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Fire and explosion hazard evaluation for the acetone aqueous solutions

Using weighting analysis of influence factors by grey system theory and 20-L-apparatus flammability investigations

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Abstract The prevention of fire and explosion is recognized as an imperative necessity that is a first priority in all operating management details of the chemical process industries. Based on significant research and original emphasis on loss control and disaster prevention, this study investigated the flammability characteristics, comprising the lower/upper explosion limit (LEL and UEL), maximum explosion overpressure (P_{max}), maximum rate of explosion pressure rise [$(\mathrm{d}P\ \mathrm{d}t^{-1})_{max}$], gas or vapor deflagration index (K_g), and explosion class (*St* class) of four acetone aqueous solutions [water vapor (steam)/acetone: 75/25, 50/50, 25/75, and 0/100 vol.%], and discussed the effect of inert steam ($H_2O_{(g)}$) on them. Interactive influences of various loading fuel concentrations and initial testing conditions of 150, 200 °C, and 101, 202 kPa on flammability characteristics were revealed via a 20-L-apparatus. Weighting analysis of the above influence factors was explored by employing the GM(h,*N*) grey system theory for rating their fire and explosion hazard degrees both specifically and quantitatively. The results indicated that the most important influence factor was the initial pressure that the manager or engineer in such a steam/acetone mixing system should consider to be well-controlled first. The second influence factor in GM(1,*N*) and GM(0,*N*) model was the initial temperature and steam/acetone mixing concentration, but the third influence factor was individual contrariwise. This study established a complete flammability hazard evaluation approach that is combined with an experimentally and theoretically feasible way for fire/explosion prevention and protection. The outcomes would be useful for positive decisions for safety assessment for the relevant practical plants or processes.

Keywords Acetone aqueous solutions · Fire and explosion · Grey system theory · Influence factors · 20-L-apparatus

List of symbols

a	Parameter of matrix method in GM(1,*N*) model (dimensionless)
a_1	Parameter of matrix method in GM(0,*N*) model (dimensionless)
a_i	Determined coefficient of GM(h,*N*) model (dimensionless)

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$\hat{a}$	Predicted value of parameter a in matrix method of GM(1,N) model (dimensionless)
B	Parameter of matrix method in GM(1,N) model (dimensionless)
B^T	Parameter of matrix method in GM(1,N) model (dimensionless)
$\hat{B}$	Predicted value of parameter B in matrix method of GM(0,N) model (dimensionless)
b_j	Determined coefficient of GM(h,N) model (dimensionless)
$\hat{b}_m$	Computing result from the matrix form in GM(0,N) model/the relationship between the major sequence and the influencing sequences in this system (dimensionless)
b_N	Computing result from the matrix form in GM(1,N) model/the relationship between the major sequence and the influencing sequences in this system (dimensionless)
BP	Boiling point (°C)
$(\mathrm{d}P\ \mathrm{d}t^{-1})_{\max}$	Maximum rate of explosion pressure rise (kPa sec^{-1})
FP	Flash point (°C)
h	Order of differential equation of GM(h,N) model (dimensionless)
IE	Ignition energy (J)
K_g	Gas or vapor explosion (m kPa sec^{-1})
LEL	Lower explosion limit (vol.%)
LFL	Lower flammable limit (vol.%)
MOC	Minimum oxygen concentration (vol.%)
N	Number of variables of GM(h,N) model (dimensionless)
P	Initial pressure (kPa)
$P_{\max}$	Maximum explosion pressure (kPa)
St	Explosion class (dimensionless)
t	Time (sec)
UEL	Upper explosion limit (vol.%)
UFL	Upper flammable limit (vol.%)
V	Volume of test apparatus (m^3, L)
$x^{(i)}$	Generating operation sequence of GM(h,N) model/i means the number of times of generating operation, $i = 1, 2, 3, \ldots, n$ (dimensionless)
$x_1^{(1)}(k)$	Major sequence of GM(h,N) model (dimensionless)
$x_j^{(1)}(k)$	Influencing sequences of GM(h,N) model (dimensionless)
$x_1^{(0)}(k)$	Main factor of the $\mathrm{x}_\mathrm{i}^{(0)}(\mathrm{k})$ .sequence ($i = 1, 2, 3, \ldots, n$) in GM(1,N) model (dimensionless)
$x_N^{(0)}(k)$	Influence factor of the $x_i^{(0)}(k)$ sequence ($i = 1, 2, 3, \ldots, n$) in GM(1,N) model (dimensionless)
X	Parameter of matrix method in GM(0,N) model (dimensionless)
Y	Parameter of matrix method in GM(0,N) model (dimensionless)
Y_N	Parameter of matrix method in GM(1,N) model (dimensionless)
Y_T	Parameter of matrix method in GM(0,N) model (dimensionless)
$z_1^{(1)}(k)$	Transferring factor of GM(h,N) model/ $x_1^{(1)}(k) \to 0.5x_1^{(1)}(k) + 0.5x_1^{(1)}(k-1)$, $k \geq 2 = z_1^{(1)}(k)$ (dimensionless)

