Use of computer modelling to evaluate the performance of halon alternatives: a literature review

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The Use of Computer Modeling to Evaluate the Performance of Halon Alternatives -- A Literature Review

by

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ABSTRACT

Computer modeling represents a relatively new methodology in the search for halon alternatives. The purpose of this report is to investigate the feasibility of using computer modeling to make the selection of halon alternatives more efficient and effective. This report reviews the current developments in computer modeling and the existing kinetic databases for hydrocarbon fuels and halon alternatives. The range of application of the computer models and their limitations are discussed in the report.

This review shows that computer modeling is capable of accurately reproducing some aspects of fire phenomena, and that it is being regarded as another method for evaluating agent performance. Such a "test" is better defined and much easier to carry out, in comparison with a full-scale fire test.

The main physical-chemical characteristics of hydrocarbon fuel oxidation for fuels up to C_8, halon 1301 (CF_3Br) and some fluorocarbon and chlorocarbon agents up to C_2 are reproduced with reasonable accuracy by the established kinetic databases. Some of these agents are being considered as candidate agents for halon replacements.

The current kinetic databases for the more complex hydrocarbon fuels and inhibitors, however, need to be further developed and refined. Also, large computer power and long calculation times are required for the calculation of higher hydrocarbon fuels and inhibitors.

A combination of experiments and computer modeling can make the selection of halon alternatives more efficient and effective.

1.0 INTRODUCTION

With the recent phase-out of halon agents, there is a need to develop alternatives to halons, to establish a ranking order of the relative fire-fighting effectiveness of alternative agents, and to understand the extinguishing mechanisms of these new agents [1]. Until now, the evaluation of the performance of halon alternatives for specific applications was mainly based on full-scale fire tests. Also, the information obtained from such tests about the extinguishing mechanisms of halon alternatives is limited by the severe test conditions and the capabilities of the test instruments. This results in delays and high costs for the development of halon alternatives.

Computer modeling represents a relatively new methodology in the search for halon alternatives [2]. This type of analysis can provide insights into many of the fundamental kinetic and fluid mechanical processes that occur between suppressants and fuel-air mixtures. Thus, the inhibiting behavior of halon alternatives under different fire suppressing conditions can be understood and assessed effectively using computer simulations. Computer modeling is becoming better defined and much easier to carry out, in comparison with full-scale fire tests. A combination of laboratory and numerical studies with validation by fire tests, will make the selection of halon alternatives much more efficient and effective.

The National Research Council of Canada (NRCC) has been actively involved in the search for halon replacements. This report documents an initial literature review conducted

to investigate the feasibility of using computer modeling in the selection of halon replacements.

The first part of this report reviews the current developments in computer modeling used in evaluating the performance of halon alternatives. The potential application of the computer models and their limitations are then discussed. The second part of the report reviews existing kinetic databases of hydrocarbon fuels and some halon alternatives. The third part of the report reviews the current application of computer modeling in the evaluation of halon replacements. A summary is given in the last part of the report.

2.0 DEVELOPMENTS IN COMPUTER MODELING

The current computer models used in evaluating the performance of halon alternatives can be considered as belonging to two categories: computational fluid dynamics (CFD) field models with simple kinetics, and quasi-dimensional computational models with detailed kinetics.

2.1 Computational Fluid Dynamics (CFD) Modeling

For Computational Fluid Dynamics (CFD) models, the computational domain is divided into a large number of small control volumes which are used to follow the propagation of the flame or combustion front [3]. Each small volume incorporates the equations for the numerical calculation of mass, momentum, energy and species-

conservation. In addition, simplistic chemistry sub-model are employed in each control volume to describe the chemical reactions of the fuel-air mixture, because of the power limitations of current computers.

CFD models are capable of providing detailed spatial information about the physical interaction between fires and fire suppressants, such as fire spread, the distribution of fire suppressants in the compartment, fluid dynamics, mass and heat transfer and thermal effects. CFD models can also be used to solve a variety of problems by specifying the geometry, the boundary conditions and other characteristics of the problem.

CFD models have been used to evaluate the performance of water mist in fire suppression. Water mist, as a halon alternative, mainly displays physical mechanisms in fire extinguishment and does not behave as a "total-flooding" agent in fire suppression. The National Research Council of Canada (NRCC) has carried out research using a CFD model to study liquid pool fire extinguishment by water mist [3-6]. Results obtained from the computer modeling showed that the fire created a strong upward plume directly over the fire pan. A low-momentum water spray was not able to penetrate the fire plume and reach the region near the fuel surface. However, the water mist rapidly cooled the fire plume and produced a flow of cool gases over pans, resulting in fire suppression.

