Suppressant-enhanced overpressure in the FAA Aerosol Can Simulator: Thermodynamic Considerations

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The effective fire suppressant CF_3Br (Bromotrifluoromethane, Halon 1301) has been banned from production by the Montreal Protocol due to its destruction of stratospheric ozone. While a critical-use exemption has been granted to the aviation industry for use of recycled Halon in cargo bay fire suppression, the European Union requires Halon replacement in new design aircraft by 2018 and in existing aircraft by 2040. Several replacements have been proposed, but they have all been found to produce enhanced burning in the FAA Aerosol Can Test simulator [1], and hence they fail FAA's Minimum Performance Standard [2]. In particular, C_2HF_5 (pentafluoroethane; HFC-125), and bromotrifluoropropene ($C_3H_2F_3Br$, 2-BTP) produce higher peak pressures in a simulated cargo bay when they are added at concentrations less than that required to completely suppress a simulated aerosol can explosion.

The particular tests in which the unwanted enhanced pressure rise occurred were performed in the aerosol can test simulator at the FAA Technical center by Reinhardt and co-workers [1,3]. The test consisted of a pressure vessel, 11400 L, simulating an aircraft cargo bay container in which a fire causes the rupture of an over-heated aerosol can. In the simulator, a fast-acting valve releases a mixture of propane, ethanol, and water from a heated container (16.2 bar \pm 0.33 bar) into the chamber, which is filled with either air or air with added suppressant. Sparks from a DC arc, located 91.4 cm downstream of the value opening, ignite the fuel from the aerosol can simulator, creating an expanding fire ball (if the overall mixture is explosive). The resulting heat release from reaction of the fuel and oxidizer raises the temperature, and hence the pressure, of the contents of the chamber. Without agent, the aerosol can contents ignited, creating a fireball and a peak pressure rise of about 1.7 bar (25 psig) above ambient. With HFC-125 at volume fractions of 6.2 %, 8.9 %, and 11.0 %, the peak pressure rise was about 3.6 bar (53 psig), whereas for 13.5 % HFC-125, no pressure rise occurred. For 2-BTP, volume fractions of 3 % or 4 % both gave a peak pressure rise of 4.3 bar (63 psig), and volume fractions of 5 % or 6 % gave a peak pressure rise of about 6.7 bar (98 psig). The goal of the present work is to understand the reasons for the enhanced pressure rise that occurs with HFC-125 and 2-BTP addition, and the lack of this effect with added CF₃Br.

The equilibrium composition, temperature, and pressure for a mixture of gases at some given initial state can be calculated [4,5], assuming an adiabatic system at constant pressure or volume. Automated numerical techniques are available, which use the method based on minimizing the Gibbs free energy, for a large number of species typically present in combustion systems. The equilibrium conditions of the aerosol can test were calculated using both the STANJAN-III program of Reynolds [6], and CEA2 of Gordon and McBride [7]. The calculations were performed over a wide range of initial conditions.

The numerical calculations provide data on the equilibrium composition (i.e., species mole fractions), entropy, enthalpy, temperature, and pressure of the final mixture—for the gases involved in the reaction. In principle, such calculations can be used to determine the pressure rise in the FAA chamber since reaction of the fuel, air, and inhibitor cause energy release that leads to a pressure and temperature rise. Such a calculation is straightforward if one knows the initial composition of the reactants (i.e., a premixed system). For a turbulently mixing system, as in the aerosol can test, the amount of oxidizer involved in the combustion depends upon the mixing, and is not known a priori. Hence, we include η as a variable parameter, where η is the fraction of the chamber volume that mixes with the aerosol before ignition, and subsequently reacts.

The following procedure was used to determine the final pressure in the chamber. The fuel from the aerosol can simulator was specified. The amount of water vapor and agent in the premixed chamber gases was specified, along with the initial pressure and temperature (typically 1 bar and 21 °C). Next, the fraction of chamber gases to interact with the expanding fire ball was specified (from which the mass of chamber gases not involved in the combustion was also specified). For the total involved mass (propane/ethanol/water in the aerosol can; plus the oxygen, water vapor, nitrogen, and agent in the involved chamber volume), an adiabatic, constant pressure equilibrium calculation was performed to determine the conditions after complete reaction. This specified the final volume of the involved reactants, which was added to the volume of the uninvolved gases, to yield a total final volume. Finally, the ideal gas law was used to find the pressure rise from this volume change, had the volume remained constant (i.e., $V_f/V_i=P_f/P_i$). Heat losses are neglected since the duration of the event is short (~ 1 s) and flame interaction with the walls is delayed because of the large volume. Nonetheless, inclusion of heat losses would lower the predicted final pressure.

