

Short Communication

Evaluating upper flammability limit of low hydrocarbon diluted with an inert gas using threshold temperature



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HIGHLIGHTS

- Theoretical model based on temperature threshold has been developed.
- A priority hypothesis for the consumption of the available oxygen was introduced.
- A general standard temperature was suggested for low hydrocarbons.
- The R^2 -value of the model is 0.9951 for nitrogen as diluent.

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ABSTRACT

This paper proposed a method using threshold temperature to evaluate upper flammability limit of a hydrocarbon diluted with an inert gas. A priority hypothesis for the consumption of the available oxygen was introduced. A linear relation model that could be applied for evaluating upper flammability limit of any low hydrocarbon diluted with a specific inert gas was founded theoretically. Examination of the model has been conducted on existing experimental data, including the cases of methane, propane, propylene, ethylene and isobutane. Results show that, given an inert gas, there may be a general critical temperature that could fit to any low hydrocarbon in case that the inert gas is not involved in combustion kinetics. The threshold temperatures recommended for carbon dioxide and nitrogen are 1700 K and 1650 K, respectively. The model is further compared to a similar published model and is shown to be far more accurate.

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1. Introduction

Developing efficient technologies to generate more electrical energy from a given fossil fuel based heat source is an important way for the abatement of greenhouse gas emissions. Studies have illustrated that hydrocarbons such as alkanes and aromatics show good character in high temperature Organic Rankine Cycle system (Siddiqi and Atakan, 2012; Shu et al., 2014a), which is a suitable technology for engine's waste heat recovery. However, such compounds are usually flammable, which limit their practical application. Mixtures based on low hydrocarbon and retardant may be good alternatives to solve this issue (Shu et al., 2014b, Garg et al., 2013). Thus, flammability characteristics of such a mixture become important for assessing its practical application possibilities. An essential feature is the flammability limit. It includes two

parts, the lower flammability limit (LFL) and upper flammability limit (UFL), which defined the concentration range of a fuel in air in which a flame can propagate.

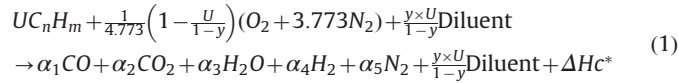
Flammability limits are related to a certain critical energy generation rate or with a certain level of reaction temperature (Himmelblau and Riggs, 2012). Accordingly, to estimate flammability limits a temperature threshold is assumed. Vidal et al. (2006) pointed out that calculated adiabatic flame temperature (CAFT) is a powerful tool for evaluating the LFL of a fuel gas diluted with an inert gas. As demonstrated (Shu et al., 2015), when applying CAFT for predicting flammability limits, the deviation between predicted UFL result and experimental data is larger against that of LFL. The prediction accuracy of UFL needs to be improved. The purpose of present study is to propose a method based on threshold temperature to evaluate UFL of low hydrocarbon diluted with an inert gas and discuss the idea that whether there is a general standard temperature that could fit to any low hydrocarbon for a specific diluent.

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2. Method

It is generally accepted that incomplete combustion is involved when combustion occurs at UFL. Considering the case of one mole hydrocarbon–air–diluent mixture combustion, a general global reaction for a typical hydrocarbon C_nH_m at its UFL in such a mixture is assumed to be:



Where y is the molar fraction of diluent in hydrocarbon–diluent mixture; U is the UFL concentration of hydrocarbon in hydrocarbon–air–diluent mixture; ΔHc^* is heat of the combustion, it can be calculated through the following equation:

$$\Delta Hc^* = U \times \Delta Hc_{C_nH_m} - \alpha_1 \times \Delta Hc_{CO} - \alpha_4 \times \Delta Hc_{H_2} \quad (2)$$

As shown in reaction Eq. (1), the amounts of reactants before the combustion are clear. But after the combustion, the product compositions are not distinct, not to mention the quantity of them. The product compositions at rich conditions depend on combustion kinetics and chemical equilibria. Researchers often use chemical equilibria to analyze the product compositions. On the other hand, there is few work has been devoted to employing kinetic analysis for the same purpose which is also an important factor (Vidal et al. (2006), Shebeko et al. (2002)). This paper attempts to introduce a priority hypothesis for the kinetic analysis which in turn analyzes the product compositions. Assuming oxygen is reacted completely and consumed on the following priority basis. Firstly, hydrocarbon is oxidized to carbon monoxide and hydrogen; secondly, depending on how much oxygen remains unutilized and using it to oxidize hydrogen to water vapor; finally to oxidize carbon monoxide to carbon dioxide if there were still oxygen left. Accordingly, the composition and contents of the products could be determined. Furthermore, CO_2 is hard to form while combustion occurs at upper flammability limit owing to the fact that air is poor, so the products will be mainly made up of H_2 , CO and H_2O . Combining the mass conservation law with the priority basis assumption, all the parameters could be figured out and the results are illustrated in Table 1.