The current CFD models require significant computer power. This requirement increases the cost and time required for the evaluation of halon alternatives. Also, in order to improve the accuracy of the models, a more comprehensive knowledge of the spray

characteristics, fuel evaporation and combustion models is required. In addition, the CFD models cannot be used to evaluate the performance of gaseous agents, because these gaseous agents suppress fires mainly by chemical inhibition.

2.2 Quasi-Dimensional Computational Modeling

For quasi-dimensional computational models, the computational domain is divided into one zone or multi-zones according to the combustion phenomena simulated [7]. In each zone, the equations of conservation of mass, momentum, and energy are solved together with the chemical species conservation equations, including the kinetics terms. Since the numerical simulation is limited to a few zones, a detailed kinetic database can be incorporated into the quasi-dimensional computational modeling to describe the elementary reaction steps of the combustion process. Such models are widely used to investigate the combustion phenomena involving chemical effects, including the onset of knock in internal combustion engines and the chemical inhibition effect of gaseous agents.

Most gaseous agents that are currently being considered as halon alternatives suppress fires primarily by chemical mechanisms. Also, these gaseous agents act as total-flooding agents in the fire extinguishment process. Their efficacy in fire extinguishment is dependent on the concentration used, not on the size and location of the fires or the geometry of the compartment. Recent full-scale fire test results [8, 9] showed that, although water mist suppresses fires primarily by physical effect, it also displays certain chemical effects in fire suppression.

A quasi-dimensional computational modeling with detailed kinetics can evaluate the performance of the fire suppressants in simplified combustion processes, such as counterflow diffusion flames, one-dimensional premixed laminar flames and plug flow reactors. Detailed information on the chemical interaction between the fire and the fire suppressants, including the breaking of reaction chains, the suppression of active species and the production of combustion by-products, can be obtained from the numerical calculations. The effects of test conditions (e.g., temperatures and the concentrations of the fire suppressants) on the efficacy of the fire suppressants can be traced by the computer model.

3.0 DEVELOPMENTS IN KINETIC DATABASES OF HYDROCARBON FUELS AND FIRE SUPPRESSANTS

The kinetic databases that represent the elementary reaction steps of the fuels and fire suppressants in the combustion process, are crucial for successful computer simulations. Figure 1 shows the typical fluorinated hydrocarbon reaction pathways and their corresponding chemical species during fire suppression [10]. It can be seen that fire suppression by chemical agents involves a large number of stable and unstable chemical species as well as complex simultaneous chain reactions that proceed in the fuel mixture and suppressants. As a result, the kinetic database required for the investigation of the fire suppression by gaseous agents must includes all possible reaction routes, chemical species and the kinetic rate constants that determine the reaction rates for these elementary reactions.

Since the fire suppression process involves the oxidation of both hydrocarbon fuels and the agents, the kinetic database incorporated in the computer models consists of two distinct reaction sets. One is the reaction set to describe the oxidation of hydrocarbon fuels (C/H/O). The other is the reaction set to describe the inhibition of the combustion process by the agent. The current agent kinetic databases mainly include fluorocarbon chemistry (C/H/O/F), chlorocarbon chemistry (C/H/O/Cl), as well as the reactions with added bromine compounds (C/H/O/Br).

3.1 Hydrocarbon Chemistry

Research into the mechanism of hydrocarbon oxidation has been carried out for many years. One of the early reaction mechanisms for the oxidation of methane can be traced to a scheme developed by Norrish [11]. Since then, a significant amount of the knowledge of the flame structure and chemical data of hydrocarbon fuels has been obtained from experiments in shock tubes, flow reactors, and laminar flames. Westbrook and Pitz [12, 13] have developed some comprehensive chemical mechanisms for the oxidation of methane. These chemical schemes were used to predict a wide range of methane combustion phenomena, such as pollutant emissions, ignition delay, and the onset of knock in internal combustion engines.

Thompson [14] developed an improved chemical mechanism for the oxidation of methane. This scheme has been used to describe a broad range of ignition and combustion mechanisms of methane in shock tubes, flow reactors, and laminar flames. Good agreement

with corresponding experimental results was obtained using the improved chemical mechanism.

