Fire Suppression Modeling using Computational Fluid Dynamics

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ABSTRACT

Military ground vehicles are equipped with **A**utomatic **F**ire **E**xtinguishing **S**ystems (AFES) to protect against enemy threats causing fuel tank ruptures and resulting fuel fires inside military vehicle crew compartments. The fires must be rapidly extinguished without reflash to ensure Soldier protection from burn and toxicity risks. This summary describes the development of a simulation-based acquisition tool which will complement vehicle testing for the optimization of AFES designs for specific vehicles and address their unique clutter characteristics.

The simulation-based acquisition tool using Computational Fluid Dynamics (CFD) techniques was validated for an exploratory test box and demonstrated with the evaluation of two different suppressant nozzle configurations for an MRAP vehicle. The result is a cost-savings tool with a negligible development payback period that optimizes Soldier survivability in a fire situation. This modeling tool is currently being applied to predict the effectiveness of crew AFES in a number of Army ground vehicles.

INTRODUCTION

Military ground vehicles are equipped with **A**utomatic **F**ire **E**xtinguishing **S**ystems (AFES) to protect against enemy threats causing fuel tank ruptures and resulting fuel fires inside their crew compartments. The resulting fires must be extinguished without reflash to ensure Soldier protection from burn and toxicity risks. Following the ban on production of Halon 1301 (CF_3Br) due to environmental concerns related to the destruction of stratospheric ozone, the US Army Tank Automotive Research, Development, and Engineering Center (TARDEC) conducted research to identify and qualify selected replacement agents for Halon 1301 in combat vehicle automatic fire extinguishing systems. Test results during the replacement agent selection process demonstrated the criticality of AFES design optimization to ensure compliance with burn and toxicity risks and other crew casualty criteria. This summary describes the development of a simulation-based acquisition tool to complement vehicle testing for the optimization of AFES designs for specific vehicles with unique clutter characteristics. The result is a cost-saving tool with a negligible development payback period that optimizes Soldier survivability due to fires.

This tool resulted from TARDEC enhancements of a commercial-off-the-shelf (COTS) computational fluid dynamics (CFD) software that has automated meshing, extensive range of physics models and post-processing capabilities. The enhancements to the code accounts for the

three-dimensional (3D) growth and suppression of fuel spray fires with Halon replacement agents of interest to the Army, and the resulting toxic byproducts. The code is capable of parallel execution on platforms ranging from DoD's High Performance Computers (HPC) to low-cost, multi-core PCs and is licensed by DoD's High Performance Computing Management Office (HPCMO) for parallel execution. Visualization of the simulated fire propagation and extinction, suppressant dispersion and toxic byproduct production and transport is typically conducted on low-cost PCs.

The detailed chemical kinetics for suppressants involves thousands of reactions and hundreds of species. Performing numerous simulations with thousands of reactions with detailed kinetics for a military ground vehicle crew compartment is not practical for the purpose of optimizing the size and location of suppressant bottles inside crew compartments. A generalized global reduced kinetics model that represents the effect of inhibitors parametrically resulted in ten reactions and thirteen chemical species. The reduced model was implemented in a commercial state-of-the-art CFD code. This generalized kinetic approach is valid for Halon + Sodium Bicarbonate (SBC), HFC227ea (Heptafluoropropane or HFP or FM200) + sodium bicarbonate and water + potassium acetate. Much of the focus for this study is placed on HFC227ea+SBC since most military vehicle platforms that are in the design/modification phase use this blend as their crew fire suppressant.

Initially, the reduced suppression kinetics were used to model a cup burner (laboratory test fixture that is used to calculate the amount of agent needed to suppress the fire in the absence of turbulence) using a defined amount of nitrogen as the suppressant. After gaining confidence with the cup burner, the enhanced CFD tool was used for the exploratory test box, which is representative of a ground combat vehicle crew compartment with HFC227ea+SBC as the suppressant. Simulation results were validated with test data for ballistic over pressures, toxic acid gas levels and suppression time.

The CFD design tool was evaluated for a MRAP vehicle crew compartment with different suppressant nozzle configurations. Predicted results from simulation of crew incapacitation criteria were compared with the test results obtained at Aberdeen Proving Ground, MD. Simulation results matched very well with testing.

In summary, the simulation-based acquisition tool for fire suppression using state-of-art CFD software with global reduced kinetics was developed by TARDEC to optimize AFES systems to enhance the survivability of the war fighter. The resulting design tool is being further enhanced and validated for various vehicle crew compartments and expanded to address non-occupied spaces such as engine compartments.

Theoretical Background

Automatic Fire Extinguishing System (AFES) developments efforts usually include several design, test, and fix cycles. Modeling & simulation allows one to conduct trade studies between various layouts quickly to reduce time and cost in the comparison of multiple AFES configurations.

