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Experimental measurements and numerical calculation of auto-ignition temperatures for binary miscible liquid mixtures

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ABSTRACT

Auto-ignition temperature (AIT) is one of the most important parameters to assess potential fire and explosion hazards for chemicals. In this work, the AITs of 132 groups of binary miscible liquid mixtures were measured. Experimental results show the AITs of binary miscible liquid mixtures vary with their volume ratios. Three types of trends representing the relationship between AITs and volume ratios were found. A computational model was established to calculate the AITs of methanol + toluene, ethyl alcohol + toluene, ethyl alcohol + methanol and *n*-heptane + ethyl alcohol in 6 volume ratios. The calculation results showed that the calculated deviations were within 8% of the experimental results. For higher hydrocarbons, the model suffers from a lack of accurate chemical kinetic data to properly predict the AITs of the mixtures.

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1. Introduction

The auto-ignition temperature (AIT) is widely used to assess the potential fire and explosion hazards for chemicals in fire protection design and risk assessment (Kim et al., 2002). The auto-ignition temperature of a substance is the lowest temperature at which it spontaneously ignites in ambient air without an external ignition source, such as a flame or spark. There is extensive data on AITs of single-component fuels (Suzuki and Takahiro, 1994). For pure flammable liquids, in general AITs can be attained through lab testing or be calculated by using specific methods (Albahri and George, 2003; Pan et al., 2008; Ihme and See, 2010; Gharagheizi, 2011; Tsai et al., 2012). For instance, Borhani et al. (2016) present a predictive model for the estimation of the AIT of 813 hydrocarbons from 69 different chemical families using a quantitative structure-property relationship (QSPR) approach. In addition, there are some data about AITs of gas mixtures (Kong et al., 1995; Rota and Zanoelo, 2003; Norman et al., 2006). However, compared with pure substances, there are fewer ways to get AITs of mixtures because the AITs change with composition.

Methods using empirical formulae and chemical group contribution are often applied in studying combustion characteristics including the flash point, and auto-ignition temperature (Chen et al., 2009; Pan et al., 2015; Cheng et al., 2015). Ye et al. (2015) presented a model to predict the AITs of binary miscible liquid mixtures using the chemical group contribution method. The detailed model was established using a multiple nonlinear regression method. The average absolute percentage errors of the training set and test set were 5.18% and 7.25%, respectively. It should be noted that for a mixed system containing a benzene ring, the average absolute error was 17.24%. He et al. (2016) established a model to predict AITs for binary liquid mixtures based on electro-topological state indices. The squared correlation coefficient and average absolute error of the proposed model were 0.991 and 3.962 K, respectively. In recent years, some papers focused on the method used to predict AITs of organic mixtures (Peper et al., 2015; Sabard et al., 2017). Tak-

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ing into account the role of molecular functional groups, Zhang and Boehman (2012) studied the auto-ignition of two binary fuel blends of *n*-heptane and C_7 esters in a motored engine, namely a *n*-heptane/methyl hexanoate blend and a *n*-heptane/methyl 3-hexenoate blend. They found that the attack of radical species to the double bonds plays an important role in the oxidation of the unsaturated esters. Then, Boot et al. (2017) found that unsaturated molecules (cyclic), additional side chains, and functional oxygen groups play important roles in the auto-ignition behavior of substance. By studying the impact of the molecular structure of the fuel on auto-ignition behavior, design rules for future high-performance gasolines were derived. Li et al. (2017) investigated the effect of fuel type, fuel molar concentration, and air molar concentration (the concentration of O_2/N_2 is constant) on the AIT of *n*-heptane, methanol, ethanol, and butanol using a constant volume bomb. The experimental results indicated that the AIT generally decreases as the chain length and molecular weight increase. An increase in either fuel molar concentration or air molar concentration had a tendency to reduce the AIT. Subsequently, a numerical study was performed to identify the cause of these AIT variations using validated and comprehensive reaction mechanisms of *n*-heptane and methanol. They found that the diverse reaction routes make the *n*-heptane oxidation process less sensitive towards external factors (such as temperature, fuel molar concentration, and air molar concentration). Conversely, the methanol oxidation process is strongly dependent on external factors.

