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Equivalence Ratio Influence on the Flame Suppressant Concentration of 2-BTP and Novec 1230

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ABSTRACT
Dependence of flame suppression concentration on the equivalence ratio was analyzed using modeling premixed propane/air flame inhibited by 2-BTP, Novec 1230, CF_3Br, H_2O, CO_2, and N_2. It was obtained that the suppression concentration of additives with fuel component is increased in the fuel-lean mixtures as a result of the increase of adiabatic flame temperature with their addition. Calculations of adiabatic explosion pressure (combustion temperature) under constant volume conditions demonstrate that the addition of inhibitors with fuel component to the lean mixtures increases the combustion pressure even for CF_3Br additive. Suppression concentrations of inert additives (N_2, CO_2, H_2O) were at the maximum for slightly rich mixtures where the maximum adiabatic flame temperature is observed. Calculations for the blend (inert and effective chemical inhibitor; CO_2/2-BTP) demonstrate that their use might be effective in the lean mixtures close to the flammability limits. The suppression concentration of 2-BTP in the blend (2-BTP/CO_2 = 50/50) was less than for pure inhibitor (2-BTP), thus leading to some decrease of the combustion pressure for inhibited flames near the flammability limits in comparison with pure 2-BTP.

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Introduction

Production of the fire suppressant CF_3Br (Halon 1301) has been banned by the Montreal Protocol, because of its high ODP (ozone depletion potential). Several low ODP replacement agents have been proposed, but they have all failed the US Federal Aviation Administration (FAA) aerosol can test (Reinhardt 2004), which is part of the FAA's Minimum Performance Standard (Reinhardt 2005). It was found that the replacement agents tested, C_2HF_5 (HFC-125), $C_3H_2F_3Br$ (2-BTP, 2-Bromo-3,3,3-trifluoropropene), and $C_6F_{12}O$ (Novec 1230, 1,1,1,2,2,4,5,5,5-nonafluoro-4-(trifluoromethyl)-3-pentanone) (Reinhardt 2006), when added at concentrations less than that required to suppress an explosion in a simulated cargo bay, produce higher peak pressures than with no added agent. In contrast, the addition of CF_3Br at any concentration does not increase the pressure.

The Aerosol Can Test (Reinhardt 2005) simulates the situation in which a fire in an aircraft cargo bay container heats an aerosol can causing it to burst, creating an explosion. In the test, a heated container releases its contents (propane, ethanol, and water) as a two-

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phase impulsive spray via a fast-acting valve. The fireball expands into the chamber atmosphere of ambient air and water vapor and premixed suppressant. Enhanced combustion by fire suppressants has been noted in previous studies and was briefly reviewed in (Linteris et al. 2013). Wider lean flammability limits have been measured (Shebeko et al. 2000) in the presence of halogenated hydrocarbons and in a constant volume; pressure rise and rate of its rise have also shown promotion for some conditions.

In our previous work (Babushok and Linteris 2017; Babushok, Linteris, Meier 2012; Linteris et al.2012, 2013), it was demonstrated that the observed unexpected pressure increase with the addition of fire suppressant agents is a result of a large number of agents like 2-BTP, Novec 1230, FM200 and C_2F_5H having some fuel properties. Their decomposition and oxidation in the flame reaction zone lead to an additional heat release in the fuel-lean mixtures. Even, Halon 1301 provides some additional heat release in the lean flames (Babushok, Linteris, Meier 2012).

Computations of cup-burner propane flames (Takahashi, Katta, Babushok 2020; Takahashi et al. 2017) reveal the combustion inhibition and enhancement by the CF_3Br, 2-BTP, and Novec 1230 using a detailed kinetic model. The peak reactivity spot (i.e., reaction kernel) at the flame base stabilizes a trailing flame, which is inclined inwardly by a buoyancy-induced entrainment flow. As the volume fraction of the agent in the coflow increases, the premixed-like reaction kernel weakens, thus the flame base detachment from the burner rim is eventually observed with blow-off-type extinguishment. The two-zone flame structure (with two heat release-rate peaks) is formed in the trailing diffusion flame. It was found that the total heat release of the entire flame decreases (inhibiting) for CF3Br but increases (enhancing) for the halon alternative agents (2-BTP, Novec 1230).

