Effect of Initial Temperature and Pressure on Laminar Combustion Velocity of ABE Mixtures with Different Component Contents

Jinying Xiong1*, Yingzhe Hou1, Xiaozhe Yan1, Qiguan Cui1, Yiwen Liu1
1Wuhan Second Ship Design and Research Institute, Wuhan, Hubei, 430064, China
*Corresponding author’s e-mail: 13554161079@163.com

Abstract: One-dimensional planar flame was numerically simulated to study the premixed laminar combustion characteristics of acetone-n-butanol-ethanol (ABE) mixtures under different component contents. The results showed that as the initial temperature was elevated, the laminar combustion velocity of ABE mixtures was gradually increased under different component contents, and the increase rate was not obviously changed. With the increase in the initial pressure, however, the laminar combustion velocity presented a declining trend, and the descent speed was gradually lowered.

1. Introduction
Fossil fuels like petroleum, natural gas and coal are the main energy sources at present in the world. However, the heavy use of the fuels will lead to environmental pollution and gradual reduction of resources, so numerous scholars have been devoted to studies regarding new-type fuels. n-Butanol is a high-quality biomass fuel, but as a large quantity of energy needs to be consumed in the purification process, some scholars have put forward using the intermediate product—acetone-n-butanol-ethanol (ABE) mixture—of n-butanol purification as the new-type alternative fuel, and found that the component contents of this mixture can be controlled by adjusting the zymophyte type and fermentation environment. In related studies, ABE mixture has been applied as fuel to internal combustion engines. For instance, in 2016, Sithyanandan et al. [1] screened out the optimal component content ratios of ABE (A:B:E = 6:3:1; 3:6:1; 5:14:1) and used this mixture as the fuel mixed with gasoline. Studies showed that compared with n-butanol, the ABE mixture with component content ratio of 6:3:1 was a more suitable alternative fuel in the aspect of thermal efficiency. The above studies have verified that the ABE mixture is a favorable alternative fuel, and the volume ratios of acetone, n-butanol and ethanol commonly applied to engines are 6:3:1, 3:6:1 and 0:10:0. Therefore, the ABE mixtures with different component contents, when used as additives, will exert a certain influence on the combustion characteristics of mixed fuel in engines.

Studying the characteristic parameters of laminar combustion will facilitate the subsequent studies on the chemical kinetics mechanism of fuels and lay a foundation for the future exploration into turbulent combustion. The influences of initial conditions on the laminar velocity of ABE single-component fuels have been investigated at present. In 2011, Gu et al. [2] used the spherical flame spreading method to study the influence of nitrogen dilution on the laminar combustion characteristics of n-butanol-air mixture under initial temperature of 428-488 K, pressure of 1-5 atm and equivalence ratio of 0.8-1.5. However, few studies have involved the influences of initial conditions on the laminar combustion velocity of ABE mixtures under different component contents. Therefore, the influences of the changes...
in initial temperature and pressure on the laminar velocity of ABE mixtures under different component contents were probed in this study. In 2012, Sarathy et al. [3] constructed a detailed chemical kinetics combustion model for four butanol isomerides, and this mechanism included 426 components and 2,335 elementary reactions. Sarathy et al. measured the combustion characteristic parameters of butanol using constant-volume combustion bomb, rapid compression machine, shock tube and jet flow stirrer, compared the simulated values with experimental values, and the comparison results showed favorable consistency. Compared with the butanol mechanism studied by predecessors, the characteristics and innovation of this mechanism lied in that it contained detailed high-temperature and low-temperature reaction paths, and derived the reaction rate constant. In addition, Sarathy et al. perfected all reaction types of butanol isomerides, thus better predicting the combustion characteristics from low-temperature segment to high-temperature segment. The above mentioned butanol oxidation mechanism remains to be further verified with the related laminar combustion characteristic parameters of ABE mixtures under different component contents.