The modeling & simulation approach involved for this simulation-based acquisition tool had to be computationally feasible to simulate the chemistry efficiently. The detailed chemical kinetics for fire suppression is complex and involves thousands of reactions and hundreds of chemical species. The simulation model for fire suppression must have the capability to model different types of heat transfer, buoyancy, turbulence, the ability to use different time steps to capture the transient phenomenon, the ability to transport and evaporate Lagrangian liquid and solid particles, the interaction of suppressant droplets with the chamber walls, the combustion of fuel, suppression chemistry, and generation and transport of toxic gases. The COTS software had the capability to simulate fire suppression, but without the suppressant chemistry responsible for fire suppression, or the production and mitigation of toxic gases. The current technical achievement is unique as the capability was not previously available in a general purpose CFD code.

Fire suppression chemistry deals with the prediction of the termination rate of chemical reactions related to the combustion of fuel with oxygen. Suppressant chemistry involves the details of chemical kinetics to predict intermediate species, but this is not practical for a vehicle simulation with detailed geometry. To be computationally efficient, a global reduced kinetics *phenomenological model* representing the effect of inhibitors was implemented parametrically into the CFD code.

R1: $JP\text{-}8 + O_2 => CO + CO2 + H_2O$
R2: $CO + O_2 <=> CO_2$
R3: $HFP + JP\text{-}8 + O_2 => HF + COF_2 + CO + H_2O$
R4: $COF_2 + H_2O => CO_2 + HF$
R5: $NaHCO_3(s) => CO_2 + NaOH(g)$
R6: $NaOH(g) <=> NaOH(hvy\_gas)$
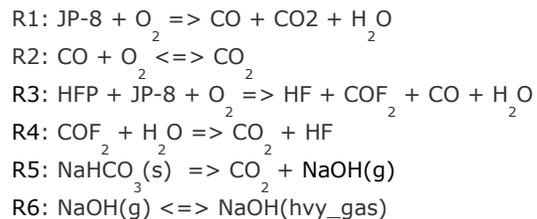
(hvy_gas = heavy-gas approximation)

R7: NaOH(hvy_gas) + HF => NaF(hvy_gas) + H_2O

R8: $NaHCO_3$(s) + HF => NaF(hvy_gas) + H_2O + CO_2

R9: JP-8 + O_2 => C (soot) + H_2O

R10: C (soot) + O_2 => CO_2
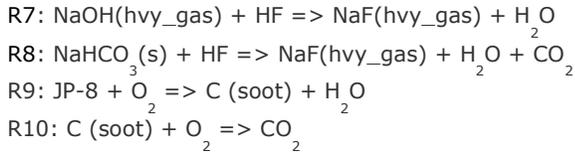
The reduced kinetics phenomenological model resulted in ten equations with thirteen species. Reactions 1 & 2 represent an uninhibited combustions process Ref [1]. Jet Propellant 8 fuel (JP-8) is represented with a surrogate fuel ($C_{12}H_{23}$) in simulation. Reaction R2 can occur faster in the presence of a flame but also can proceed in the absence of a flame. For the fire to go out, the reaction rate of R1 must reach zero.

Fuel, oxygen, carbon monoxide, carbon dioxide, water, HFC227ea, hydrofluoric acid (HF), carbonyl fluoride (COF_2), sodium hydroxide (gas + liquid), sodium bicarbonate (solid), sodium fluoride (solid) and soot scalars are modeled in the simulation. Some simplifications have been made to represent the formation of condensed liquid sodium hydroxide (NaOH) and solid sodium fluoride (NaF) through heavy gas approximation for computational reasons without affecting predicted accuracy.

The suppression mechanisms can be classified as a combination of physical and chemical inhibition as shown below:
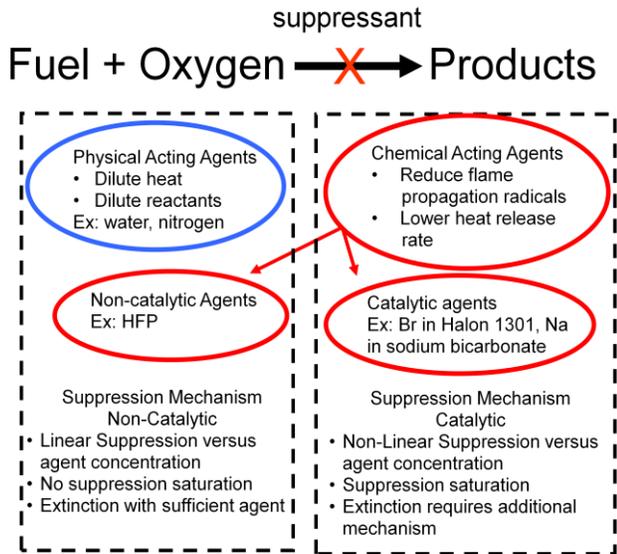
Categorization of Fire Suppression Mechanisms

Physical inhibition attributed mainly to diluting heat and reactants was implicitly accounted for in the CFD code and did not require any special treatment. Chemical inhibition includes catalytic inhibition, $\Delta R\_{catalytic}$ and non-catalytic inhibition, $\Delta R\_{non\text{-}catalytic}$ is not captured by the standard CFD software.