In this work, we studied the influence of the equivalence ratio on the flame suppression concentrations of suggested Halon 1301 replacements: 2-BTP, Novec 1230, and their blends with inert compounds (2-BTP/CO_2). It is commonly believed that the combustion of stoichiometric mixtures is more difficult to extinguish than lean or fuel-rich mixtures. However, a large number of fire suppressant agents possess some fuel component as discussed above thus contributing some heat to the overall heat release. The aim of this work was a study of the behavior of suppression concentration with the change of the equivalence ratio using modeling of the propane flame propagation with a detailed kinetic model. The obtained results demonstrate that suppression concentrations of Novec 1230 and 2-BTP are increased in the lean mixtures in comparison with stoichiometric mixtures. In contrast, CF3Br behaves similarly to the suppression concentrations of inert gases with the change of the equivalence ratio. The results of the work indicate that the blend of an effective flame inhibitor (2-BTP) and an inert additive (CO_2) demonstrates better performance than pure 2-BTP at the equivalence ratios close to the lower flammability limit. The 50/50 and 30/70 blends do not show the widening of the lower flammability limit.

Kinetic model. Modeling procedure

The kinetic model consists of five sub-models: (1) hydrocarbon combustion; (2) C_1-C_2 fluorocarbon flame inhibition; (3) bromine-species flame inhibition (Babushok et al. 2015b; Noto et al. 1996); (4) 2-BTP decomposition in flames (Babushok et al. 2015b; Burgess et al. 2015) and (5) Novec 1230 related reactions (Linteris et al. 2013). The C_1–C_3 optimized model of Qin et al. (Qin et al. 2000) is used for the hydrocarbon flame. The mechanism to describe reactions of the hydrofluorocarbons (HFCs) in hydrocarbon flames is based on the C_1–C_2 NIST HFC mechanism (Burgess et al. 1995) including modifications described in (Babushok et al. 2015b; Babushok, Linteris, Meier 2012; Linteris et al. 2013). The set of thermodynamic and transport data for fluorine-containing species was updated as described in (Babushok et al. 2020). The thermodynamic data for fluorine-containing species were modified in comparison with the previous set of data (Burgess et al. 1995) using two main sources (Ganyecz, Kallay, Csontos 2018; Goos, Burcat, Ruscic 2012). One of the relatively large changes was for CF_2O (Goos, Burcat, Ruscic 2012).

The open-source software package Cantera (Goodwin, Moffat, Speth 2016) and Chemkin set of programs (Kee et al. 1991; Kee, Rupley, Miller 1989, 1990) were used for combustion equilibrium calculations and laminar flame modeling in mixtures of propane/air with added flame inhibitors.

A decrease in the fuel concentration in the air/fuel mixture or increase in the inhibitor concentration leads to the flame extinguishment. The conditions corresponding to the flame extinguishment determine the flammability limits: the lower flammability limit (LFL, lean mixtures) and upper flammability limit, rich mixtures. Under normal conditions, the heat losses from the reaction zone and fluid dynamic disturbances extinguish flames at the flammability limits. For typical ambient conditions, it is difficult to observe flames with burning velocities below 1–4 cm/s (Ju, Masuya, Ronney 1998; Rozlovski 1980; Spalding 1957). The burning velocity of 5 cm/s was considered as the burning velocity at the flammability limit (Egerton and Powling 1948; Westbrook 1982). This value is, to some extent, device dependent. Nonetheless, it can be used as a metric for flammability limits, and it was used earlier for the estimation of flammability limits (Babushok, Linteris, Meier 2012; Westbrook 1982). The assumed level of burning velocity at the flammability limit actually defines the level of the heat release rate which becomes comparable with the heat losses at the flammability limits.