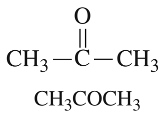
Introduction

Acetone (CH_3COCH_3), also known as propanone, dimethyl ketone or 2-propanone, is the simplest representative of the ketones industrially [1, 2]. For the high volatility and readily soluble properties in water, ethanol, ether, and so on, acetone serves as an important solvent and raw material mixed with chemical substances for many pivotal applications, such as in making drugs, fibers, plastics, and some other chemicals in petrochemical industrial processes [1]. Acetone can be employed for thinning and cleaning fiberglass resins and epoxies; the prevailing household application is as the active ingredient in nail polish remover [3]. It is also used as a general purpose cleaner in paint and ink manufacturing operations, and is a strong solvent for the majority of plastics and synthetic fibers [1].

Although the invention and application of chemicals is a great contribution to human civilization, not only in petrochemical plants but also in the daily lives [4–8], they originally exist with particular inherent hazards that might inevitably cause specific damages. History is filled with regrettable accidents involving the use of chemical materials [9]. Though acetone and its aqueous solutions, or even the acetone-involved chemicals, have played a very important role for human beings and the environment in multiple functions, their hidden intrinsic flammability hazard is a troublesome issue we have to confront.

Organic solvents are the most dominant source of fires and explosions in chemical industries [10]. Flammable liquids such as acetone aqueous solutions [$\mathrm{acetone}_{(\mathrm{aq})}$] might have momentous incidents. In fact, the boiling point (BP, 101 kPa) and flash point (FP) of acetone are 56 and –20 °C, and its vapor pressure is 80 mmHg at 25 °C, respectively [3]. Owing to its high volatility and great capability of reacting with many chemicals in the gas phase, acetone is grouped into “flammability liquid Class IB” according to National Fire Protection Association (NFPA) criteria 30 and 704 [11–13]. In short, acetone is a liquid or vapor that can be readily ignited under almost all ambient temperature conditions. Once it ignites or burns a serious issue could occur during preparation, storage, operation, or transportation [13]. At present, the most imperative objective for industrial fires and explosions prevention is to confirm beforehand the flammability characteristics of utilizing materials under working conditions. Practically, it is driven by the strong need to recognize their fundamental but crucial flammability characteristics in detail, including the explosion limits [lower explosion limit (LEL)/upper explosion limit (UEL)], maximum explosion pressure ($P_{\max}$), pressure to time record, i.e., maximum rate of explosion pressure rise $(\mathrm{d}P\ \mathrm{d}t^{-1})_{\max}$, gas or vapor deflagration index (K_g), and explosion class (St class) [14] that are interacting with various influence factors within operating scenarios. Therefore, the authors need to make it a priority to leave the flammability risk behind of acetone$_{(aq)}$, and attempt to find a feasible way both experimentally and theoretically for fire/explosion prevention and protection.