Suppression chemistry capability has been added to the CFD code through user coding. The majority of the achievement for this initiative was in implementing, modifying and validating this chemical inhibition. Catalytic inhibition has a nonlinear dependence on inhibitor concentration due to scavenging of flame radicals and non-catalytic inhibition has linear dependence on inhibitor concentration. The kinetic rates of all chemical reactions are expressed using Arrhenius rate expression. The kinetics rates were obtained through literature search, analysis of test data and derivation using reaction enthalpy. A generalized modification of the kinetic rate for inhibition for non-catalytic and catalytic inhibition is made for fuel oxidation rate of reaction, **R1** as follows:

R1(uninhibited)=$[C_{12}H_{23}]^{0.25}*[O_2]^{1.5}*3.8*10^{11}*exp(-30/RT)$

Where the calculated rate on the left-hand side of the equation is in moles/cm^3-s, the reactant concentrations in brackets are in moles/cm^3, the gas constant R is in units of kilocalories/mole-Kelvin, and T is the absolute temperature in Kelvin.

R1 (inhibited) =

R1(uninhibited) $- \Delta R\_{noncatalytic} - \Delta R\_{catalytic}$

$$\Delta R\_{noncatalytic} = R1_R^u * \Sigma_i X_i E_i$$

$$\Delta R\_{catalytic} = R1_R^u *(0.9 \cdot \Sigma_i X_i F_i)/(1 + \Sigma_i X_i \cdot F_i)$$

where X_i, E_i, F_i are mole fractions, and noncatalytic and catalytic suppression factors, respectively, for each inhibitor. The noncatalytic, E and catalytic, F suppression factors are derived from laboratory experiments or detailed kinetics.

Typical suppressants used in military ground vehicles are Halon 1301, Heptafluoropropane (HFC227ea) + sodium bicarbonate (SBC) and water-based agents. The generalized modification of kinetic rate for inhibition is valid for all the suppressants of interest to the Army. Most of the focus of the current modeling and simulation effort is related to HFC227ea combined with SBC Ref. [2].

Various best practices for representing the domain of interest with high mesh quality (resembling hexahedron elements), boundary condition specification for liquid and solid droplets at the walls, solver Lagrangian parameters, specification of suppressant spray parameters, and empirical parameters for extinction strain rate and minimum reaction rate are, just a few of the items that have been incorporated into the simulation. The kinetic reaction rate parameters have been refined based on CFD modeling of fire suppression events, and may be subject to further refinement in the future based on validation of computational predictions against experimental data. Thirteen species mentioned in R1- R10 are transported along with mass, momentum, energy, turbulence. Spray equations for suppressant droplets are solved in the computational domain.

Simulation Results

A cup-burner is a laboratory test method used to experimentally determine the suppressant concentration required for extinguishing a premixed flame.

The enhanced CFD suppression tool was validated for suppression flame extinction in a cup-burner with nitrogen where the suppressant effect is purely thermal and should be already accounted for in the CFD calculation since the conservation of energy lowers the temperature. Based on published literature Ref [3], as the oxygen mole fraction drops to 16.2%, the cup burner should extinguish – the flame detaches from the cup rim and travels along the chimney.

Two-step mechanism Ref [1] was used to simulate the combustion of fuel and oxygen as shown in Figure I (a). Simulation of the cup-burner is done in 2-D, assuming axial symmetry. Temperature contours are shown on the left and Oxygen contours are shown on the right. Results from suppression with nitrogen are shown in Figure I (b). As shown in the Figure I (b), the flame is lifted from the cup rim and is moved downstream which is a transient phenomenon. Ability to predict suppression with Nitrogen using two-step mechanism gave us confidence that physical suppression due to dilution is being captured in the CFD code.
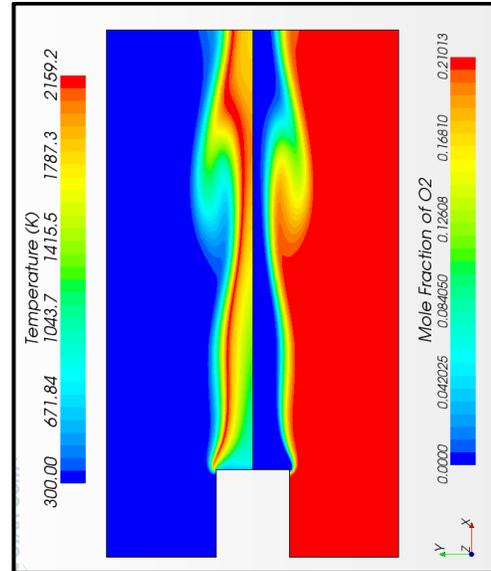
Fig. I (a) Uninhibited
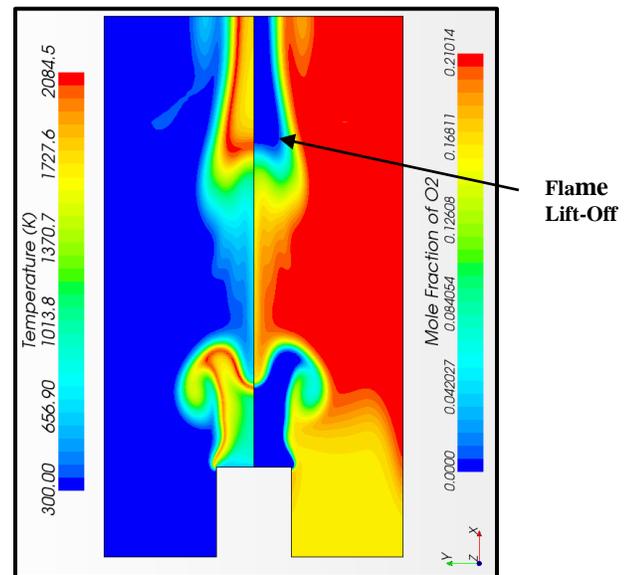
Fig. I (b) Inhibited with Nitrogen