Burgess et al [10] developed a set of reactions for the oxidation of hydrocarbon fuels of up to C_2. This kinetic database is based on the chemical models of Miller and Bowman [15] and Egolfopoulos et al [16]. Some of the rate constants have been adjusted on the basis of a review by Tsang and Hampson[17]. The NIST C/H/O reaction set, which consists of about 30 species and 140 elementary reactions, can be used to describe the oxidation of hydrogen (H_2), methane (CH_4), and formaldehyde (CH_2O). The simulations of the hydrocarbon oxidation were validated on the basis of experiments.

Tsang [17] summarized the chemical kinetic data for the combustion chemistry of methane based on a comprehensive review of the relevant literature. Some comments and recommendations on the chemical kinetic data in the publications were made in his work. It was found that the chemical mechanisms of hydrocarbon fuels of up to C_2 were relatively well understood and validated by a broad range of experiments.

The chemical reaction mechanism for the oxidation of propane was developed later. Its chemistry is more complex than the mechanism for methane. The pyrolysis of propane has been studied in tubular flow reactors and shock tubes by many investigators [12, 13, 18, 19] while the oxidation of propane was examined in flow reactors, static vessels and shock tubes by Hautman et al [20].

Westbrook et al [21] developed a detailed chemical kinetic reaction mechanism to describe the oxidation and pyrolysis of propane. The kinetic mechanism consists of 163 elementary reactions with 41 chemical species. Some rate constants were obtained by estimation. This scheme was then tested by a comparison between computed and experimental results in shock tubes and a turbulent flow reactor. They reported that the resulting comprehensive mechanism accurately reproduced experimental data for pressures from 1 to 15 atm and temperatures from 1000 to 1700 K.

Recently, a literature review on the oxidation of propane and methane was conducted by Karim and Liu [22]. A "comprehensive" reaction mechanism of propane, methane, and other hydrocarbon fuels, that consists of 145 reaction steps with 35 species (see Table 1) was established based on a literature review and sensitivity analysis. The calculation results obtained using this kinetic database were in good agreement with corresponding experimental results.

Tsang [23] also summarized the chemical kinetic data for the combustion chemistry of propane based on a comprehensive review of the relevant literature. Both evaluated and estimated data of the kinetics of reactions involving propane, isopropyl radical, n-propyl radical and various inorganic species in small concentrations were considered in his work. He also made comments on and recommendations for the chemical kinetic data in the publication, which are important for a proper understanding of the chemistry of propane pyrolysis and combustion.

Heptane is one of the main components of diesel fuel and is widely used in various fire tests. Its chemistry is much more complex than the chemistries of methane and propane. Westbrook [24] has developed a chemical kinetic mechanism involving hydrocarbon fuels of up to C_8, such as n-heptane and other complex hydrocarbon fuels. This scheme consists of 1972 elementary reaction steps with 380 species. Considerable computer power and long calculation times are needed to run such a complex kinetic scheme.

Khalil et al [25], on the basis of Westbrook's n-heptane model, developed a compact kinetic scheme for the oxidation of n-heptane fuel using sensitivity analysis for the reaction rates and species consumption path. This compact kinetic scheme consists of only 502 elementary reaction steps with 170 species, and is capable of being incorporated into computer programs for different calculation purposes. This chemical scheme was validated by comparing the calculated results with corresponding experimental values in internal combustion engines.

The chemical mechanisms of hydrocarbon fuels of up to C_2, combined with the chemical mechanisms of halon alternatives, are widely used to evaluate the inhibition efficiencies of various gaseous agents, because of their relatively simple and well established chemistry. For more complex hydrocarbon fuels, such as n-heptane, a compact kinetic scheme chemistry must be incorporated into the model to reduce the calculation time. For example, Sekiuji et al [26] used a very compact n-heptane kinetic scheme to evaluate the performance of polyfluoroalkylamines in fire suppression. This compact n-heptane scheme consists of only 102 elementary reaction steps and 32 species. However, the compact

chemistry scheme may lead to increasing uncertainties during the simulation, unless a wide range of sensitivity analysis and corresponding experimental validations are conducted.

3.2 Fluorocarbon and Chlorocarbon Chemistry (C/H/O/F/Cl/Br)

In comparison with the development of hydrocarbon chemistry, research into the chemistry of fire suppressants started very late. In the 1970's, Biordi et al [27, 28], and Lewis and Simpson [29, 30] completed experimental and modeling studies of halon (CF_3Br) flame chemistry. The role of bromine atoms in fire suppression and several key reactions were determined and identified. Westbrook [31], on the basis of this research, developed the first comprehensive chemical mechanisms to describe in detail the chemistry of CF_3Br (halon 1301) and its halogenated products in hydrocarbon flames. This chemical scheme consists of 56 elementary reactions and 16 species, including such important species as CF_3Br, CF_3H, HBr, etc. The decomposition of these species, their chemistry, and their influence on hydrocarbon flames can be determined from this scheme.

