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EFFECTS OF FLAMMABILITY CHARACTERISTICS OF STEAM INERTING TO SOLUTION OF ACETONE IN WATER

C.-H. Lin[1], *Y.-M. Chang*[1], *J.-C. Lee*[2], *S.-Y. Lin*[2] *and C.-M. Shu*[1]*

[1]Doctoral Program, Graduate School of Engineering Science and Technology, National Yunlin University of Science and Technology (NYUST), 123, University Rd., Sec. 3, Douliou, Yunlin, Taiwan 64002, Republic of China
[2]Department of Safety, Health, and Environmental Engineering, NYUST, 123, University Rd., Sec. 3, Douliou, Yunlin Taiwan 64002, Republic of China

Preventing accidental explosions of flammable liquid/gas mixtures is very important. As far as flammability characteristics are concerned, we simulated the effects of inert liquid/gas, which was filled with reactors, vessels, or closed space, employed in the chemical process industries. The inert liquid/gas (H_2O) weakened the oxygen concentration and reduced solvent vapor concentration in a 20-L-Apparatus. This study investigated the flammability characteristics of acetone/water solutions (100/0, 75/25, 50/50, and 25/75 vol.%) that are controlled at a temperature of 150°C and pressures of 101/202 kPa, respectively. The flammability parameters included flammability limits (LEL and UEL), maximum explosion pressure ($P_{\max}$), maximum explosion pressure rise ($(\mathrm{d}P\,\mathrm{d}t^{-1})_{\max}$), and vapor deflagration index (K_g). The results of a series of experimental tests showed that UEL, $P_{\max}$, and K_g all decreased with steam rising under the experimental conditions. The results can be applied to process safety design/operation for identifying whether the inert liquid/gas (H_2O) content has any substantial effects in reducing the fire and explosion hazard of the solution of interest.

Keywords: *acetone/water solutions, explosion accidents, flammability parameters, inert liquid/gas (H_2O), 20-L-Apparatus*

Introduction

Acetone is an important organic raw material with a wide range of applications; it can be mixed with water, ethyl alcohol, ether, and so on [1]. It is a raw material for making epoxy resin and polyurethane; also, it is a crucial medical raw substance for producing vitamin C industrially. The most well-known household use of acetone is as the active ingredient in nail polish remover. Annually, the import and export of acetone in Taiwan [2] is quite extensive; the throughput of acetone in Taiwan is 307,873 tons per year mainly produced by Formosa Petrochemical Co., Ltd. and Lee Chang Yung Chemical Industry Co., Ltd.

The common method for manufacturing acetone industrially is the cumene hydroperoxide process. The cumene hydroperoxide is cleaved under acid conditions with agitation in a vessel at 60–70°C. A large number of nonoxidizing inorganic acids are useful for this reaction, e.g., sulfur dioxide. A crude acetone product is recovered by distillation from the reaction mass, as depicted in Fig. 1. Acetone in liquid or vapor phase is highly flammable. Thus, various fires and/or explosions might occur if flammable liquids and vapors are ignited within flammability limits in manufacturing processes. The evaluation and analysis of fire and explosion accidents caused by flammable mixtures must take into account whether the ratio of fuel and air on top of the flammable is under the flammable and explosion limits. In the past, many flammability characteristics of single chemicals or binary mixtures have been studied [3–16]. Many flammability characters lack of little information about flammable mixtures at added inert gases for preventing fires and explosions. Generally, it may be by weakening oxygen concentrations to the minimum oxygen concentration (MOC) by adding nitrogen, carbon dioxide, or water vapor until reaching the MOC [17].