This study aimed at elucidating the safety-related properties of LEL, UEL $P_{\max}$ $(\mathrm{d}P\ \mathrm{d}t^{-1})_{\max}$, K_g, and St class for four acetone$_{(aq)}$ solutions with various mixing ratios by water vapor (steam)/acetone: 75/25, 50/50, 25/75, and 0/100 vol.%, which are typical of practical processing prescriptions. Experimental investigations were carried out via a 20-L-apparatus (or so-called 20-L spherical explosion vessel) under initial temperatures (150, 200 °C) and initial pressures (101, 202 kPa). The authors undertook to identify the influence of inert steam [$H_2O_{(g)}$] on the flammability attributes of several loading fuel concentrations, i.e., the above-mentioned acetone$_{(aq)}$ solutions, so as to determine if steam was effective in alleviating the fire and explosion hazard degree. Likewise, the experimentally derived data were further employed for weighting analysis via a soft computing by way of GM(h,*N*) grey system theory [GM(1,*N*) and GM(0,*N*) model]. According to the references [15], the grey system theory is a quantitative analysis that has been extensively applied [15, 16] to explore the most important factor among the foregoing interacting testing scenarios. Here, the influence factors include “initial temperature”, “initial pressure”, and “steam/acetone mixing concentration”. The concept and equations of GM(h,*N*) model are delineated in the following section. In this study it was strove to get more complete flammability hazard evaluations of acetone$_{(aq)}$ solutions, and preferably provide a more specific and quantified consideration of decision for fire and explosion assessment. By means of the traditional way for measuring the flammability properties of acetone$_{(aq)}$ solutions experimentally, and further proven via the grey system theory approach theoretically, the authors learned that the most important factor should be actually considered to be controlled first for definitely minimizing the potential risk under the fire and explosion prevention and protection purposes.



$$\mathrm{CH_3-\overset{\displaystyle O \atop \|}{C}-CH_3}$$

CH_3COCH_3

Fig. 1 Chemical structure of acetone [1]

Experimental setup

Experimental steam/acetone mixing samples

Acetone, or so-called 2-methyl ketone, is a clear, colorless but irritant liquid at room temperature. Figure 1 [1] shows its chemical structure (CH_3COCH_3). The fundamental physical and chemical properties of 99.5+% acetone are given in Table 1 [1, 2]. Acetone is viewed as a “flammable liquid IB” due to its low FP (–20 °C) and BP (56 °C), as listed and according to Table 2 [11–13]. It flames quite readily when in contact with an effective ignition source, so vapors should be avoided before its particular explosion limits are reached.

In this study, more than 99.5% purity acetone (99.5+%) from Lee Chang Yung Chemical Industry Corp. was

Table 1 Basic physical and chemical properties of acetone [1, 2]

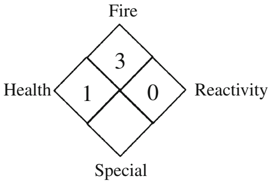
Characteristic	Acetone (99.5 + %)
CAS no.	67-64-1
Chemical formula	CH_3COCH_3
Molecular weight	58.08 g mol^{-1}
Flash point	–20 °C
Boiling point/101 kPa	56 °C
Melting point	–94.6 °C
Vapor pressure	247 kPa (20 °C)
Specific gravity/H_2O = 1	0.791
Explosion limits	2.5 (LEL)–13.0 (UEL) vol.%
Flammability hazard (Liquids and solids that can be ignited under almost all ambient temperature condition.)	The Hazardous Materials Information System (HMIS) Rating  Health = 1, Flammability = 3, Reactivity = 0
Flammability liquid	Class IB (NFPA 30) [11, 12]

Table 2 Definition and classification of flammable/combustible liquids [11–13]

	Flammable liquids (Class I liquids)		Combustible liquids (Class II and III liquids)
Class IA	FP < 73°F (23 °C); BP < 100°F (38 °C)	Class II	100°F (38 °C) < FP < 140°F (60 °C)
Class IB	FP < 73°F (23 °C); BP > 100°F (38 °C)	Class IIIA	140°F (60 °C) < FP < 200°F (93 °C)
Class IC	FP > 73°F (23 °C); BP > 100°F (38 °C)	Class IIIB	200°F (93 °C) < FP

FP flash point, *BP* boiling point

Table 3 Four simulated concentrations (vapor mixing ratios) for steam and acetone

Mixing vapor ratio	vol.%	vol.%	vol.%	vol.%
Steam	0	25	50	75
Acetone	100	75	50	25

employed for presenting the "pure" acetone sample to the flammability testing series. The authors deliberately selected four acetone$_{(aq)}$ solutions with different steam/acetone mixing concentrations, i.e., 0/100 (pure acetone), 25/75, 50/50, and 75/25 vol.%, as the experimental samples (Table 3). Each acetone$_{(aq)}$ solution represented an individual component of inert steam once being heated to total vapor situation while being investigated, so as to measure the flammability properties of interest for mimicking every particular "inerting efficiency" during practical operating processes. The authors undertook to find the variations of potential fire and explosion hazard while adding various inert steam portions to loading fuel concentrations in this study.

