

Screening of halogenated compounds for hydrogen flame (turbulent) inhibition

Background

Efficient hydrogen flame inhibition is a core part of nuclear power plants and hydrogen safety as a whole. A number of substances was proposed including halogenated compounds. The large scale experiments of hydrogen flame inhibition are very costly. Obviously there is a need in evaluating efficiency of different compounds in prevention of hydrogen combustion before experimental evaluation will be made.

Problem statement

The efficiency of halogenated inhibitors for hydrogen flames should be performed.

Theoretical preface

Combustion limits arise only in the system with losses (thermal, mass, momentum, etc.) [1]. The least and always present losses in any combustion process are radiation losses of energy from reaction zone [1]. For the hydrogen the most widespread regime of combustion is turbulent flame. When chemical reaction time become comparable characteristic time of radiative heat losses, combustion stops.

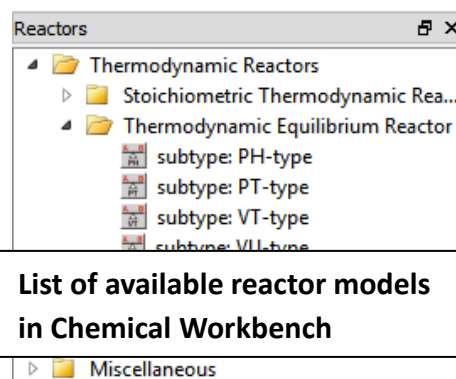
The ideal model of hydrogen turbulent combustion is well-stirred reactor, which is characterized by residence time (residence time in turbulent eddies). In frame of this model it is possible to plot the stable combustion diagram (lower limit due to short residence time and upper limit due to heat losses) in the coordinates “inhibitor concentration”-“residence time”. The concentration of inhibitor, which fully quench the combustion for any residence time will be used for screening purposes.

Problem setup in Chemical Workbench

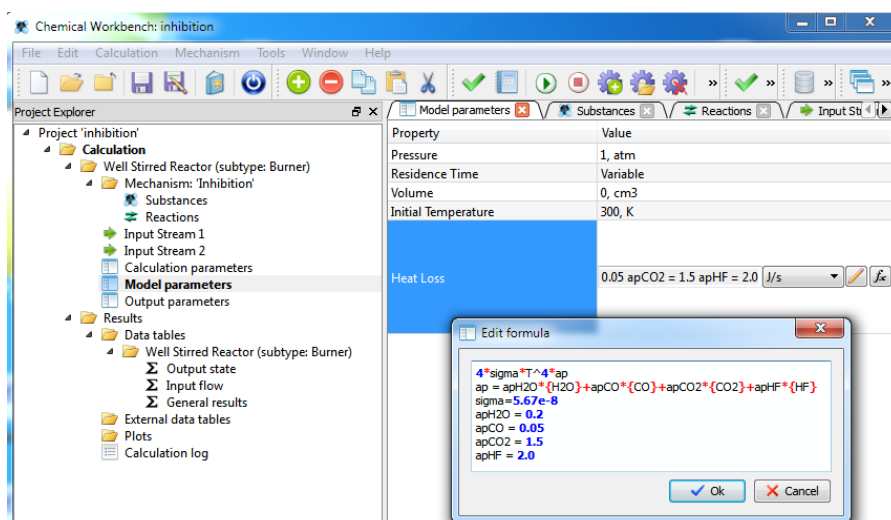
To **simulate the turbulent combustion** of stoichiometric hydrogen-air-inhibitor mixture, the WSR reactor model (sub-type burner) was used. State of the initial mixture: Inhibitor:H₂:O₂:N₂=X:2:1:3.76 (by volume), temperature 300K, pressure 1 atm. Two parameters are independent variables: residence time from 10⁻⁷ s to 10000 s, inhibitor molar fraction from 0 to 0.5 by volume.

The radiative heat loss are implemented as user-defined heat loss intensity based on actual mixture composition (primary radiating species H₂O, CO, CO₂, HCl) and temperature. The combustion mechanism of Babushok et al. [2, 3] was loaded from CHEMKIN format into Chemical Workbench software.