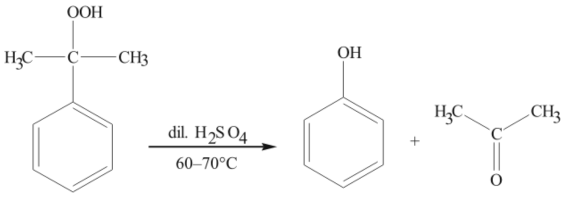

Fig. 1 Reaction pathways on CHP catalyst in the oxidation for producing acetone and phenol

The purpose of this study was to investigate the flammability for various proportions of flammable aqueous solutions in an acetone/water system as experimental samples. To determine the fire and explosion characteristics, our study included lower explosion limit (LEL), upper explosion limit (UEL),

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* Author for correspondence: shucm@yuntech.edu.tw

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Springer, Dordrecht, The Netherlands

maximum explosion overpressure ($P_{\max}$), rate of maximum explosion pressure rise $(\mathrm{d}P\ \mathrm{d}t^{-1})_{\max}$, gas or vapor deflagration index (K_g), and MOC, all at 150°C of initial temperature with 101 and 202 kPa of initial pressures, respectively. Concerning the hazards of various mixing ratios in this research, we studied the different ratios of acetone and water in 100/0, 75/25, 50/50, and 25/75 vol.% to identify the potential hazards in terms of the water and to see if the inert steam content was effective in alleviating the fire and explosion hazard of the solutions. The results can help related industries prevent unexpected accidents and provide specific information on relevant properties for fires and explosions in flammable chemicals, especially with steam.

Experimental

Materials

Acetone, or so-called 2-methyl ketone which has the chemical formula of C_3H_6O, is a colorless, liquid. Figure 2 shows its chemical structure. The basic physical and chemical properties of acetone are given in Table 1.

In this study, we prepared four acetone aqueous mixtures with different concentrations as experimental samples (100, 75, 50 and 25 vol.%). We deliberately mixed the pure acetone with water to simulate various vapor mixing ratios produced in a practical process.

Initial conditions

We set initial pressures of 101 and 202 kPa, along with the initial temperature of 150°C, four vapor mixing ratios and various oxygen concentrations (21,17, 14…vol.%) until to MOC. We established the initial temperature as 150°C for transcending acetone/water normal boiling points (56.3/100°C) forming a complete flammable vapor, to ensure a good mixing state in the gas phase.

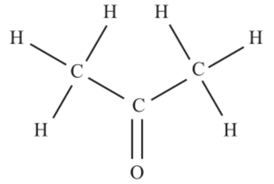

Fig. 2 Chemical structure of acetone

Table 1 Basic physical and chemical properties of acetone

Characteristics	Acetone
Formula	C_3H_6O
Molecular mass/g mol^{-1}	58.08
Flash point/°C	–18
Boiling point (1 atm)/°C	56.3
Vapor pressure (25°C)/101 kPa	180
Specific gravity (H_2O=1)	0.791
Flammability limits/vol.%	2.5–12.8
CAS No.	67-64-1

Methods, procedures and parameters

Figure 3 delineates a schematic of the experimental setup of the 20-L-Apparatus (or 20 Liter Spherical Explosion Vessel) which was purchased from Adolf Kühner AG. The test chamber is a stainless steel hollow sphere with a personal computer interface. The top of the cover contains holes for the lead wires to the ignition system. The opening provides for ignition by a condenser discharging with an auxiliary spark gap, which is controlled by a KSEP 320 unit of the 20-L-Apparatus [15]. The KSEP 332 unit uses piezoelectric pressure sensors to measure the pressure as function of time [18]. A comprehensive software package KSEP 6.0 was available, which allowed safe operation of the test equipment and an optimum evaluation of the explosion test results [19].

The test system enables one to determine the inherently safer properties in accordance with internationally recognized test procedures, e.g., ASTM 1226 (American Society for Testing and Materials, USA) and VDI 2263 (Verein Deutscher Ingenieure, Germany). In essence, it is suitable for measuring explosion behaviors of combustible materials, such as solvent vapors, flammable gases, or combustible dusts and to derive the flammability properties of LEL, UEL, $P_{\max}$, $(\mathrm{d}P\ \mathrm{d}t^{-1})_{\max}$, K_g, MOC in a series of testing procedures. We could consider the normal operation and set the various simulating conditions for preventive measures *vs.* fire and explosion hazards by investigating the flammability safety-related properties with this equipment.