Experimental conditions

As for the experimental initial conditions, it was established the initial pressures of 101, 202 kPa and initial temperatures of 150, 200 °C for the flammability investigations herein. To exceed both the normal BPs of acetone (56 °C) and water (100 °C) when dosing the samples, the initial temperature had to be set at least more than 100 °C to insure that total flammable acetone vapors and steam/$H_2O_{(g)}$ could be generated and in a well-mixed state in gas phase during the tests [17].

Experimental apparatus and procedures

20-L spherical explosion vessel

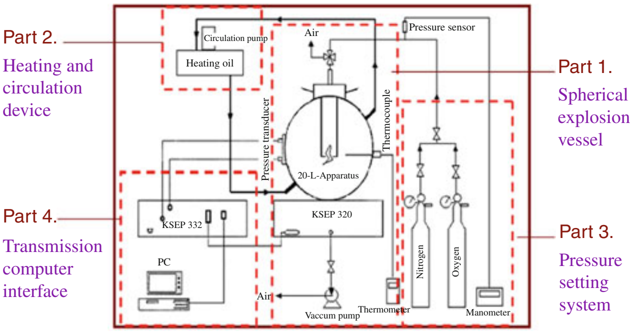


Fig. 2 Schematic diagram of the experimental set-up and its control system [14, 18–20]

Figure 2 schematizes the experimental apparatus of a 20-L spherical explosion vessel, or so-called 20-L-apparatus, and its control system sections [14, 18–20], which was purchased from Adolf Kühner AG and was feasible for flammability surveys of this study. The 20-L test chamber is a stainless steel hollow sphere. The top of the cover includes 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 dictated by a KSEP 320 unit of the 20-L-apparatus [19, 20]. The mixtures are ignited by a pyrotechnic igniter, which consists of a total of 10 J electric current employed as ignition source for the gas/vapor system, and is placed at the center of this vessel [19, 21]. The KSEP 332 unit uses piezoelectric pressure sensors to measure the pressure as a function of time [19]. In addition, a personal transmission computer interface was established for catching the explosion pressure–time corresponding records after an explosion. 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 [17, 22].

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) [23] and VDI 2263 (Verein Deutscher Ingenieure, Germany) [23]. Essentially, it is for observing explosion behaviors of combustible materials, such as solvent vapors, flammable gases, or combustible

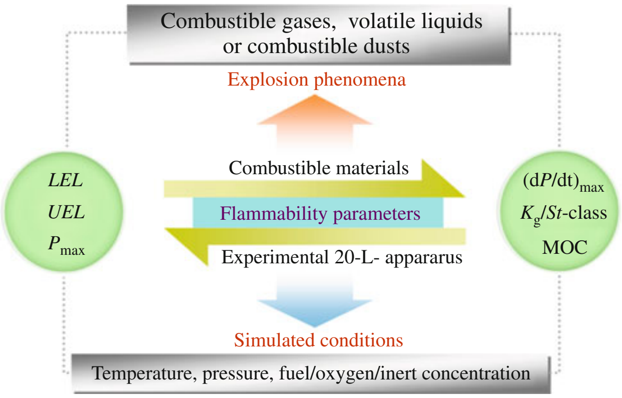


Fig. 3 Various applications of 20-L-apparatus [14, 18–20]

dusts. The flammability properties of LEL, UEL, P_{max} $(dP\ dt^{-1})_{max}$, gas, or vapor deflagration index (K_g), explosion class (St), and minimum oxygen concentration (MOC), etc., are detected in a series of testing procedures.