For every combination of residence time and inhibitor concentration the combustion success was identified by steady-state value of temperature: 1) mixture is burning if steady state temperature >> then initial temperature, 2) combustion failed if steady-state temperature is close to initial one (300 – 310 K)



List of available reactor models in Chemical Workbench

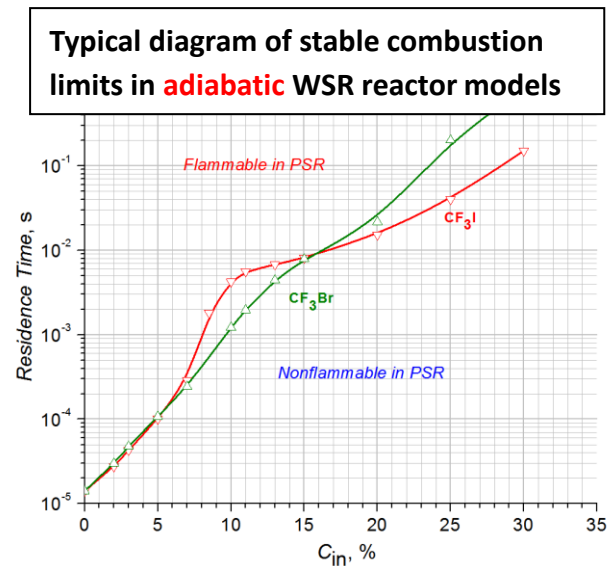
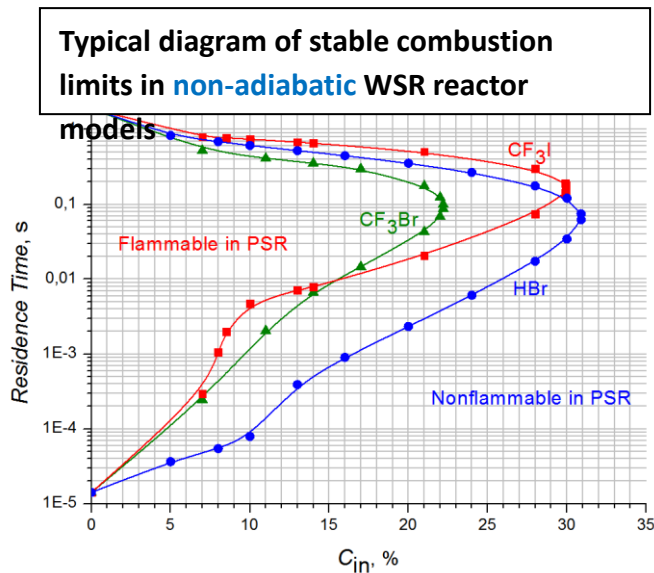


User-defined heat loss based on actual mixture composition for WSR reactor model in Chemical Workbench

Results

The screening of the different halogenated inhibitors was performed using developed model of combustion limits. Typical “flammable/non-flammable” diagrams in adiabatic WSR and non-adiabatic WSR reactor models are shown on the figures.

In case of adiabatic reactor only lower combustion limit is present, when chemical time becomes comparable with residence time. In case of non-adiabatic reactor both limits are present, when chemical time becomes comparable either with residence time (lower limit) or with heat loss time (upper limit). Also the limiting inhibitor concentration exists, when stable combustion in the system is not possible for any residence time of the reactive mixture.



Based on such a diagrams all candidate inhibitors can be ranked based on the limiting concentration, which completely prevents combustion. In the presented case the ranked set of inhibitors: $CF_3Br > CF_3I > HBr$ (from most efficient to least efficient).

Next steps

1. Keep only $C_{10}H_{22}$, O_2 , N_2 , CO , CO_2 , H_2 , N_2 in the species list and see how the combustion temperature will increase due to lack of dissociation of combustion products
2. Put fuel $C_{10}H_{22}$ with temperature 300K as a separate input stream of TER_PH of reactor model. Allow reactor model automatically account for different temperatures of separate streams. Thus tedious calculation of initial mixture temperature is omitted.

References

- [1] Ronney, P. D., “Premixed-Gas Flames,” in: Microgravity Combustion: Fires in Free Fall (H. Ross, Ed.), Academic Press, London, U.K., 2001, pp. 35-82.
- [2] T. Noto, V. Babushok, A. Hamins, W. Tsang, 1998, Combust. Flame, vol. 112, pp. 147 – 160.
- [3] V. Babushok, T. Noto, D.R.F. Burgess, A. Hamins, W. Tsang, 1996, Combust. Flame, vol. 107, pp. 351 – 367.