Once confidence was gained with the cup-burner, suppression methodology was applied to an exploratory test box. This exploratory test box as shown in Figure II (a) has volume similar to a combat vehicle crew compartment but does not represent any particular combat vehicle. The exploratory box tests were conducted at the Army's Aberdeen Test Center (ATC) in a 260 ft³ box with relatively little clutter, no HVAC system and hatches closed. Extensive

test data are available for this configuration with different agents, nozzles and amounts of suppressants Ref [4].

The exploratory test box was meshed with COTS software Ref [5] using pre-dominantly hexahedral finite volume cells with prism cells near the wall as shown in Figure II (b). Multiple simulations were performed with cell sizes varying from 0.5 inch to 2.0 inch. One inch cell size was chosen as a compromise between the number of cells with a reasonable turn-around time and ability to capture the physics of interest.

The fire ball is simulated by spraying a surrogate fuel for JP-8. Multiple hollow cone angle nozzles are used to obtain the simulation spray pattern to match testing as shown in Figures III (a) & (b). The fire ball is generated based on a coarse estimate of the threat scenario using a specified amount of heated fuel at high pressure and an igniter to initiate the fire.

Suppressant nozzle cone angle and droplet distribution are based on the testing that was done using Particle Image Velocimetry (PIV) instruments. The droplet distribution is specified using a Rosin-Rommler distribution. Mass flow rate for the nozzle discharge is specified using output from Jet Propulsion Lab software that models a two-phase mixture of suppressant and pressurized nitrogen Ref. [6]. Heat transfer coefficient for energy transfer and the Sherwood number for the evaporation rate are calculated using the Ranz-Marshall approach. Drag coefficient is calculated using Schiller-Naumann method. Devolatization of dry powder is specified using a particle reaction rate. Two-way coupling between the Eulerian phase and Lagrangian phase is used to account for mass, momentum and energy transfer between the two phases.

Radiation from the fire ball is modeled using the discrete ordinate method to account for the radiative heat transfer in participating media. Absorption and the scattering coefficient of participating media are modeled using weighted sum of gray gases. However, this method considers only the local gas species concentration of CO_2 and H_2O as participating gases.

Turbulence is modeled using K-epsilon turbulence model. Energy is modeled using a segregated enthalpy. For the droplet interaction with walls, the composite mode is specified with selected probability from escape, rebound, and stick or vaporize based on local conditions. Various parameters are optimized for numerical stability, accuracy and turn-around time. Most of the stability issues are related to rapid evaporation of the suppressant.

Properties of liquid phase suppressants are based on published literature. These include temperature-dependent, polynomial expressions for density, specific heat capacity, latent heat of vaporization and critical temperature. Vapor pressure is calculated using Antoine Equation. Gas Phase properties such as specific heat capacity, enthalpy and entropy were modeled using NASA polynomials Ref [7].