The peak pressure in the FAA tests was successfully predicted when η (chamber volume fraction involved in the reaction with the aerosol can contents) was selected as that which yielded either the peak final adiabatic temperature T_{aft} or peak final [CO₂] (which of course varies with η). This value of η corresponds to typical diffusion flame behavior (stoichiometric proportions of reactants meeting at the reaction zone). The predicted pressure rise as a function of initial agent volume fraction in the oxidizer is shown in Figure 1, for the agents HFC-125, 2-BTP, and CF₃Br. As indicated, the predicted pressure rise for HFC-125 and 2-BTP are both a strong function of X_i , while for CF₃Br is not. Also, CF₃Br inhibits the explosion at all values of X_i , HFC-125 inhibits the explosion only at 13.5 %, and 2-BTP, if it inhibits at all, only does so at 6 %.



Figure 1 – Calculated pressure rise based on equilibrium thermodynamics evaluated at η of peak T_{aff} , as a function of inhibitor volume fraction in the chamber air, for addition of HFC-125, 2-BTP, or halon 1301 (small symbols and lines: calculation with polynomial curve fits; large circles: FAA experimental data).

The calculations indicate that for the agents HFC-125 and 2-BTP, complete reaction of the fuel and agent, at a fueloxidizer ratio pertaining to peak temperature, is required to produce the pressure rise in the FAA tests. As one of these agents is added to the oxidizer, the amount of oxidizer required increases geometrically, since the inhibitor itself has a significant oxygen requirement. Nearly complete reaction to equilibrium products is required to reproduce the observed pressure rise for all inhibitor concentrations except at the highest concentrations tested (13.5 % for HFC-125, and 6 % for 2-BTP). At these concentrations, however, the overall system is oxygen limited, so any suppression effects may have been due to oxygen starvation (as opposed to the expected chemical inhibition). Conversely, CF3Br was found to cause no over-pressure enhancement for two reasons: 1.) it reduces the extent of reaction at all concentrations, and 2.) it does not increase the oxygen demand of the system. This latter effect is due to the unique stoichiometry of the system with added CF₃Br. With added HFC-125 or 2-BTP at high loading, variation in T_{aft} is very mild near the peak in T_{aft} . Hence, energetically, there is a very wide range of η over which the flame might burn. Additional research (e.g., chemical kinetic calculations) is suggested to explain the lack of expected chemical inhibition by the HFC compounds, as well as to explore the possibility of extinction by these HFCs only when the systems reach their rich limit or inerting concentration. The present results are of significance not only for fire suppression, but for other applications of HFCs as well. For example, new HFC refrigerants (and blends) are likely to be slightly flammable [8,9]. Hence, understanding their flammability in the presence of hydrocarbons (and any anomalous behavior) is important for their fire-safe use in buildings.

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REFERENCES

- [1] Reinhardt, JW. Behavior of bromotrifluoropropene and pentafluoroethane when subjected to a simulated aerosol can explosion. DOT/FAA/AR-TN04/4, Washington, D.C.: Federal Aviation Administration; 2004.
- [2] Reinhardt, JW. Minimum performance standard for aircraft cargo compartment halon replacement fire suppression systems (2nd update). DOT/FAA/AR-TN05/20, Washington, D.C.: Federal Aviation Administration; 2005.
- [3] Reinhardt, JW. Prevention of a simulated aerosol can explosion with a mixture of Halon 1301 and nitrogen. DOT/FAA/AR-TN08/49, Washington, D.C.: Federal Aviation Administration; 2008.
- [4] Glassman, I. Combustion. San Diego, CA: Academic Press; 1996.
- [5] Turns, SR. An introduction to combustion. Boston: McGraw-Hill; 2000.
- [6] The element potential method for chemical equilibrium analysis: implementation in the interactive program STANJAN. ME 270 HO no 7, Stanford, CA: Stanford University; 1986.
- [7] Gordon, S, McBride, BJ. Computer program for calculation of complex chemical equilibrium compositions and applications. NASA Reference Publication 1311, Cleveland, OH: NASA Glenn Research Center; 1996.
- [8] Linteris, GT. Burning Velocity of 1,1 difluoroethane (R-152a). ASHRAE Transactions 2006; 112:448-458.
- [9] Kondo, S, Takizawa, K, Takahashi, A, Tokuhashi, K, Sekiya, A. Flammability limits of five selected compounds each mixed with HFC-125. Fire Safety Journal 2009; 44:192-197.