Recently, different approaches were suggested for modeling of flammability limits using detailed kinetic models (Bertolino et al. 2019; Lakshmisha, Paul, Mukunda 1990; Mascarenhas and Westmoreland 2020). In this work, we employ the combination of the empirical criterion with modeling of burning velocity using the detailed kinetic models for the simulation of the flammability range of propane with suggested replacements of Halon 1301. In the work, we assumed that the adiabatic laminar burning velocity of 5 cm/s correlates with flammability limits. A burning velocity of 5 cm/s correlates well with a lower flammability limit of methane, a calculated value of equivalence ratio 0.52 (methane volume fraction of 5.17%) represents the lower flammability limit. Available experimental data for lower flammability limit are in the range 4.6–5.4% (Cui, Li, Yang 2016), with 5.0% of CH4 measured in the works of (Cashdollar et al. 2000; Kondo et al. 2011). We can compare the calculated LFL for propane using the criteria 5 cm/s with available experimental data. In accordance with Cashdollar et al. (2000), the LFL of propane is 2.05 ± 0.05%. Our results indicate that 5 cm/s correspond to the equivalence ratio of approximately 0.497 and propane concentration of 2.04%, which is in good agreement with experimental measurements. Another comparison can be made for a minimum concentration of additive, or inerting concentration, to make propane/air mixture nonflammable. The report of Coward and Jones (Coward and Jones 1952) contains results for the inerting concentrations of CO_2 and N_2 for propane combustion. The calculated peak value for CO_2 (Figure 1a) is about 27% and experimental results demonstrate 29.5%, and for N_2, calculated inerting