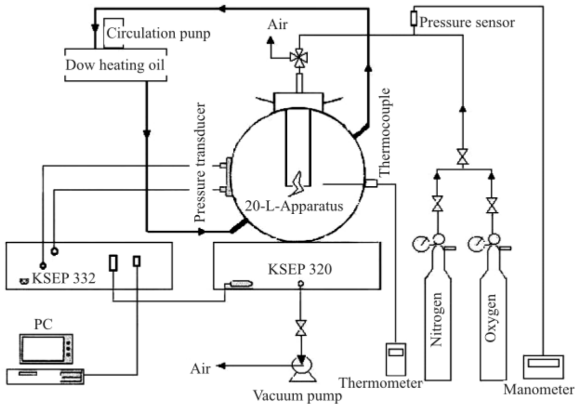

Fig. 3 Schematic diagram of the experimental set-up and its control system [15]

LEL and UEL for gas and solvent vapors

Explosion limits include the LEL and the UEL, and the explosion range is from LEL to UEL of a specific substance. Vapor-air mixtures will ignite and combust only over a well-specified range of compositions [20]. By definition, the LEL/UEL of a gas or vapor is the lowest/highest concentration, at which a gas or vapor explosion is not detected in three successive tests [18].

Maximum explosion pressure (P_{max}), maximum rate of explosion pressure rise ($(dP\ dt^{-1})_{max}$), and gas or vapor deflagration index (K_g)

The explosion indices, P_{max} and $(dP\ dt^{-1})_{max}$, are defined as the mean values of the maximum values of all three series. Subsequently, the gas or vapor deflagration index (K_g) is calculated from $(dP\ dt^{-1})_{max}$ by means of the cubic law [21]:

$$V^{1/3}(dP\ dt^{-1})_{max} = K_g \qquad (1)$$

where K_g and V are the maximum gas explosion constant specific to the gas and the volume of test apparatus (i.e., 0.02 m^3), respectively.

As there are many gas products in industrial practices, it is appropriate to assign this maximum constant to one of several explosion classes (St), and to use these as a basis for identifying explosive relief according to NFPA 68 [18, 21, 22].

Minimum oxygen concentration (MOC)

MOC is a useful parameter, because explosions and fires are preventable by lessening the oxygen concentration regardless of the concentration of the fuel. This concept is the basis for the common procedure called inerting [20, 23]. When oxygen concentration is less than the MOC, the reaction cannot generate enough energy to heat the entire gas mixture (including the inerts) to the extent required for self-propagation of the flame [20]. Under such a circumstance, oxygen is the key element that is required for propagating a flame.

Results and discussion

Effects of inert steam on acetone

In this study, four concentrations of acetone aqueous solution were measured in compliance with their typical acetone/water mixing ratios (100/0, 75/25, 50/50 and 25/75 vol.%) for various simulated inerting. The effects of the presence of steam on flammability limits of fuel mixtures were investigated with two initial pressures (101 and 202 kPa) under 150°C, and various oxygen concentrations (21, 17 vol.%,…) to MOC for four different compositions. It showed four acetone/water mixing vapors forming an expanded bell-type curve with P_{max} at different temperatures, as disclosed in Figs 4 to 5. In Fig. 4, the P_{max} and UEL was 5.6 bar and 12.8 vol.% measured from 100/0 vol.% acetone/water mixture, with increasing water vapor, the P_{max} and UEL was decreased to 2.6 bar and 2.82 vol.% measured from 25/75 vol.% acetone/water mixture. In Fig. 5, at elevated pressure to 202 kPa, with four typical acetone/water mixing ratios (25, 75, 50 and 100 vol.%), the P_{max} and UEL was 6.2 and 3.08 vol.% increased to 12.4 and 14.9 vol.%.