Figure 3 outlines and combines various applications of the 20-L-apparatus [14, 18–20]. It was applied it to establish several scenarios to simulate the operating conditions in a practical process for preventive measurements against fire and explosion hazards by investigating these safety-related parameters.

LEL and UEL for gas and solvent vapors

The lower flammability limit (LFL) and upper flammability limit (UFL) are also referred as the LEL and UEL, respectively [24]. 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. Commonly used units are volume percent fuel (percentage of fuel plus air, vol.%) [10]. In this study, the test series was continued with a systematic increase and decrease of the sample concentration until a concentration was reached at which no ignition was observed in three successive tests [9, 19].

P_{max} $(dP\ dt^{-1})_{max}$ K_g parameters and St class measurements

The peak values that accompany the explosion of a combustible vapor are the P_{max} and $(dP\ dt^{-1})_{max}$. Experimentally, they can be obtained from tests over a wide range of concentrations ignited by electric spark [10]. The explosion indices, P_{max} and $(dP\ dt^{-1})_{max}$, are defined as the mean values of the maximum values of all three series. As for the K_g index, it is calculated from $(dP\ dt^{-1})_{max}$ by means of the cubic law [25]:

$$V^{1/3} \times \left(dP\,dt^{-1}\right)_{max} = K_g \tag{1}$$

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 gaseous products and industrial practices, it is appropriate to assign this maximum constant to one of several explosion classes (or so-called *St* classes in this study), as given in Table 4 [19, 20, 25], and to use these as a basis for sizing explosive relief. Furthermore, the *St* class detected at each testing scenario most stood for each explosion damage class significantly and with quantification among the whole investigations in this study. Herein is presented an important final "output" result estimated for the grey system theory approach.

Grey system theory approach

In this section, the authors introduce the basic concept of the GM(h,*N*) model.

GM(h,*N*)

In grey system theory, the main function of the GM(h,*N*) model is a method to calculate the measurement among the discrete sequences, and to compensate for the weaknesses in the traditional statistics methodology. The GM(h,*N*) model is suitable for the situation with h order differential equation and *N* variables, which is defined as [16, 26]:

$$\sum_{i=0}^{h} a_i \frac{d^{(i)} x_1^{(1)}}{dt^{(i)}} = \sum_{j=2}^{N} b_j x_j^{(1)}(k) \tag{2}$$

where a_i and b_j are determined coefficients, $x_1^{(1)}(k)$: major sequence, $x_j^{(1)}(k)$: influencing sequences. AGO represents accumulated generating operation in grey system theory:

$$\begin{aligned} \text{AGO } x^{(0)} &= x^{(1)} \\ &= \left[\sum_{k=1}^{1} x^{(0)}(k), \sum_{k=1}^{2} x^{(0)}(k), \sum_{k=1}^{3} x^{(0)}(k), \ldots \sum_{k=1}^{n} x^{(0)}(k), \right] \end{aligned} \tag{3}$$

The GM(h,*N*) model is separated into two sections: GM(1,*N*) model and GM(0,*N*) model [16]. In the following

Table 4 K_g and explosion classes (St) [19, 20, 25]

K_g/m kPa/sec	Explosion classes/St
<1,000	St-0
1,000–200,000	St-1
201,000–300,000	St-2
>300,000	St-3

paragraphs, the authors continued to explain the two models.

GM(1,*N*)

With sequences $x_i^{(0)}(k)$, $i = 1, 2, 3, \ldots, N$, $x_1^{(0)}(k)$ is the main factor in the system, and sequences $x_2^{(0)}(k), x_3^{(0)}(k), x_4^{(0)}(k), \ldots, x_N^{(0)}(k)$ are the influence factors; then the authors can use GM(1,*N*) to analyze the system. The GM(1,*N*) model is shown below.

$$x_1^{(0)}(k) + a_1 z_1^{(1)}(k) = \sum_{j=2}^{N} b_j x_j^{(1)}(k) \tag{4}$$

where $k = 1, 2, 3, \ldots, n$

Equation 4 is derived from Eq. 2 by means of the transferring factor $z_1^{(1)}(k)$ according to the basic concept of grey system theory: $x_1^{(1)}(k) \to 0.5x_1^{(1)}(k) + 0.5x_1^{(1)}(k-1)$, $k \geq 2 = z_1^{(1)}(k)$ [16]. The analytic steps are shown as below.