Unsteady CFD solver simulation runs were made with different time steps to capture the development of the fire ball, discharge of suppressant particles, fire suppression, toxic acid generation and mitigation. This optimization of time steps for different stages of the suppression event was chosen such that appropriate time scales were used to capture the suppression phenomenon that spanned hundreds of milliseconds. The simulation needed to run for about ten seconds duration to compare toxic gas concentration as measured with a Fourier transform infrared spectroscopy (FTIR) test method.
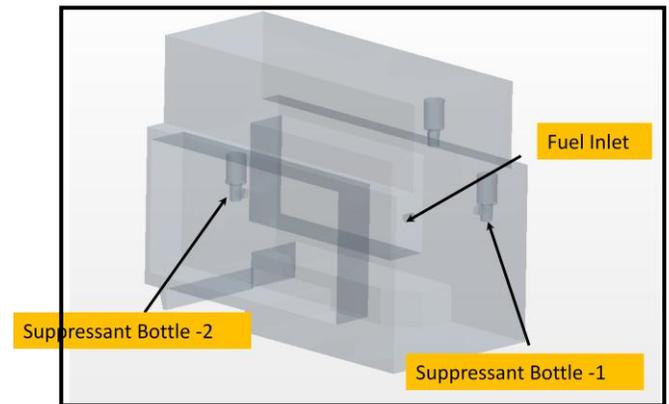
Fig. II (a) Exploratory Test Box
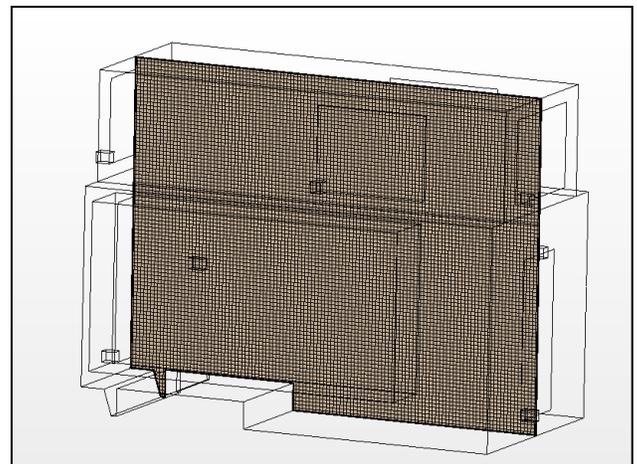
Fig. II (b) Finite Volume Mesh for the Test Box

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In the CFD simulation, the strength of the fireball is matched with a volume-normalized speed of explosion, K as used in industrial explosion protection tests Ref. [4]. As shown in Figure III (a) & (b), the fuel spray pattern was achieved in simulation through a combination of specification of multiple injectors and other injector parameters such as cone angle and diameter of the injector.

The strength of the fire ball is calculated as follows:

$$K = \frac{\Delta P}{\Delta t} \sqrt[3]{V}$$

K is calculated using a predetermined time interval for simulation. The value computed from simulation is compared with testing in Figure IV. In testing, a "K" value of 1 to 2 bar-meter/second is targeted and quite a bit of fluctuation is observed due to variation in testing parameters such as fuel pressure, cooling of fuel in the lines due to ambient conditions and ignition energy. Predicted values achieved from simulation of around 1.5 bar-meter/second are close to the targeted value.
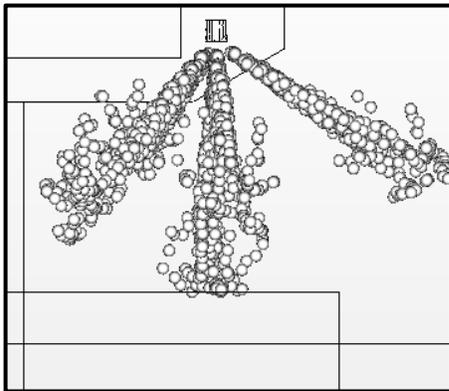
Fig. III (a) Fuel Spray Pattern (simulation)
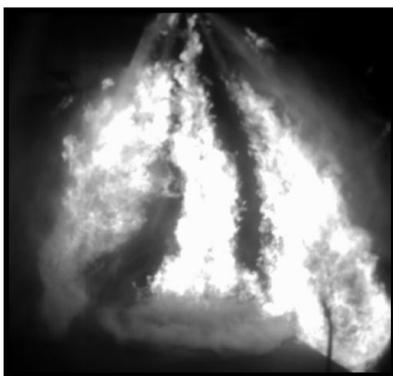
Fig. III (b) Fuel spray pattern (testing)
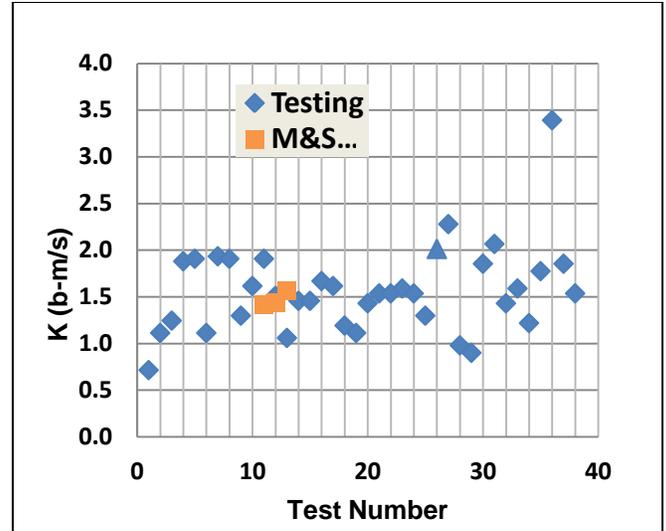
Figure IV. Exploratory Test Box Validation for Strength of the Fire Ball

The crew casualty criteria defined in Ref [8] were used to assess the simulation results. Out of eight required criteria summarized in Table I, six criteria were able to be assessed using the CFD simulation. Discharge forces and impulse noise resulting from the agent discharge were not captured in the simulation as modeling of the suppressant discharge from the bottle was not included.