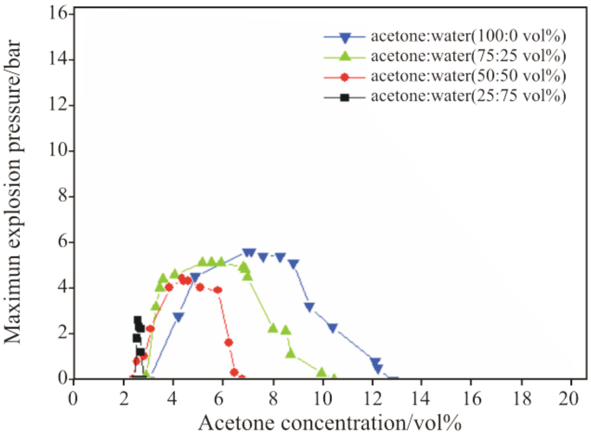

Fig. 4 P_{max} *vs.* acetone$_{(aq)}$ with four vapor mixing ratios at 101 kPa, 150°C and 21 vol.% oxygen

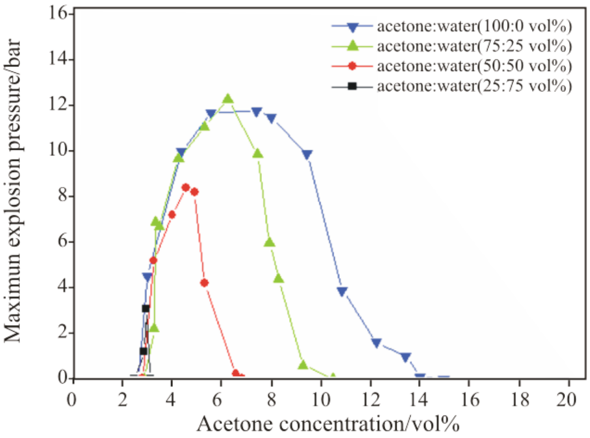

Fig. 5 P_{max} *vs.* acetone$_{(aq)}$ with four vapor mixing ratios at 202 kPa, 150°C and 21 vol.% oxygen

Effects of inert oxygen concentrations

The flammability characteristics of various acetone/water mixtures curved with the different oxygen concentrations at 101 and 202 kPa, as diagrammed in Figs 6 to 12. In 150°C, 101 kPa and 21 vol.% O_2, it showed that with four typical acetone/water mixing ratios (25, 75, 50 and 100 vol.%), the P_{max} and UEL

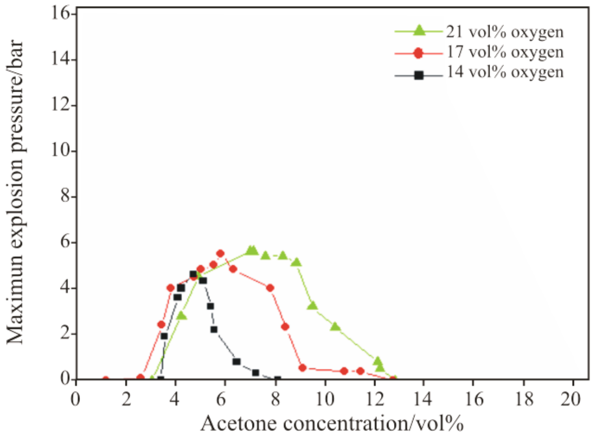

Fig. 6 P_{max} *vs.* pure acetone with three oxygen concentrations at 150°C and 101 kPa

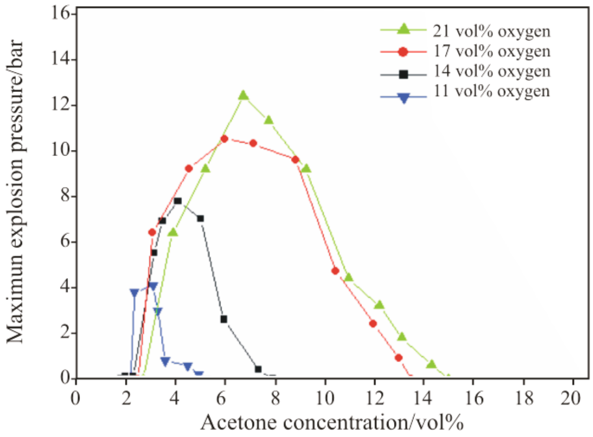

Fig. 7 P_{max} *vs.* pure acetone with four oxygen concentrations at 150°C and 202 kPa