The calculated results obtained from Westbrook's halon 1301 chemical model show good agreement with corresponding experimental results [10, 31]. The flame suppression mechanisms of CF_3Br (halon 1301) is well understood from Westbrook's chemical model. As a result, the kinetic database developed by Westbrook for the description of the chemical mechanisms of CF_3Br (halon 1301) is considered a well-established chemistry and is the basis for the description of chemical mechanisms of other bromine-containing compounds

[10]. Recently, some reaction rates in Westbrook's CF_3Br model were adjusted to reflect more recent measurements [10].

On the basis of a significant amount of experimental and modeling work over many years that investigated the effectiveness of halogenated fire suppressants, Burgess et al [10] at the National Institute of Standards and Technology (NIST) recently developed a thermochemical and chemical kinetic database for C_1 and C_2 fluorinated hydrocarbon destruction and fire suppression. The fluorinated hydrocarbons presented in this kinetic database include four of the candidate agents specifically being considered as halon replacements: CH_2F_2, CF_3-CH_2F, CF_3-CHF_2 (HFC-227 ea), and CF_3-CF_3 as well as all of the other possible fluoromethanes and fluoroethanes. Larger fluorinated hydrocarbon agents (e.g., C_3F_8) and chlorine-substituted agents (e.g., CHF_2Cl) are not included in this kinetic database due to their complex chemistry. But the effectiveness of these agents can be estimated to some degree by analogy to the other agents that have already been studied. The set of reactions containing bromine species in the NIST database is based on the mechanisms of Westbrook [31]. The reaction set of the kinetic data consists of 520 elementary reactions and the chemistry of 48 species containing one and two carbons with H, O, OH, H_2O and other flame species.

Daniel et al [32] used a diode laser and the NIST kinetic database developed by Burgess et al to study the HFC chemistry in a low pressure flame. It was found that for the limited number of species investigated, the calculated results obtained from the NIST model were in good agreement with the corresponding experimental results. Linteris and his

coworkers [33] have used the NIST model to investigate the fire suppression properties of fluoromethanes and other agents. They found that flame speeds calculated from the NIST model were in good agreement with experimental results. The NIST model was also successfully used to evaluate the inhibition ranking of the halon alternatives by Babushok et al's work [34]. The NIST chemical database, however, is considered as a framework for future model development, rather than a finished model. Future refinements will require experimental validation using high-temperature flow reactor, premixed flame and diffusion flame measurements as well as the determination of rate constants [10].

CF_3I is considered one of the promising halon alternatives for many applications. Its chemistry was also studied by McIlroy [35, 36]. The experimental investigations of iodine based fire suppression have shown that the performance of CF_3I for fire suppression is similar to that of the analogous bromine compounds (CF_3Br), but slightly less effective [35]. However, there are not many high temperature experimental kinetic data involving species containing iodine. Westbrook's CF_3Br model is accepted as a basis for describing the chemistry of CF_3X (X=H, Br, and I). Iodine compound reaction rates are substituted for the bromine compound reaction rates to develop the CF_3I reaction mechanism [36]. The numerical simulations for CF_3I chemistry demonstrate good agreement with corresponding experimental results.

For the chlorogenated fire suppressants, Wang et al [37] have recently developed a detailed reaction mechanism of chloromethane oxidation, based on a methane combustion mechanism [38], and a CH_3Cl and CH_2Cl_2 oxidation mechanism by Ho and coworkers [39,

40]. This scheme, including the chemistry of CH_3Cl, CH_2Cl_2, $CHCl_2$, CClO, C_2H_5Cl and other important species, consists of 132 elementary reactions and 46 species. The numerical results were found to be in close agreement with corresponding experimental and literature data.

4.0 THE APPLICATION OF COMPUTER MODELS IN THE EVALUATION OF HALON ALTERNATIVES

There are many computer models available for the evaluation of the inhibition effects of fire suppressants. Sandia's CHEMKIN code [41, 42] is one such typical commercial computer model. The CHEMKIN model can simulate counterflow diffusion flames, one-dimensional premixed laminar flames, plug flow reactors, and well-stirred reactors. The computer model developed by Karim and Liu [7, 22, 43] can also be used to simulate plug flow reactors, well-stirred reactors, and other types of combustion phenomena. In these models, the changes in the ignition delay, burning velocity, heat release rates, and the production of active species by the addition of agents are considered as criteria to evaluate the inhibition efficiencies of halon alternatives.