Parameter	Requirement	M&S
Fire Suppression	Extinguish all flames without reflash	Y
Skin Burns	Less than second degree burns (<1315°C-sec & heat dose < 3.9 cal/cm² over 10 seconds)	Y
Overpressure	Less than 11.6 psi	Y
Agent Concentration	Not to exceed Lowest Observed Adverse Effects Level	Y
Acid Gases (HF + HBr + 2·COF$_2$)	Less than 746 ppm-min (5 min dose)	Y
Oxygen Levels	Not below 16%	Y
Discharge Impulse Noise	No hearing protection limit: <140 dBP Single hearing protection limit: <165 dBP	N
Discharge Forces	Not to exceed 8 g and <20 psi at 5 inches	N

Table I. Crew Survivability Criteria

Results from simulation of the exploratory test box are discussed here using HFC227ea + SBC. One simulation was done with the amount of agent above the design concentration required to suppress the fire and another simulation with the amount of agent below the design concentration required to suppress the fire. The objectives of these simulations are to assess the effectiveness of the simulation methodology.

Simulations are done with a fuel spray for about 50 msec before agent discharge to allow the fire ball to grow. Dry chemical is sprayed for about 10 msec and HFC227ea is sprayed after the dry powder. Typically, dry chemical is released initially from the bottle due to gravity before the liquid HFC227ea discharges due to pressurized nitrogen. Simulations are run on High Performance Computing Linux clusters using 48 CPUs. Typical turn-around time for a simulation is about a week.
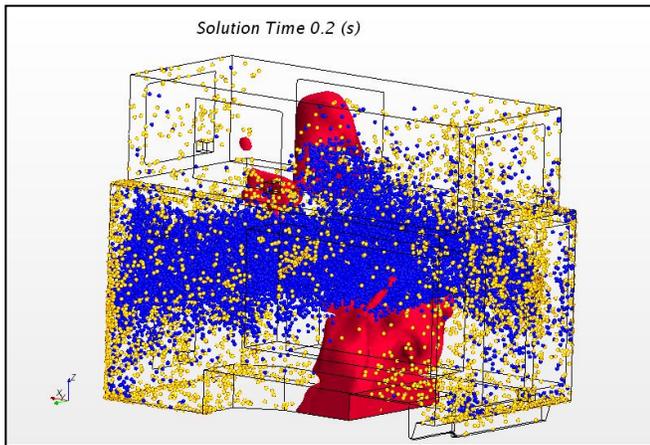
Figure V (a). Test Box (Successful Suppression)
Fire Ball (Red), SBC (Gold), HFC227ea (Blue)
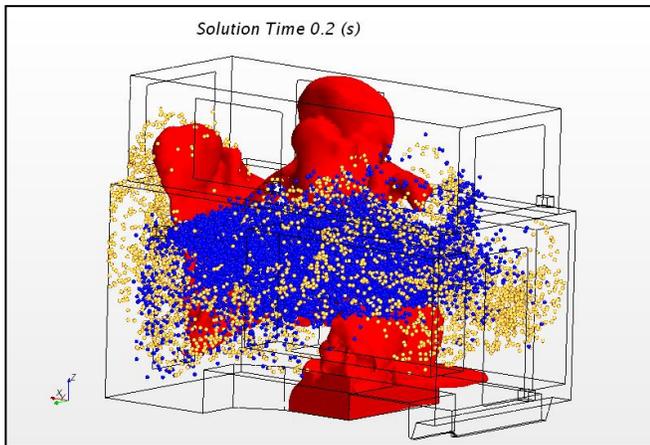
Figure V (b). Test Box (Failed Suppression)
Fire Ball (Red), SBC Powder (Gold), HFC227ea (Blue)

Simulation results from the two cases are shown in Figures V (a) & (b). The fireball is represented with an iso-surface of 800K temperature. Parcels of dry chemical are shown in yellow color and HFC227ea parcels in blue color are shown at 200 msec. As clearly can be seen, the fireball size is much bigger in Figure V (b) compared to V (a).