Providing the temperature of combustion products could reach to a critical temperature while the combustion reaction occurs under adiabatic condition. Through the energy balance analysis of Eq. (1) yields,

$$\alpha_1 H_{CO}^0 + \alpha_2 H_{CO_2}^0 + \alpha_3 H_{H_2O}^0 + \alpha_4 H_{H_2}^0 + \alpha_5 H_{N_2}^0 + \frac{y \times U}{1-y} H_D^0 + \Delta Hc^* \rightarrow \alpha_1 H_{CO}^c + \alpha_2 H_{CO_2}^c + \alpha_3 H_{H_2O}^c + \alpha_4 H_{H_2}^c + \alpha_5 H_{N_2}^c + \frac{y \times U}{1-y} H_D^c \quad (3)$$

Wherein, the superscripts '0' and 'c' refer to the initial temperature (298 K) and the critical temperature, respectively.

Table 1

Mass balance for hydrocarbon combustion occurs at its upper flammability limit in hydrocarbon–air–diluent mixture.

Compounds	No. of moles before reaction	No. of moles after reaction
Hydrocarbon	U	0
Diluent	$U \cdot y / (1-y)$	$U \cdot y / (1-y)$
Air		
Oxygen	$(1 - U / (1-y)) / 4.773$	0
Nitrogen	$3.773(1 - U / (1-y)) / 4.773$	$3.773(1 - U / (1-y)) / 4.773$
Carbon monoxide	0	$U \cdot n$
Carbon dioxide	0	0
Water vapor	0	$2(1 - U / (1-y)) / 4.773 - U \cdot n$
Hydrogen	0	$U \cdot (n+m/2) - 2(1 - U / (1-y)) / 4.773$

Assuming the combustion process at UFL occurs at the atmospheric pressure, Eq. (3) could be converted to (4):

$$\left[\alpha_1 C p_{CO} + \alpha_2 C p_{CO_2} + \alpha_3 C p_{H_2O} + \alpha_4 C p_{H_2} + \alpha_5 C p_{N_2} + \frac{y \times U}{1-y} C p_D \right] \Delta T = \Delta Hc^* \quad (4)$$

Wherein, ΔT is the difference between the threshold temperature and initial temperature. Substituting Eq. (2) and relevant parameters in Table 1 into Eq. (4), through a series of deduction (see supplementary information A) yields,

$$\frac{1}{U} - \frac{1}{U_0} = k \left(\frac{1}{1-y} - 1 \right) \quad (5)$$

$$k = \frac{(2C p_{H_2} - 2C p_{H_2O} - 3.773C p_{N_2} + 4.773C p_D) \Delta T + 2\Delta Hc_{H_2}}{2\Delta Hc_{H_2} - (2C p_{H_2O} - 2C p_{H_2} + 3.773C p_{N_2}) \Delta T} \quad (6)$$

Wherein, U_0 is UFL concentration of pure hydrocarbon in air. Eq. (5) is the theoretical model for predicting UFL of a hydrocarbon diluted with an inert gas. An amazing point was discovered that the slope (k) has nothing to do with the number of carbon or hydrogen atoms in the hydrocarbon molecule. It is a constant once a critical temperature was defined. Thus, for a specific diluent, an idea that whether there is a general critical temperature that could fit to any hydrocarbon was formed and would be confirmed.

Coincidentally, the formula (5) developed in present study is similar to the one drawn by Chen et al. (2009a, b), the difference is the slope expression. As Eq. (7) shown, the one developed by them is denoted with a '*'. The predictive effectiveness of models determined by Eqs. (6) and (7) would be compared in next section.

$$k^* = \frac{U_0 C p_f + (1 - U_0) C p_D}{U_0 C p_f} \quad (7)$$

3. Results and discussion

For UFL prediction, a threshold temperature must be chose in the first place to determine the slope value. As a corollary, the selected threshold temperature may have a significant impact on prediction precision. Di Benedetto (2013) applied ignition temperatures as the threshold temperature for the flammability limits estimation. The results indicate that a much higher threshold temperature may be used to improve the prediction accuracy. For the sake of caution, a series of temperatures were chose for the evaluation and verification of their effectiveness was conducted on existing experimental data. Experimental data reported in recent works by Kondo et al. (2006a, b; 2007) were adopted for examination, including the cases of methane, propane, isobutane, ethylene and propylene.

3.1. Hydrocarbon diluted with carbon dioxide

For various threshold temperatures, the slope value and coefficient of determination (R^2 -value) of predicted lines could be seen in Table 2. A temperature of 1700 K could fit best to all of the hydrocarbons and the R^2 -value is 0.9830, which indicates a high accuracy was achieved. Figure 1 shows an intuitive representation

Table 2

Calculated slope (k) and R^2 -value of predicted lines with different threshold temperatures for carbon dioxide as diluent.

Temperature	1500 K	1550 K	1600 K	1650 K	1700 K	1750
Slope	1.969	2.044	2.124	2.209	2.300	2.397
R^2 -value	0.9518	0.9651	0.9753	0.9816	0.9830	0.9787

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