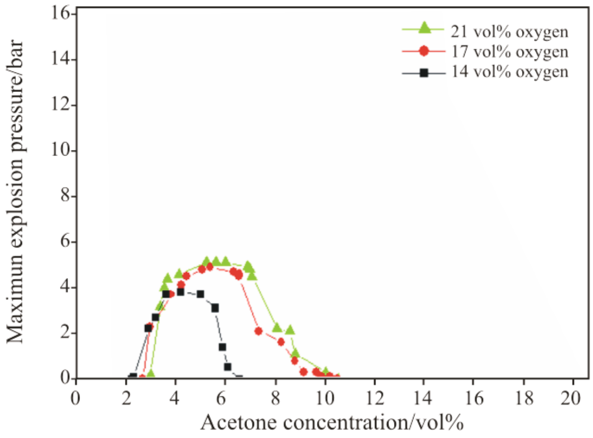

Fig. 8 P_{max} *vs.* 75% acetone$_{(aq)}$ with three oxygen concentrations at 150°C and 101 kPa

was 5.6 and 12.8 vol.%, with increasing to 202 kPa, the P_{max} and UEL increased to 12.4 and 14.9 vol.% all measured from 100/0 vol.%. Whereas increasing water vapor, at 150°C, 101 kPa, the flammability limit was 10.11 vol.% measured from 100/0 vol.% decreased to 0.33 vol.% measured from 25/75 vol.%.

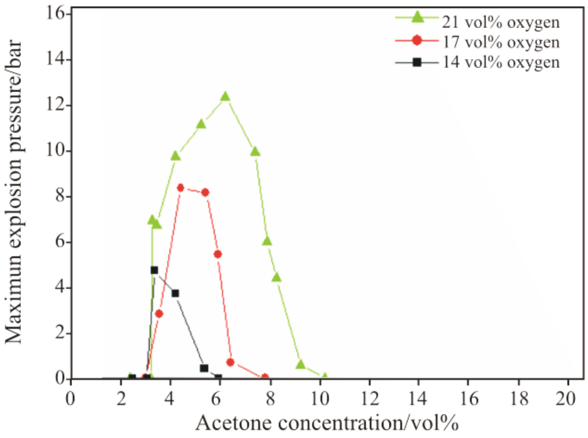

Fig. 9 P_{max} *vs.* 75% acetone$_{(aq)}$ with three oxygen concentrations at 150°C and 202 kPa

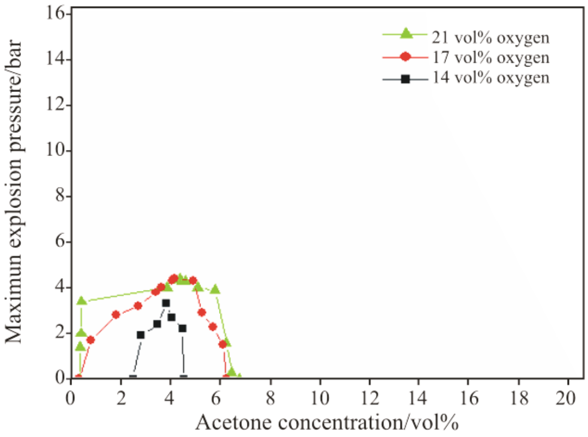

Fig. 10 P_{max} *vs.* 50% acetone$_{(aq)}$ with three oxygen concentrations at 150°C and 101 kPa

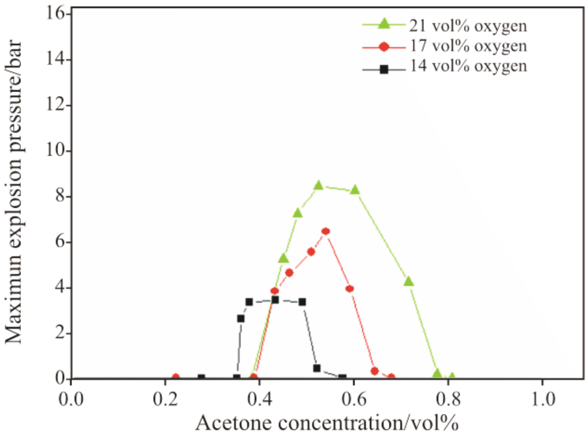

Fig. 11 P_{max} *vs.* 50% acetone$_{(aq)}$ with three oxygen concentrations at 150°C and 202 kPa

Besides, Fig. 12 shows the relationship between P_{max} and 25% acetone$_{(aq)}$ only in the oxygen concentration status of 21 vol.%, especially. Owing to explosion is impossible under observation; thus there is no data of other oxygen concentrations shown in this picture.