- Building the original sequences

$$\begin{aligned}
x_1^{(0)} &= (x_1^{(0)}(1), x_1^{(0)}(2), \ldots, x_1^{(0)}(k))\\
x_2^{(0)} &= (x_2^{(0)}(1), x_2^{(0)}(2), \ldots, x_2^{(0)}(k))\\
x_3^{(0)} &= (x_3^{(0)}(1), x_3^{(0)}(2), \ldots, x_3^{(0)}(k)) \qquad k = 1, 2, 3, \ldots, n\\
&\cdots\cdots\cdots\cdots\cdots\cdots\cdots\\
x_N^{(0)} &= (x_N^{(0)}(1), x_N^{(0)}(2), \ldots, x_N^{(0)}(k))
\end{aligned} \tag{5}$$

- Creating the AGO sequences

$$\begin{aligned}
x_1^{(1)} &= (x_1^{(1)}(1), x_1^{(1)}(2), \ldots, x_1^{(1)}(k))\\
x_2^{(1)} &= (x_2^{(0)}(1), x_2^{(1)}(2), \ldots, x_2^{(1)}(k))\\
x_3^{(1)} &= (x_3^{(1)}(1), x_3^{(1)}(2), \ldots, x_3^{(1)}(k)) \qquad k = 1, 2, 3, \ldots, n\\
&\cdots\cdots\cdots\cdots\cdots\cdots\\
x_N^{(1)} &= (x_N^{(1)}(1), x_N^{(1)}(2), \ldots, x_N^{(1)}(k))
\end{aligned} \tag{6}$$

- Substituting all AGO values into Eq. 6, then we acquired

$$\begin{aligned}
x_1^{(0)}(2) + a z_1^{(1)}(2) &= b_2 x_2^{(1)}(2) + \cdots + b_N x_N^{(1)}(2)\\
x_1^{(0)}(3) + a z_1^{(1)}(3) &= b_2 x_2^{(1)}(3) + \cdots + b_N x_N^{(1)}(3)\\
&\cdots\cdots\cdots\cdots\cdots\cdots\\
x_1^{(0)}(n) + a z_1^{(1)}(n) &= b_2 x_2^{(1)}(n) + \cdots + b_N x_N^{(1)}(n)
\end{aligned} \tag{7}$$

The authors further, convert Eq. 7 into matrix form in $Y_N = B\hat{a}$pattern as below.

$$\begin{bmatrix} x_1^{(0)}(2)\\ x_1^{(0)}(3)\\ \vdots\\ x_1^{(0)}(n) \end{bmatrix} = \begin{bmatrix} -z_1^{(1)}(2) & x_2^{(1)}(2) & \cdots & x_N^{(1)}(2)\\ -z_1^{(1)}(3) & x_2^{(1)}(3) & \cdots & x_N^{(1)}(3)\\ \vdots & \cdots & & \\ -z_1^{(1)}(n) & x_2^{(1)}(n) & \cdots & x_N^{(1)}(n) \end{bmatrix} \begin{bmatrix} a\\ b_2\\ \vdots\\ b_N \end{bmatrix} \tag{8}$$

Here, $\hat{a}$ means the predicted value of parameter *a*.

- Applying the matrix method, formula $\hat{a} = (B^T B)^{-1} B^T Y_N$. (according to "least square" approach) to obtain the values of parameters $\hat{a}$, *B*, and b_N, where

$$\begin{aligned}
Y_N &= \begin{bmatrix} x_1^{(0)}(2)\\ x_1^{(0)}(3)\\ \vdots\\ x_1^{(0)}(n) \end{bmatrix}, \hat{a} = \begin{bmatrix} a\\ b_2\\ \vdots\\ b_N \end{bmatrix},\\
B &= \begin{bmatrix} -z_1^{(1)}(2) & x_2^{(1)}(2) & \cdots & x_N^{(1)}(2)\\ -z_1^{(1)}(3) & x_2^{(1)}(3) & \cdots & x_N^{(1)}(3)\\ \vdots & \cdots & & \\ -z_1^{(1)}(n) & x_2^{(1)}(n) & \cdots & x_N^{(1)}(n) \end{bmatrix}
\end{aligned} \tag{9}$$

Hence, the relationship between the major sequence and the influencing sequences can be found by comparing the values of b_N.