Computer models for the screening and selection of potential halon alternatives can be used to investigate the followings: 1) understanding the fire-fighting mechanisms of halon alternatives; 2) evaluating the inhibiting efficiencies of halon alternatives; and 3) evaluating the formation of the combustion by-products (e.g., HF and HCl) generated during the fire suppression process.

In Westbrook's early work [31], a computer model that incorporated the detailed chemical kinetic reaction mechanisms of fuels and Halon 1301 (CF_3Br) was used to investigate the properties of laminar flames inhibited by the agent. Fuels considered in the model included hydrogen, methane, methanol and ethylene. The effects of variations in pressure, unburned gas temperature, and equivalence ratio on the inhibition efficiency of CF_3Br were examined using the computer model. The calculation results showed good agreement with corresponding experimental results.

Babushok et al [44] investigated the effect of a number of possible flame suppressants (Br_2, HBr, CH_3Br, CF_3Br, CF_3H, CF_2H_2, CF_4, C_2F_6, C_2HF_5 and $C_2H_2F_4$) on the ignition behavior of a variety of combustible gases (H_2, CH_4, CH_3OH and C_2H_6). The conditions simulated using the model included temperatures between 900 and 2000 K, pressures between 0.5 to 1.5 atm, equivalence fuel ratios of 0.5 to 1.3 and additive concentrations ranging from 0 to 30%. The ignition behavior of the fuels was used to give a rank ordering of the inhibition effectiveness of the various agents. Their findings showed that the agent can promote or inhibit fire reactions depending on the reaction conditions. It was also concluded that ignition delay was not a good measure of the inhibition efficiency of the additives.

Babushok et al [2] also investigated the acid gas formation for two of the leading near-term halon alternatives (FE-13 (CF_3H) and HFC-125 (C_2F_5H)) using the CHEMKIN code developed by Sandia. They used the NIST kinetic database [10], as it was assumed to

substantially capture the chemistry of these two halon alternatives. Fuels considered in the study included hydrogen, methane, methanol and ethylene. It was found that in order to obtain the same suppression effectiveness as halon 1301 (CF_3Br), these two halon alternatives could produce larger quantities of HF during fire suppression. The calculated inhibition rankings were in accord with existing experimental results. They also suggested that a higher hydrocarbon, such as propane or some mixture, may be a more appropriate fuel for the evaluation of halon alternatives in computer modeling.

Linteris and Truett [33] investigated, both experimentally and numerically, the inhibition of premixed methane-air flames by the two-carbon fluorinated species (C_2F_6, C_2HF_5, $C_2H_2F_4$) and the three-carbon species (C_3F_8 and C_3HF_7), all of which are being considered as halon replacements. The NIST detailed chemical kinetic mechanism for the two-carbon fluorinated species [10] was employed in the computer modeling. The calculations illustrated that all these inhibitors were not inert in the flames and the reduction of the burning rate was mainly attributed to the chemical inhibition by these agents. The NIST fluorine-inhibition mechanism predicted reasonably well the burning rate reduction for the flames. It was also suggested that as the mechanism is further developed and refined, better agreement should be possible, and that it can also be extended to investigate more complex fuels and inhibitors.

Sekiuji et al [26] evaluated the inhibition effect of polyfluoroalkylamines ($(CF_3)_2NCF_2CF_3$, $(CF_3)_2NCF_2CHF_2$ and $(CF_3)_2NCF=CF_2$) both experimentally and numerically. The fuel considered in their work was n-heptane. A compact chemistry, that

consists of only 152 elementary reaction steps and 49 species, was used to describe the reactions involving n-heptane, bromic and fluoric species. Table 2 compares the calculated and experimental burning velocities for n-heptane flames containing CH_3Br, CF_3Br and CF_4 additives. The calculated inhibition rankings were in accord with the existing experimental results. Although there was no available kinetic data for polyfluoroalkylamines, they were able to calculate the physical inhibition effect of polyfluoroalkylamines and compare it with the experimental results. It was determined that polyfluoroalkylamines had a strong chemical inhibition effect and all of the polyfluoroalkylamines inhibited flame propagation less than CF_3Br (Halon 1301), but more than CF_3CHFCF_3 (FM200).