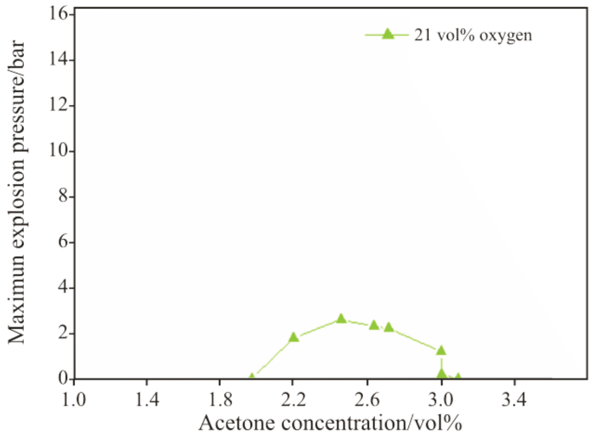

Fig. 12 P_{max} *vs.* 25% acetone$_{(aq)}$ with 21 vol.% oxygen concentrations at 150°C and 101 kPa

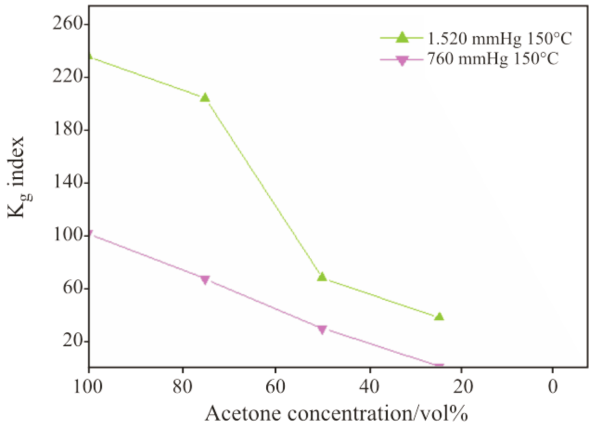

Fig. 13 K_g *vs.* acetone$_{(aq)}$ with four vapor mixing ratios (acetone/water solutions of 100/0, 75/25, 50/50 and 25/75 vol.%)

Significantly, while the water vapor was increasing, the oxygen concentration was dropping gradually in the test. Once the oxygen concentration was controlled below the MOC, an explosion was no longer possible.

Effects of vapor deflagration index (K_g) in different initial pressure

The effects of the presence of water vapor deflagration index (K_g) of fuel mixtures was investigated with two initial pressures under 150°C, and 101 and 202 kPa. Figure 13 reveals a large slope of K_g value in acetone/water vapor mixing ratios from 100 to 25 vol.%. Obviously, the results indicate the relationship between acetone/water concentrations and vapor deflagration index (K_g) under the specific operation conditions.

Conclusions

By augmenting the water vapor, the flammable range or flammability zone became narrower. These flammability parameters (P_{max}, $(dP\,dt^{-1})_{max}$) and degree of hazard were reduced accordingly. The results were also reduced from 101 and 202 kPa. The addition of steam component to the acetone/air mixtures determined the decrease of UEL. With increasing the steam, the oxygen concentration was reduced in the 20-L-Apparatus. Therefore, the effect of decreasing the oxygen concentration is tantamount to the increasing of steam for preventing an explosion. Explosion class was also increased from St–0 to St–2 with acetone solutions increased from 101 and 202 kPa. Moreover, with the initial pressure being decreased, the explosion class would be dropped from St–1 to St–0. Hence, changes in inert steam can result in large variation in K_g and explosion classes. According to the experimental data, the flammability parameters would be damped by doping steam inerting to solution of acetone as well as reducing the initial pressure to prevent fires and explosions. We can dictate oxygen concentration to be lower than LOC in an operating process through the effect of inerting.

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