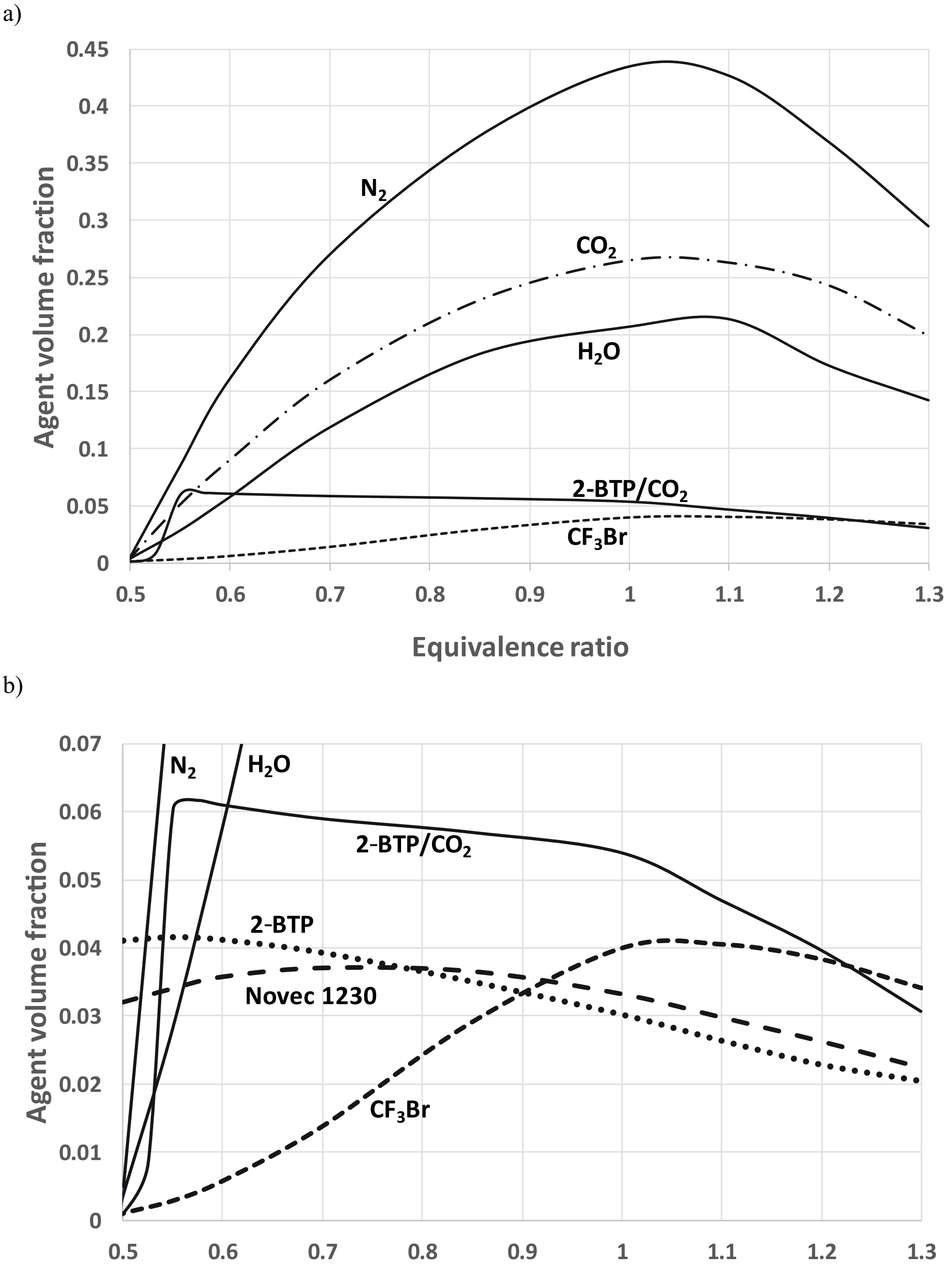

Figure 1. (a,b). Dependence of suppression concentrations (CF_3Br, 2-BTP, Novec 1230, N_2, CO_2, H_20, blend 2-BTP/CO_2 = 50/50) on the equivalence ratio for propane/air flame (298 K, 1 atm).

concentration is about 44%, and the report (Coward and Jones 1952) shows a value of 43%. The detailed comparison of the influence of 2-BTP and Novec 1230 on the burning velocity was conducted in earlier work and demonstrates good agreement with experimental measurements (Babushok et al. 2015b; Pagliaro, Bouvet, Linteris 2016; Pagliaro and Linteris 2017).

Results and discussion

The influence of the following agents was analyzed: CF_3Br, 2-BTP, Novec-1230, blend 2-BTP/CO_2 (50%/50%), and inert additives: N_2, H_2O and CO_2. Figure 1(a,b) contains the results of calculations of the dependence of suppression concentration for 2-BTP, Novec-1230, CF_3Br, N_2, CO_2, H_2O and blend 2-BTP/CO_2 (50/50) on the equivalence ratio. Results of calculations with H_2O were included for comparison purposes. Water was added as a liquid assuming a quick evaporation in a flame zone. Note that the equivalence ratio refers to that of the propane-air mixture prior to the addition of the agent. Figure 1(b) is an insert to Figure 1(a), showing in more detail the behavior of suppression concentrations for effective flame inhibitors (2-BTP, Novec 1230, CF_3Br, and blend 2-BTP/CO_2) in the concentration range from 0 to 0.07 of mole fraction.

The results (Figure 1a,b) demonstrate that as expected, the inerting concentrations of inert gases (CO_2, N_2, H_2O) correspond to the propane concentration close to the stoichiometric concentration where the maximum of adiabatic combustion temperature occurs. Similar behavior is observed for CF_3Br. Naturally, when the fuel concentration becomes close to the flammability limits, the suppression concentration decreases down to zero. However, the suppression concentrations of Novec-1230 and 2-BTP increase with the decrease of the equivalence ratio, and they are at the maximum at concentrations close to the lower flammability limit as a result of the fuel component of agents. Figure 1(a,b) demonstrates that the suppression concentrations increase with the decrease of the equivalence ratio in the range of the equivalence ratios from 1 to 0.5. The suppression concentration of 2-BTP increases from approximately 3% to 4.1%; the suppression concentration of Novec 1230 increases from 3.2% (equivalence ratio – 1) to 3.7% (0.7 equivalence ratio); and the concentration of the blend 2-BTP/CO_2 increases from 5.4% (1) to 6.1% at the equivalence ratio 0.55.

The behavior of the dependence of suppression concentration of 2-BTP and Novec 1230 with the decrease of equivalence ratio indicates that the addition of these agents widens the range of the flammability limits. The concentration of propane at the lower flammability limit becomes less than the concentration of C_3H_8 at the lean flammability limit without additives. The presence of maximum suppression concentrations close to the flammability limits indicates also that the addition of Novec 1230 and 2-BTP makes the flammability range wider. The lower flammability limit of propane decreases with the addition of 2-BTP or Novec 1230, or an increase of flammability range is observed. Thus, for a certain range of suppressant concentrations, the mixture of the suppressant agent with C_3H_8 can be flammable for propane concentration below the LFL concentration. Figure 2 demonstrates the decrease of propane concentration at the lower flammability limit with the addition of 2-BTP and Novec 1230 and demonstrates the increase of the flammability range. The mixture may be flammable below the equivalence ratio 0.45 for the concentration of 2-BTP in the relatively narrow range around 3.8–4.1%. For Novec 1230 the increase of