2. Research method

2.1. Basic control equations and CHEMKIN software
The Premixed Laminar Flame-speed calculation module [5] (abbreviated as PREMIX model) in the gaseous chemical kinetics software CHEMKIN [4] was used in this study to establish 1D steady flat flame of ABE mixture, followed by numerical solution. The module selected in this paper and its establishment process are shown in Figure 1, including fluid inlet, outlet and flat flame simulation module.

![Figure 1. Establishment of PREMIX Module in CHEMKIN](image)

3. Results and Analysis

3.1. Influence of temperature on laminar combustion velocity of ABE Mixtures under different component contents

![Graphs](image)
The mechanism constructed by Sarathy et al. [3] was selected to simulate the 1D flat flame. Figure 2(a) shows the influences of acetone content on the laminar combustion velocity of $n$-butanol-acetone mixture at different temperatures. It could be known that as the initial temperature rose, the laminar combustion velocity of this mixture was gradually elevated, and the increase rate was not obviously changed. When the acetone content reached 60%, the laminar combustion velocity of this mixture started being different from that of $n$-butanol to some extent. Figure 2(b) presents the influences of ethanol content on the laminar combustion velocity of $n$-butanol-ethanol at different temperatures, and it could be observed that with the increase in initial temperature, the laminar combustion velocity of $n$-butanol-ethanol mixture was gradually increased, and the increase rate was basically unchanged. As the ethanol content was increased, the difference in the laminar combustion velocity of $n$-butanol-ethanol mixture under different ethanol contents was gradually enlarged. With the increase of initial temperature, the difference in the laminar combustion velocity of mixtures under different ethanol contents was basically unchanged. Figure 2(c) displays the influences of acetone content on the laminar combustion velocity of mixture with and without ethanol at different temperatures, and it could be seen that as the temperature was elevated, no matter whether ethanol was adulterated or not, the laminar combustion velocity presented a rising trend. At different temperatures, the laminar combustion velocity of ABE mixture added with 10% ethanol was higher than that of the $n$-butanol-acetone mixture not added with ethanol. Moreover, as the initial temperature was increased, the difference between ABE mixture and $n$-butanol-acetone mixture in the aspect of laminar combustion velocity was slightly enlarged. With the increase in acetone content, such difference was gradually increased. Figure 2(d) shows the influences of ethanol content on the laminar combustion velocity of mixture with and without acetone at different temperatures, and it could be known that as the temperature was increased, no matter whether 30% acetone was added or not, the laminar combustion velocity presented a rising trend. With the increase in ethanol content, the difference between ABE mixture and $n$-butanol-ethanol mixture in the laminar combustion velocity was gradually enlarged. At different temperatures, the laminar combustion velocity of ABE mixture added with 30% acetone was obviously higher than that of $n$-butanol-ethanol mixture not added with acetone under a large ethanol content (60%). Furthermore, as the temperature was increased, the difference between ABE mixture and $n$-butanol-ethanol mixture in the laminar combustion velocity was slightly increased.
3.2. Influence of pressure on laminar combustion velocity of ABE under different component contents

Figure 3. Influences of Changes in Component Contents on Laminar Combustion Velocity of ABE Mixtures under Different Pressures