Table 2 Comparison of calculated and experimental burning velocities of heptane flames with C1-compounds [26]

Inhibitor	Calculated Burning Velocity (m/s)	Experimental Burning Velocity. (m/s)
None	0.43	0.45
CF_4	0.41	0.39
CH_3Br	0.36	0.34
CF_3Br	0.34	0.32

Linteris and Truett [45] recently examined the burning velocity of premixed hydrocarbon flames inhibited by CH_2F_2, CF_3H and CF_4 using model calculations and experimental measurements. The inhibitors were tested over a range of concentrations and fuel-air equivalence ratios. The calculation results showed that CF_3H and CH_2F_2 were totally

consumed in the flame and the inhibition effect was produced by a reduction in the H-atom concentration due to the formation of stable HF molecules. In contrast, only about 10% of CF_4 was consumed in the main reaction zone and the inhibition effect of this agent CF_4 was due to a lowering of the final temperature of the burned gases. The calculated results were in good agreement for CH_2F_2 and CF_4 and within 35% for CF_3H.

Recently, Babushok et al [34] investigated the influence of halogenated fire suppressants (CF_3Br, CF_3I, CF_4, CHF_3, C_2F_6 and C_2HF_5) on the combustion of C_1-C_2 hydrocarbons (CH_4, CH_3OH, C_2H_6, C_2H_4 and C_2H_2). The simulations were conducted for plug flow and a well-stirred reactors using the Sandia CHEMKIN code. The general ordering of the inhibition effectiveness of the halogenated fire suppressants was CF_3Br > CF_3I > C_2F_6 > C_2HF_5 > CHF_3 > CF_4. The first two compounds were clearly superior to the others.

The chemical and physical inhibition effect of water vapor on the structure of counterflow diffusion flames was initially investigated both experimentally and theoretically by Suh and Atreya [46]. The detailed C_2 chemistry was employed in their numerical calculations. They found that the fire temperature as well as OH and CO_2 production increased with an increase in water vapor concentration. After approximately 30% water vapor substitution, the flame temperature and OH production began to decrease. Hence, at low water vapor concentrations, the addition of water vapor into fires improved combustion efficiency. At 30% water vapor concentration, the predominant effect of the water vapor changes from chemical to physical.

5.0 SUMMARY

Computer simulation represents a relatively new methodology for the evaluation of the performance of halon alternatives. The models can accurately reproduce some aspects of fire phenomena and can be regarded as another testing method [2]. Such a "test" is better defined and much easier to carry out, in comparison with full-scale fire tests. Detailed information about fire extinguishment using fire suppressants, including the breaking of reaction chains, the suppression of active species and the production of combustion by-products, can be obtained using the numerical simulations. The computer models can be used to obtain a better understanding of the inhibition process and to reduce the cost and time required for experimental tests.

The accuracy of computer models for the evaluation of the performance of halon alternatives depends on the availability of adequate chemical kinetic data for hydrocarbon fuels and fire suppressants. The reaction mechanisms of hydrocarbon fuel oxidation of up to C_2 are relatively well known and established. The reaction mechanisms can be used to evaluate the effectiveness of halon and its alternatives in fire suppression. The reaction mechanisms of more realistic fuels, such as propane and n-heptane, are also established and validated in a wide range of experiments, although there are some uncertainties for some species and reactions due to the complex chemistry. The chemical mechanisms can be used to evaluate the chemical inhibition effects of water mist and other inerting agents on hydrocarbon fires.

The suppression mechanisms of Halon 1301 (CF_3Br) are relatively well known and established. The chemistry of some of the fluorocarbon and chlorocarbon agents is also established. These agents include CF_2H, CF_3I, CH_2F_2, CF_3-CH_2F, CF_3-CHF_2 (HFC-227 ea), CF_3-CF_3, CH_3Cl, CH_2Cl_2, $CHCl_2$, CClO, and C_2H_5Cl. The effectiveness of more complex fluorinated hydrocarbon agents (e.g., C_3F_8) and chlorine-substituted agents (e.g., CHF_2Cl) can be approximated by analogy to other agents that have already been studied. Some of these agents have been investigated as candidate agents for halon replacements. The main physical-chemical characteristics of these agents during fire suppression are reproduced with reasonable accuracy by the established kinetic databases.

Current chemistry for hydrocarbon fuels and fire suppressants still need to be further developed and refined, especially for more complex hydrocarbon fuels and inhibitors. Also, large computer capacity and long calculation times are required for the calculations with complex hydrocarbon fuels and inhibitors.

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