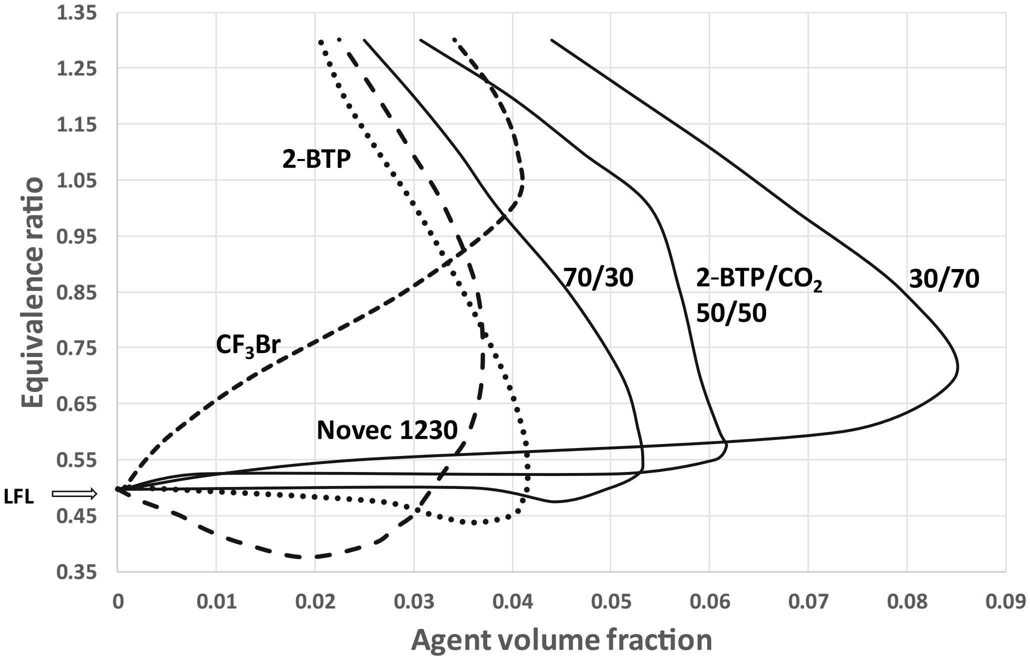

Figure 2. Flammability limits of propane/air mixtures containing various amounts of added agents: CF_3Br, 2-BTP, Novec 1230, 2-BTP/CO_2 (298 K, 1 atm).

the flammability range is even larger. The approximate decrease of propane concentration is about 0.2% of C_3H_8 for 2-BTP and about 0.45% for Novec 1230 for the assumed kinetic model. In the range of concentrations of propane between 1.8% and 2% of C_3H_8 (equivalence ratios – 0.437–0.497) there exists the range of 2-BTP concentrations, where propane/air mixture becomes flammable; correspondingly for Novec 1230, the propane/air mixture can be flammable in the range from 1.55% to 2% of C_3H_8 in the presence of Novec 1230 (equivalence ratios – 0.375–0.497). The increase of the flammability range of hydrocarbons with the addition of additives with fuel components was experimentally demonstrated in many works, e.g., CH_2FCF_3 (Molnarne, Mizsey, Schroder 2005), CH_3Br (Zabetakis 1965), $C_2H_2Cl_2$, C_2HCl_3 (Coward and Jones 1952). Particularly, Shebeko et al. (2000) demonstrated experimentally the widening of LFL for hydrogen and methane combustion with the addition of several fluorohydrocarbon agents (CHF_3, C_4F_8).

The behavior of the blend 2-BTP/CO_2 (Novec 1230/CO_2) is of interest. Calculations were performed for the blends with compositions: 30/70, 50/50, and 70/30 (Figure 2). The presence of 2-BTP and Novec 1230 in the blend significantly decreases the suppression concentration. In comparison with the pure CO_2 addition, the inerting concentration of the 50/50 blend was decreased approximately 5 times, and it was increased approximately 1.5 times in comparison with the pure 2-BTP. Due to the presence of 2-BTP, the suppression concentration of the blend increases with the decrease of the equivalence ratio. However, at the concentrations close to the lean flammability limit the suppression concentration of the blend decreases sharply (Figure 1b). Blend 70/30 shows a slight increase in the flammability range (Figure 2) as a result of the large content of 2-BTP in the blend. Figure 3 demonstrates