Figure 3(a) presents the influences of acetone content on the laminar combustion velocity of \( n \)-butanol-acetone mixture under different pressures, and it could be known that with the increase in initial pressure, the laminar combustion velocity presented a declining trend under all acetone contents, and the descend speed was gradually lowered. As the initial pressure was increased, the difference in the laminar combustion velocity of acetone-\( n \)-butanol mixture under different acetone contents was gradually expanded. Figure 3(b) shows the influences of ethanol content on the laminar combustion velocity of \( n \)-butanol-ethanol mixture under different pressures: with the increase in initial pressure, the laminar combustion velocity of \( n \)-butanol-ethanol mixture was gradually lowered, and the descent rate was also on the decrease. As the initial pressure was increased, the difference in the laminar combustion velocity of \( n \)-butanol-ethanol mixture under different ethanol contents was gradually reduced. Figure 3(c) displays the influences of acetone content on the laminar combustion velocity of mixture with and without ethanol under different pressures, and it could be known that as the pressure was increased, the laminar combustion velocity of ABE mixture added with 10% ethanol and that of \( n \)-butanol-acetone mixture not added with 10% ethanol both presented a declining trend. Under the acetone content of 0-60%, the laminar combustion velocity of ABE mixture added with 10% ethanol was always not obviously different from that of \( n \)-butanol-acetone mixture not added with 10% ethanol as the pressure was increased. Furthermore, as the pressure was elevated, the difference between acetone-ethanol mixture added with 10% ethanol and acetone not adulterated with ethanol in the laminar combustion velocity was not obviously changed. Figure 3(d) displays the influences of ethanol content on the
laminar combustion velocity of mixture with and without acetone under different pressures, and it could be known that with the increase in pressure, the laminar combustion velocity of ABE mixture added with 30% acetone and that of n-butanol-ethanol mixture not added with acetone both presented a declining trend. As the pressure was increased, the difference between ABE mixture added with 30% acetone and n-butanol-ethanol mixture not added with acetone in the laminar combustion velocity was gradually reduced. Under a high ethanol content and low pressure, the laminar combustion velocity of ABE mixture added with 30% acetone was higher than that of n-butanol-ethanol mixture not added with acetone, and higher ethanol content and lower pressure would result in a larger difference between the two mixtures in the laminar combustion velocity.

4. Conclusion
Through the numerical simulation method of 1D plane, the influences of changes in temperature and pressure on the laminar combustion velocity of ABE mixtures under different component contents were studied by using the mechanism established by Sarathy et al., and the influence laws were analyzed. The following conclusions were drawn:

1) With the increase in initial temperature, the laminar combustion velocity of ABE mixtures was gradually increased under different component contents, and the increase rate did not go through any obvious change. The laminar combustion velocity of ABE mixture added with 10% ethanol was higher than that of n-butanol-acetone mixture, and that of ABE mixture added with 30% acetone was higher than that of n-butanol-ethanol mixture, and moreover, the difference between the two mixtures in the laminar combustion velocity was gradually enlarged with the increase in ethanol content.

2) As the initial pressure was increased, the laminar velocity of ABE mixtures under all component components presented a declining trend, and the descent rate was gradually reduced. When the pressure was elevated under the acetone content of 0-60%, the ABE mixture added with 10% ethanol was not obviously different from the n-butanol-acetone mixture in the aspect of laminar combustion velocity, and the difference between ABE mixtures added with 30% acetone and n-butanol-ethanol mixture in the laminar combustion velocity was gradually reduced with the increase in initial pressure.

References
[1] Nithyanandan K, Zhang J, Li Y, et al. (2016) Improved SI engine efficiency using acetone–butanol–ethanol (ABE). Fuel, 174: 333–343.
[2] Gu X, Li Q, Huang Z. (2011) Laminar burning characteristics of diluted n-butanol/air mixtures[J]. Combustion Science and Technology, 183(12): 1360-1375.
[3] Sarathy S M, Thomson M J, Togbé C, et al. (2009) An experimental and kinetic modeling study of n-butanol combustion[J]. Combustion and Flame, 156(4): 852-864.
[4] Kee R J, Rupley F M, Meeks E, et al. (1996) CHEMKIN-III: A fortran chemical kinetics package for the analysis of gas-phase chemical and plasma kinetics[R]. Sandia National Laboratories: Albuquerque, NM. Report SAND96-8216.
[5] Kee R J, Grcar J F, Smooke M D, et al. (1998) PREMIX: A fortran program for modeling steady laminar one-dimensional premixed flames[R]. Sandia National Laboratories: Livermore, CA. Report SAND85-8216.