Figure [VI] shows the comparison of chemical heat release from the two simulations. Heat release predicted from simulation seems to correlate with the estimation of heat released per unit of mass of oxygen consumed. Chemical heat release from the unsuccessful suppression does not reach zero as can be seen for the suppression case within 400 msec. With unsuccessful suppression, the fire is not suppressed and rapidly grows. As the fire is not suppressed quickly, higher concentrations of HF and COF2 acids are generated due to interaction of the fire ball with the agent as shown in Figures VII and VIII.
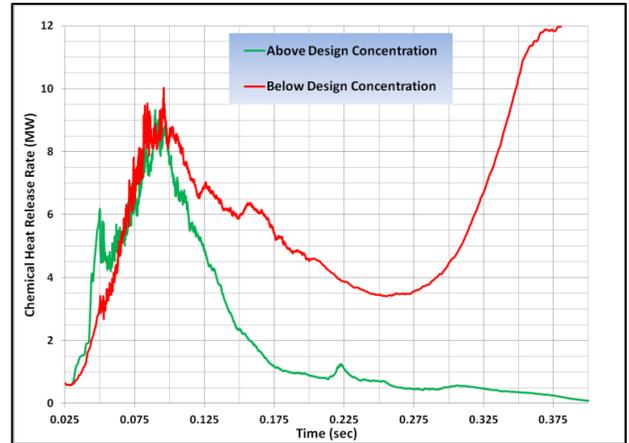
Figure VI. Chemical Heat Release Comparison
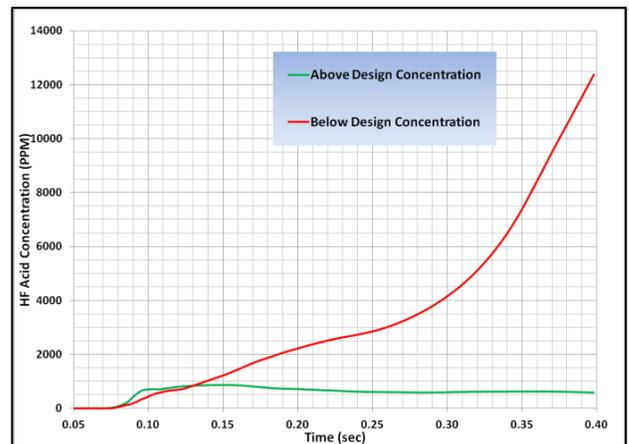
Figure VII. HF Acid Comparison

Volume averaged pressure and oxygen from simulation are shown in Figures IX and X. As can be seen from the comparison, pressure rises rapidly due to continued growth of the fire ball for the unsuccessful suppression and oxygen concentration drops below 16%.
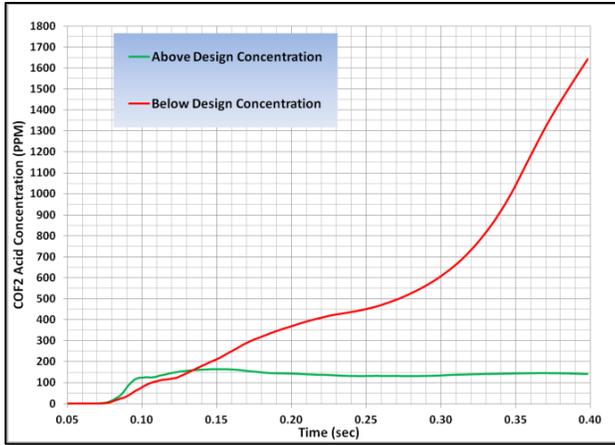
Figure VIII. COF2 Acid Comparison
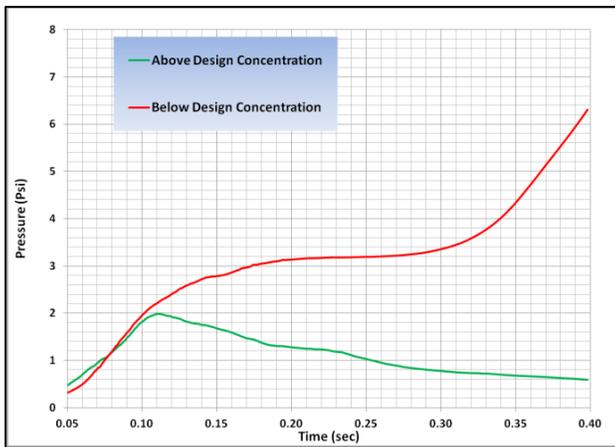
Figure IX. Pressure Comparison
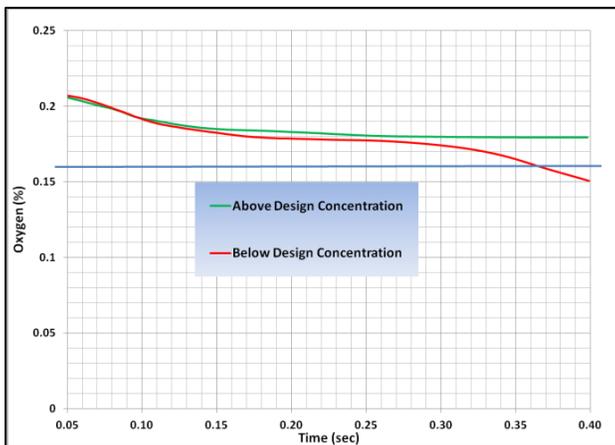
Figure X. Oxygen Comparison

Simulation results for the exploratory test box match with test results very well for the above design concentration scenario both qualitatively and quantitavely as shown in Table II. However, simulation results match only qualitatively with test results for agent concentrations below the design concentration. The reduced chemical kinetics based on Ref [1] are only valid for a certain range of fuel/oxygen ratios. With the below design concentration case, the fireball grows in regions with unrealistically lean concentrations of oxygen zones. A modification to the reduced kinetics is being validated to account for low oxygen concentration scenario.