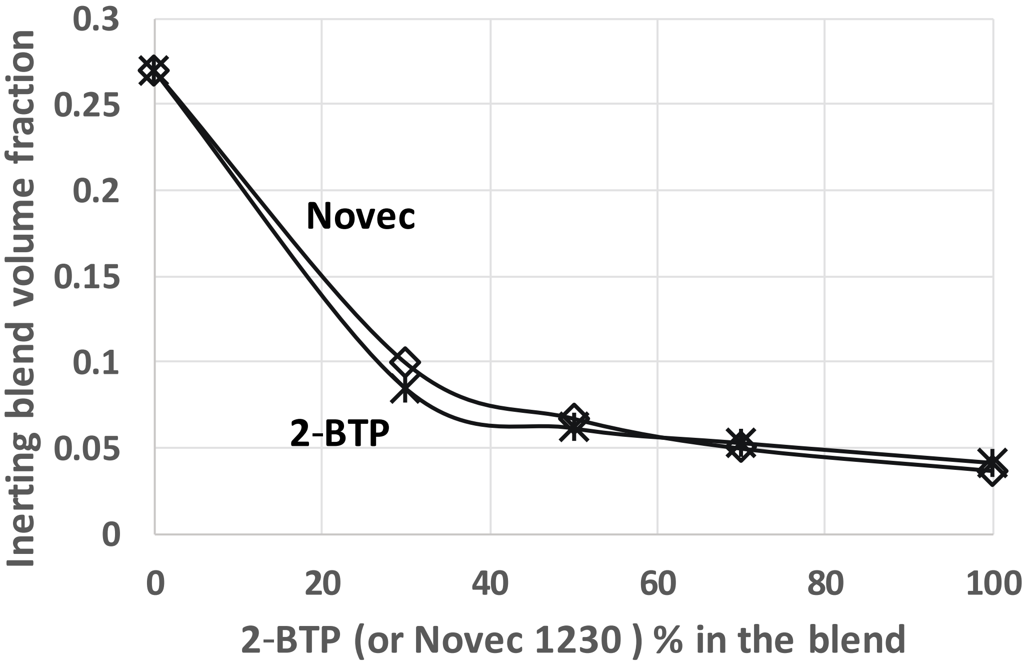

Figure 3. Dependence of the inerting volume fraction of the blend on the blend composition (2-BTP + CO_2; Novec 1230 + CO_2).

the dependence of the inerting concentration of the blends, 2-BTP/CO_2 and Novec 1230/CO_2, on the blend composition. The presented results show that even the blend with 70% of CO_2 demonstrates a rather good performance, and it can be considered as a possible CF_3Br replacement, as well as the 50/50 blend.

It is of interest that a shift of the maximum suppression concentration to the range of lean mixtures also leads to the increase of F/H ratio of mixtures, and correspondingly to the increase of the possibility of water vapor promotion influence as a result of a sharp increase in F atom concentration at $F/H > 1$ and of increase in the rate of the $F + H_2O = OH + HF$ reaction (Babushok, Linteris, Baker 2015a). Particularly it is the case for Novec 1230. Thus, for stoichiometric mixture F/H ratio is approximately 1.2 for Novec 1230 and 0.4 for 2-BTP at the suppression level of concentrations. Numerical experiments demonstrate a rather large F atom concentration in the combustion products of flame inhibited by Novec 1230 (1–2%). Note that the use of blends decreases the F/H ratio.

Figure 4 presents the results of equilibrium calculations of the explosion pressure developed during combustion in a closed constant volume as a function of added agent concentration (2-BTP, CO_2, CF_3Br, blend 2-BTP/CO_2) for different equivalence ratios (1, 0.7, and 0.5) of propane/air mixtures. The calculations were performed for ideal conditions: constant volume system without heat losses. It can be seen (Figure 4) that the addition of inert compound, CO_2, decreases naturally the explosion pressure for all equivalence ratios. The addition of an additive with a fuel component increases the explosion pressure for lean mixtures because it increases the fuel content of the mixture. Thus, the addition of 2-BTP to the lean propane mixtures increases the combustion pressure until the overall mixture

