+215\,kJ/mol)\,(R1719) \end{split}$$

The reactions to form CF_2O are particularly exothermic because of its exceptionally low (negative) heat of formation (-640 kJ/mol).



Fig. 5. Calculated reaction kernel coordinates of propane-ethanol-water mixture (ACT fuel) flames in air with agent. $\triangle \blacktriangle$, CF₃Br; $\bigcirc \blacklozenge$, C₂HF₅; $\nabla \blacktriangledown$, C₂HF₃Cl₂; $\boxtimes \blacksquare$, C₃H₂F₃Br.

3.2. Flame characteristics

Figure 5 shows the effects of the agent volume fraction in the coflowing oxidizer on the calculated axial (z_k) and radial (r_k) positions of the reaction kernel from the burner exit on the axis. In the present unsteady calculations, as X_a was increased incrementally, the flame-stabilizing reaction kernel in the flame base detached from the burner rim and moved downstream (i.e., the inward and upward direction) gradually and then more steeply as the extinguishment limit approached ($X_a > 0.02$ for CF₃Br, $X_a > 0.084$ for C₂HF₅). For each X_a , a stable stationary flame was obtained. For CF₃Br (and, to a lesser extent, C₂HF₅), the flame base



Fig. 4. Calculated radial variations of the (a) species production rates, and (b) species and total heat-release rates at z = 5.6 mm in a propane–ethanol–water mixture (ACT fuel) flame in air with C₂HF₅ at $X_a = 0.083$.

oscillated, until finally, blowoff-type extinguishment occurred, whereas for C2HF3Cl2 and $C_{3}H_{2}F_{3}Br$, the calculation abruptly diverged at $X_a = 0.049$ and $X_a = 0.0187$, respectively. As X_a was increased, r_k decreased and z_k increased slightly, thereby more premixing occurred over the standoff distance. The calculated minimum extinguishing concentrations (MECs) of CF₃Br, C_2HF_5 , $C_2HF_3Cl_2$, and $C_3H_2F_3Br$ were $X_{\rm a} = 0.0225, 0.084, 0.049, 0.0187,$ respectively, for the ACT fuel. No measured MECs for the ACT fuel are available in the literature. The measured MEC values of CF₃Br, C₂HF₅, C₂HF₃Cl₂ (HCFC Blend B), and C₃H₂F₃Br for *n*-heptane [44] are $X_{\rm a} \approx 0.031$, ≈ 0.089 , ≈ 0.065 , and ≈ 0.026 , respectively. The calculated MECs of these agents for the ACT fuel are 73%, 94%, 75%, and 72%, respectively, of the measured values for *n*-heptane.

The incoming flow velocity around the flame base is important in diffusion flame stability as it represents the reciprocal of the residence time through the reaction kernel. Figure 6 shows the effects of the agent volume fraction in the oxidizer on the calculated total $(|\mathbf{v}_k|)$, axial (U_k) , and radial velocity (V_k) at the reaction kernel. For all agents, as $X_{\rm a}$ was increased, the absolute values of $|\mathbf{v}_{\rm k}|$ increased moderately and then increased steeply as the flame lifted off. Figure 7 shows the temperature, heat-release rate, and a ratio of the heatrelease rate and the total velocity at the reaction kernel. For all agents, as X_a was increased, the reaction kernel weakened (lower heat-release rate), but the flame stabilized at higher temperature and velocity $(|\mathbf{v}_k|)$. Nevertheless, the quantity $\dot{q}_{\rm k}/|{\bf v}_{\rm k}|$ (which relates to a ratio of the residence time and the reaction time, i.e., local Damkhöler number, at the reaction kernel [40]) decreased



Fig. 6. Calculated axial (U_k) and radial (V_k) velocity components and total velocity $(|v_k|)$ in propane–ethanol–water mixture (ACT fuel) flames in air with agent. Symbols: same as Fig. 5.