Criteria	Above Design Conc.		Below Design Conc.	
	Test	Simulation	Test	Simulation
Overall	Pass	Pass	Fail	Fail
Extinguish Flames without reflash	YES	YES	YES	No
K Value	1.56	1.44	1.14	1.44
HF Acid (PPM)	<20	47	3975	NA
COF2 Acid (PPM)	<20	97	1550	NA
Oxygen Levels	17.4%	18.0%	16.5%	NA

Table II. Exploratory Test Box Results Comparison

After successful validation, the tool was used to simulate a fire in a crew compartment where the fire ball generator (FBG) was located on the rear wall of the crew compartment. The suppressant nozzle was located in the center of the roof of the vehicle.

Two different simulations were done with hatch open and no active air flow with different nozzle configurations and suppressant spray characteristics as shown in Figures XI & XII. The purpose of the suppression-enhanced CFD tool simulation was to evaluate whether the simulation tool could distinguish between nozzle designs given that the other parameters such as nozzle location and type, amount of agent and vehicle configuration remained the same.

Results from the simulation of two different nozzle configurations are summarized in Table III. The predicted results for blast overpressure, agent concentration, and oxygen concentration, correlate very well with test data. Overall, acid concentrations predicted for the two configurations qualitatively match with test data. Configuration I did not pass the toxicity criteria in testing compared to configuration II which is consistent with the simulations.

**Figure XI. Nozzle Configurations:
configuration I (left) and configuration II (right)**
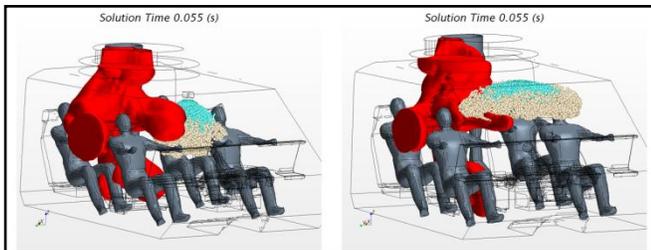
**Figure XII. Suppressant discharge patterns for
configurations I (left) and II (right).**
Fire Ball (red), SBC (yellow), HFC227ea (light Blue)

Heat flux data from the simulation are also being compared with testing for skin burn assessment. Quantitative results for skin burn are not included since the study is on-going but trends for predicted results are very encouraging.

Criteria	Configuration I		Configuration II	
	Test	Simulation	Test	Simulation
Overall	Fail	Fail	Pass	Pass
Extinguish Flames without reflash	YES	YES	YES	YES
Overall Pressure (psi)	0.59	0.48	0.35	0.31
Agent Concentration	Below LOAEL	Below LOAEL	Below LOAEL	Below LOAEL
HF Acid (PPM)	708	656	<20	96
COF2 Acid (PPM)	161	518	<10	169
Oxygen Levels	15.9%	15.9%	17.1%	17.2%

LOAEL (Lowest Observed Adverse Effects Level)
Table III. Comparison of simulation results with testing

Conclusions & Future Work

The results summarized in this paper represent TARDEC's effort to develop a simulation-based acquisition tool that can accurately predict fire-suppression trends. More vehicles are being simulated with the CFD tool to gain confidence and modeling improvements are being identified to increase its accuracy. This methodology has been extensively validated for HFC227ea+dry chemical combination.

Validation work with Halon + dry chemical, water + potassium acetate, dry chemical alone, and HFC-125 are in process. Enhancements to improve the accuracy of the simulation include a detailed description of the suppressant nozzle discharge, enhancements to chemical kinetic rates, oxygen depletion factor to account for low oxygen concentration, radiative properties calculation to include gases other than CO_2 and H_2O and specification of initial atmospheric conditions to take into account moisture content for hydrolysis of COF_2.

Assessment of the impact of mesh quality on overall prediction accuracy needs to be evaluated further. Optimal solver settings need further refinement to reduce overall turn-around times. Numerical stability of the simulation is a challenge due to rapid evaporation of the suppressant and enhancements to the software such as implicit treatment of latent heat contribution to the energy equation will improve the robustness of the simulation.

Also, this methodology is being applied to simulate fire suppression in an engine compartment with HFC-125. Challenges associated with meshing complicated geometry and numerical stability are being addressed.

Acknowledgements

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