GM(0,*N*)

The GM(0,*N*) model is a special case of the GM(h,*N*) model [15, 16]; the function is the same as the GM(1,*N*) model. According to the definition of the GM(0,*N*) model,

$$\begin{aligned}
a z_1^{(1)}(k) &= \sum_{j=2}^{N} b_j x_j^{(1)}(k)\\
&= b_2 x_2^{(1)}(k) + b_3 x_3^{(1)}(k) + \cdots + b_N x_N^{(1)}(k)
\end{aligned} \tag{10}$$

where $z_1^{(1)}(k) = 0.5x_1^{(1)}(k-1) + 0.5x_1^{(1)}(k)$, $k = 2, 3, 4, \ldots, n$.

- Substituting the AGO value, then

$$\begin{aligned}
a_1 z_1^{(1)}(2) &= b_2 x_2^{(1)}(2) + \cdots + b_N x_N^{(1)}(2)\\
a_1 z_1^{(1)}(3) &= b_2 x_2^{(1)}(3) + \cdots + b_N x_N^{(1)}(3)\\
a_1 z_1^{(1)}(4) &= b_2 x_2^{(1)}(4) + \cdots + b_N x_N^{(1)}(4)\\
&\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\\
a_1 z_1^{(1)}(n) &= b_2 x_2^{(1)}(n) + \cdots + b_N x_N^{(1)}(n)
\end{aligned} \tag{11}$$

- Dividing a_1 at both sides, then translating into matrix form

$$\begin{bmatrix} 0.5x_1^{(1)}(1)+0.5x_1^{(1)}(2) \\ 0.5x_1^{(1)}(2)+0.5x_1^{(1)}(3) \\ \vdots \\ 0.5x_1^{(1)}(n-1)+0.5x_1^{(1)}(n) \end{bmatrix} = \begin{bmatrix} x_2^{(1)}(2) & \cdots & x_N^{(1)}(2) \\ x_2^{(1)}(3) & \cdots & x_N^{(1)}(3) \\ \vdots & \cdots & \vdots \\ x_2^{(1)}(n) & \cdots & x_N^{(1)}(n) \end{bmatrix} \begin{bmatrix} \frac{b_2}{a_1} \\ \frac{b_3}{a_1} \\ \frac{b_4}{a_1} \\ \vdots \\ \frac{b_N}{a_1} \end{bmatrix} \tag{12}$$

Assume $\frac{b_j}{a_1} = \hat{b}_m$, where $m = 2, 3, 4, \ldots, N$,then Eq. 12 can be rewritten into

$$\begin{bmatrix} 0.5x_1^{(1)}(1)+0.5x_1^{(1)}(2) \\ 0.5x_1^{(1)}(2)+0.5x_1^{(1)}(3) \\ \vdots \\ 0.5x_1^{(1)}(n-1)+0.5x_1^{(1)}(n) \end{bmatrix} = \begin{bmatrix} x_2^{(1)}(2) & \cdots & x_N^{(1)}(2) \\ x_2^{(1)}(3) & \cdots & x_N^{(1)}(3) \\ \vdots & \cdots & \vdots \\ x_2^{(1)}(n) & \cdots & x_N^{(1)}(n) \end{bmatrix} \begin{bmatrix} \hat{b}_2 \\ \hat{b}_3 \\ \hat{b}_4 \\ \vdots \\ \hat{b}_N \end{bmatrix} \tag{13}$$