Thus far, extensive research programs have studied the auto-ignition delay of mixture of fuels under different combustion conditions (Bounaceur et al., 2009; Thiessen et al., 2010; Kim et al., 2015). Among these extensive studies, Holton et al. (2010) performed autoignition delay experiments in an atmospheric flow reactor using typical natural gas components, namely, methane, ethane and propane. Autoignition delay measurements were also performed for binary and ternary fuel mixtures. Equivalence ratios for the experiments ranged between 0.5 and 1.25, and temperatures ranged from 930 K to 1140 K. The results showed that increasing the equivalence ratio and increasing the inlet temperature over these ranges decreased autoignition delay times. Sante (2012) and Zhang et al. (2013) measured the ignition delay times of *n*-heptane/toluene mixtures and *n*-heptane/*n*-butanol mixtures respectively. Both used different experimental equipment, being a rapid compression machine and reflected shock waves methodologies respectively. Sante (2012) developed a single-zone model using CHEMKIN software with Lawrence Livermore detailed oxidation mechanisms to model the combustion of the *n*-heptane/toluene mixtures, Zhang et al. (2013) also conducted kinetic modeling for interpreting the oxidation of the *n*-heptane/*n*-butanol mixtures. The rapid compression machine was also used in the research by Kumar et al. (2015). They studied the influence of blending *n*-butanol on the ignition delay times of *n*-heptane and iso-octane, and the ignition delay times were measured. The majority of the experiments were conducted at an equivalence ratio of 0.4 and a pressure of 20 bar, with the temperatures at the end of compression ranging from 613 K to 979 K. In addition, Troshin et al. (2016) studied the influence of C_3–C_5 alkanes on the ignition delay of their binary mixtures with methane in air at a temperature of 523–1000 K and a pressure of 1 atm. However, few studies have focused on the change in the AIT as a function of the ratio of the fuel components, which is of significant practical importance. The present work explores the AIT dependence on the ratio of the fuel components by measuring the AITs of 12 groups of binary miscible liquid mixtures in 11 volume ratios by using an AITTA 551 auto-ignition temperature tester. In addition, it is also an objective to provide an experimental database for these 12 groups. In the present study, a computational model will be established and validated using the experimental data, and the AITs of four binary miscible liquid mixtures in different volume ratios will be calculated using this model in combination with detailed chemical kinetic mechanisms.

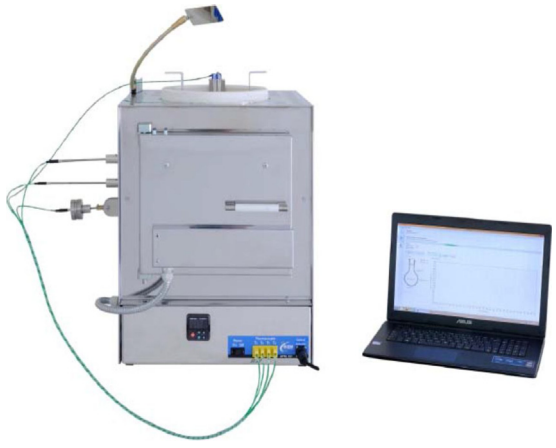

Fig. 1 – AITTA 551 auto-ignition temperature tester.

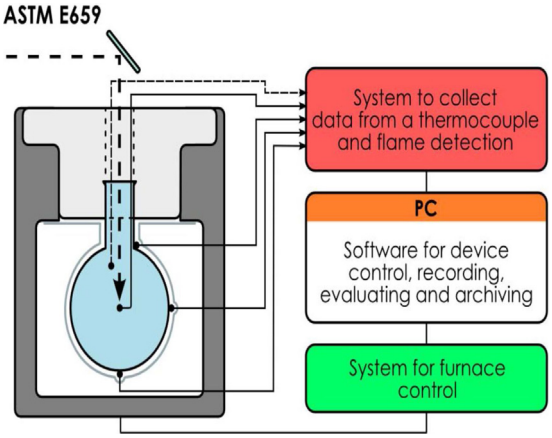

Fig. 2 – Structure chart of AITTA 551 auto-ignition temperature tester.

2. Experiments

2.1. *Experimental apparatus and chemicals*

As shown in Fig. 1, the AITTA 551 auto-ignition temperature tester (Manual AITTA 551) is used as experimental apparatus. AITs are obtained according to the ASTM E659-78 test standard. As can be seen in Fig. 2, the AITTA 551 auto-ignition temperature tester contains a heating furnace, control software and measurement unit. In the heating furnace, a 500 mL flask is installed, and three thermocouples are contacted to the outside surface of the flask to monitor its temperature variation. A fourth thermocouple is placed inside the flask. The computer controls the tester and collects data of the thermocouples simultaneously. When testing starts, the flask is homogeneously heated.

In this work, 10 analytical grade reagents were used: methanol, ethyl alcohol, *n*-butyl alcohol, 1-pentanol, *n*-hexane, *n*-heptane, acetic acid, acetone, toluene and ethyl acetate. These substances were selected due to their extensive usage in process industries.

2.2. *Experimental method*

Considering the mutual solubility of these 10 chemicals, 12 binary miscible liquid mixtures in different volume ratios were prepared. At the beginning of a test, the temperature in the heating furnace was pre-set as the estimated value of the AIT. The estimated AIT was obtained based on the AITs of the two components of the binary miscible liquid mixture. When the furnace was heated up to the estimated temperature and remained unchanged for 5 min, 100 μL miscible mixture was

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