Fig. 7. Calculated reaction kernel temperature and heatrelease rate, and its ratio to total velocity in propane– ethanol–water mixture (ACT fuel) flames in air with agent. \triangle , CF₃Br; \bigcirc , C₂HF₅; ∇ , C₂HF₃Cl₂; \boxtimes , C₃H₂F₃Br.

mildly to a minimum level (\approx 3), which was comparable to the chemically passive agents [24,25]. This result suggests that the reaction kernel shifted gradually downstream (inward) to seek a location where a subtle balance between the residence time and the reaction time can be achieved. As the flame lifted higher, it became more difficult to obtain the balance, thus leading to blowoff eventually.

3.3. Combustion enhancement

Figure 8 shows the maximum temperature in the trailing diffusion flame, the total heat-release rate (\dot{q}_{total}) , integrated over the entire flame and over the flame base region ($\dot{q} <_{z_k+3 \text{ mm}}$). Thus, both the heat-release rate per unit volume along the flame zone and the flame size affect the \dot{q}_{total} . Unlike chemically passive agents [24,25], which work thermally to reduce the flame temperature by dilution, the maximum flame temperatures in the present work were nearly constant ($\approx 1800 \text{ K}$) for C₂HF₅ and C₂HF₃Cl₂, or mildly increased for CF_3Br or $C_3H_2F_3Br$ as X_a increased until extinguishment. There was a striking difference in \dot{q}_{total} (over the entire flame) between CF₃Br and the other agents: \dot{q}_{total} decreased (i.e., inhibition) with added CF3Br, whereas it increased (i.e., combustion enhancement) with the other agents. In contrast, for all agents, $(\dot{q} <_{z_k+3 \text{ mm}})$ was nearly constant as X_a increased. Thus, the combustion enhancement occurred only in the trailing flame. In fact, the heat release in the trailing flame $(\dot{q}_{total} - \dot{q}_{< zk+3 \text{ mm}})$ almost tripled with added C_2HF_5 (at $X_a \approx 0.08$). This enhancement is $\sim 1.5 \times$ larger than the zero-gravity flames studied previously [18], because of much higher incoming flow velocity in normal gravity, resulting in higher



Fig. 8. Calculated maximum temperature and total heat release rate (integrated over the entire flame and the base region) in propane–ethanol–water mixture (ACT fuel) flames in air with agent. Symbols: same as Fig. 7.

reactants (agent and oxygen) influx into the flame zone. Although the volumetric heat-release rate in the trailing flame was an order-of-magnitude smaller than the peak \dot{q}_k , integration over the entire trailing flame zone made the total value much larger. This result suggests the significant implication that even if the reaction kernel, with premixed-like flame structure, is weakened by halogenated agent addition toward the flame stability limit, the trailing *diffusion* flame can burn more reactants (including the agent itself) because of the additional heat release to form HF and CF₂O in the aforementioned "two-zone" flame structure.

4. Conclusions

The physical and chemical effects of Halon 1301 (CF₃Br) and halon-replacement fire-extinguishing agents (C₂HF₅, C₂HF₃Cl₂, and C₃H₂F₃Br) were studied numerically to gain better understanding of the flame structure, combustion inhibition/ enhancement, and blowoff extinguishment of cup-burner flames. Addition of agent to the coflowing air weakened the flame attachment point (reaction kernel) at the flame base, thereby inducing the detachment, lifting, and blowout extinguishment. With added agent, the calculated maximum flame temperature remained nearly constant (≈ 1800 K) for C₂HF₅ and C₂HF₃Cl₂ or mildly increased for CF₃Br and C₃H₂F₃Br, while the reaction kernel temperature increased for all agents. Moreover, the total heat release increased with agent addition for all of the halon replacements (by up to a factor 2.5). In the trailing flame, H₂ and H₂O (from hydrocarbon combustion) were converted to HF and CF₂O by exothermic reactions, enhancing an inner heat-release zone, while reactions of the inhibitor, also forming of HF

and CF_2O , created a large outer heat-release zone. In contrast, CF_3Br reduced the total heat release.

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