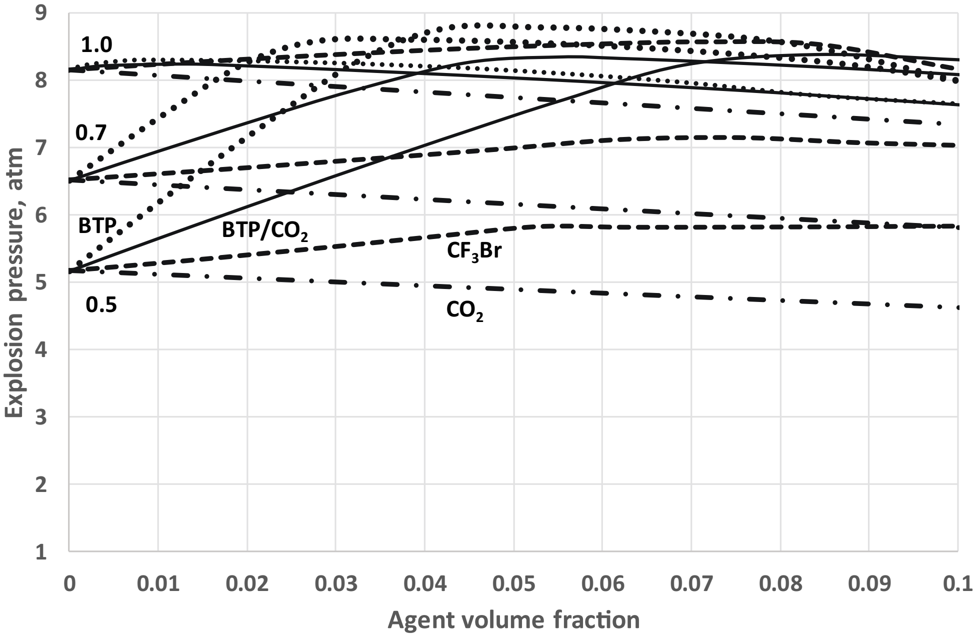

Figure 4. Dependence of adiabatic explosion pressure of propane/air on the concentration of suppressant agent (2-BTP, 2-BTP/CO_2, CF_3Br, CO_2) for different equivalent ratios (1.0, 0.7, 0.5; dotted line – 2-BTP, solid line – 2-BTP/CO_2 blend, 50/50; dashed line – CF_3Br, dash-dotted line – CO_2, 298 K, 1 atm).

composition (propane and additive) becomes the stoichiometric one. As it was indicated (Babushok, Linteris, Meier 2012), CF_3Br also has some fuel component thus leading to the pressure increases in the lean mixtures (Figure 4). It is of interest that pressure increase with the addition of CF_3Br and 2-BTP is observed also for stoichiometric mixtures. This is the result of the maximum adiabatic temperature, and the maximum burning velocity occur in the slightly fuel-rich mixtures.

Conclusions

In this work, we have studied the influence of the equivalence ratio on the suppression concentrations of 2-BTP, Novec 1230, and the blend of 2-BTP with an inert compound (CO_2) for propane/air flame. It was demonstrated that the agents with fuel component, Novec 1230 and 2-BTP, have higher suppression concentrations for the fuel-lean mixtures in comparison with stoichiometric mixtures. The suppression concentration of 2-BTP practically increases up to the lower flammability limit of propane flame. The main results of the work are as follows:

(1) For the used kinetic model the inerting concentration of 2-BTP (4.1%) is observed at about the equivalence ratio 0.6, in comparison with about 3% for stoichiometric mixture. The inerting concentration of Novec 1230 was about 3.7% at the equivalence ratio of approximately 0.8% and 3.3% for the stoichiometric mixture.

(2) The addition of 2-BTP and Novec 1230 cause wider flammability limits. Propane concentration at the lower flammability limit decreases with the addition of Novec 1230 and 2-BTP in comparison with propane concentration without additives. There exist a range of concentrations of Novec 1230 and 2-BTP where the propane/air mixture is flammable at the concentrations below the lean flammability limit. Suppression performance of 2-BTP and Novec 1230 is better than CF_3Br in the rich mixtures.

(3) Calculations of adiabatic combustion pressure in a closed constant volume demonstrate that an increase of pressure is observed for lean propane mixtures with the addition of 2-BTP and Novec 1230. Even the CF_3Br addition to the lean mixtures increases the explosion pressure in a constant volume due to its fuel component.

(4) The blend of an effective flame inhibitor (2-BTP) and an inert additive (H_2O, CO_2) demonstrates better performance than pure 2-BTP at the equivalence ratios close to the lower flammability limit. The 50/50 and 30/70 blends (2-BTP/CO_2) do not show the widening of the lower flammability limit.

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