



## Experimental and Numerical Studies on Chemically Active Flame Inhibitors

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**August 9, 2021 at 11:00 AM**

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### ABSTRACT

Fire hazards pose an increasingly potent threat to modern societies. Early identification and mitigation of fire hazards are crucial to avoid the loss of human lives and property. Recent research suggests that finely-atomized water spray consisting of droplets with a Sauter Mean Diameter (SMD) of less than  $100\text{ }\mu\text{m}$  is a superior fire-suppressant compared to traditional water sprinklers ( $\text{SMD} \sim 0.1 - 1\text{ mm}$ ). The addition of chemical inhibitors further improves the effectiveness of water mist as cooling, dilution, and chemical modes of fire suppression are combined. In the present thesis, the effectiveness of chemically active fire suppression agents for methane and LPG flames has been assessed through experiments and numerical modelling. The agents (K/Na-based compounds) are introduced in a counterflow diffusion flame of methane/LPG in the form of aqueous solutions, and their impact on the flame extinction is measured. Initial experiments conducted with pure water mist show 45% reduction in the extinction strain rate (ESR) at a  $Y_{H_2O} = 1.5\%$  in a methane flame. It is observed for both LPG and methane flames, the addition of alkali compounds further improves the inhibition effectiveness of water mist. Four potassium compounds and six sodium compounds have been tested in the present thesis. All potassium compounds show superior effectiveness compared to those of sodium. Among the tested additives, potassium bicarbonate ( $\text{KHCO}_3$ ) and potassium acetate ( $\text{CH}_3\text{COOK}$ ) are established as the most efficient in both methane and LPG flames. In methane flames, the addition of  $\text{KHCO}_3$  at 2% solute concentration to water reduces the ESR by 20% as compared that obtained using a pure water mist. Combinations of multiple compounds are also tested to identify possible synergistic/antagonistic interactions between the agents. Additive interaction is found in the  $\text{KHCO}_3$  -  $\text{NaHCO}_3$  mixture, whereas the mixture of  $\text{KHCO}_3$  –  $\text{CH}_3\text{COOK}$  shows antagonistic interaction. To understand these observations, experimental results are compared with one-dimensional simulations using detailed chemical kinetic models. Numerical predictions of the ESR under the influence of water mist are in good agreement with measured data. However, the influence of alkali solutions is only captured qualitatively in the simulations. Numerically, the analysis is extended to other classes of fire suppression agents as well. The ranking among four agents (Fe, K, P, Br-based) is obtained in a methane flame. Additionally, the work closely examines the effect of flame residence time on the inhibitor performance. The importance of regeneration coefficients and radical pool composition in determining the inhibitor effectiveness is established. The detailed chemical mechanism describing the phosphorus-based flame inhibition contains 44 species and 213 reactions, thus making the simulations computationally expensive. The thesis presents two reduced chemical mechanisms, i.e., a skeletal (4 species, 7 reactions) and a global (3 species, 3 reactions) mechanism, which lead to an 82% reduction in computational time with respect to the detailed mechanism. Overall, the thesis has led to an improved understanding of fire suppression under the influence of chemically active flame inhibitors, specifically identifying the most effective potassium-based chemical inhibitors for methane and LPG flames.

### ABOUT THE SPEAKER

Pabitra Badhuk is a Ph.D. student enrolled in the Department of Mechanical Engineering, IISc Bengaluru. He completed his B.E. from Jadavpur University, Kolkata, in 2015. After a short stint at BPCL, he joined IISc as an M. Tech student in 2016. His research interest includes chemical kinetics, combustion, and fire safety with a focus on chemically active flame inhibitors.