- Using matrix method $\hat{B} = (Y^T Y)^{-1} Y^T X$ to solve the values of a_1 and b_j, then $\hat{b}_m$ was obtained, where

$$X = \begin{bmatrix} 0.5x_1^{(1)}(1)+0.5x_1^{(1)}(2) \\ 0.5x_1^{(1)}(2)+0.5x_1^{(1)}(3) \\ \vdots \\ 0.5x_1^{(1)}(n-1)+0.5x_1^{(1)}(n) \end{bmatrix}, \quad Y = \begin{bmatrix} x_2^{(1)}(2) & \cdots & x_N^{(1)}(2) \\ x_2^{(1)}(3) & \cdots & x_N^{(1)}(3) \\ \vdots & \cdots & \vdots \\ x_2^{(1)}(n) & \cdots & x_N^{(1)}(n) \end{bmatrix}, \ \hat{B} = \begin{bmatrix} \hat{b}_2 \\ \hat{b}_3 \\ \hat{b}_4 \\ \vdots \\ \hat{b}_N \end{bmatrix} \tag{14}$$

Then, the relationship between the major sequence and the influencing sequences also can be found by comparing the value of $\hat{b}_m$ [15, 16].

Through the above-mentioned expressions of the GM(h,*N*) approach, it was finally found the computed results of b_N [GM(1,*N*)] and $\hat{b}_m$ [GM(0,*N*)], which were further used to explore the relationship between the major sequence and the influencing sequences in each model to determine which influence factors were the most important in this study.

Results and discussion

Results of 20-L-apparatus testing

In this novel finding, the inert steam effect on the series of flammability characteristics of acetone$_{(aq)}$ mixtures was revealed under scenarios for four different steam/acetone mixing ratios (75/25, 50/50, 25/75, and 0/100 vol.%). We could clearly observe significant variations in those properties, demonstrating the effects of inert steam accordingly.

Figures 4 and 5 [27, 28] show the relationships between the explosion pressure versus different acetone$_{(aq)}$ concentrations with four vapor mixing ratios at 150 °C, 101 kPa and 150 °C, 202 kPa all under 21 vol.% oxygen. Similarly, Figs. 6 and 7 [27, 28] are the situation of 200 °C, 101 kPa and 200 °C, 202 kPa, also under 21 vol.% oxygen. Both of them form expanded bell-type curves with explosion pressure and ($dP\ dt^{-1}$) versus many acetone$_{(aq)}$ concentrations, of which one curve, the highest concentration is UEL, and the lowest one is LEL. The largest explosion pressure, the so-called P_{max}, and the greatest rate of explosion pressure rise were named the $(dP\ dt^{-1})_{max}$.

In Fig. 4, the LEL and UEL are 2.69 and 12.8 vol.%, and the P_{max} is exactly 5,600 kPa measured from the 0/100 vol.%, "pure" steam/acetone mixture in this study. The authors deliberately checked and reviewed the reference acetone's basic physical and chemical properties, as displayed in Table 1 [1, 2]; the explosion limits show 2.5–13 vol.%. In other words, it is close to the explosion-surveyed results. With enhanced steam/acetone from 0/100 to 75/25 vol.% samples, the P_{max} and UEL were all reduced down in evidence. For instance, Table 5 [27–29] lists explosion limits, i.e., LEL, UEL, and P_{max} for different steam/acetone mixing ratios at 150 °C, 101 kPa and 21 O_2 vol.%; it also tells us that while the steam/acetone component was

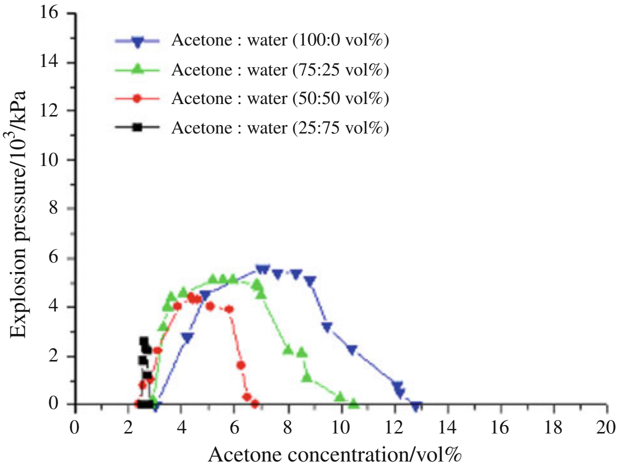


Fig. 4 Explosion pressure versus acetone$_{(aq)}$ with four vapor mixed ratios at 150 °C, 101 kPa and 21 vol.% oxygen [27, 28]

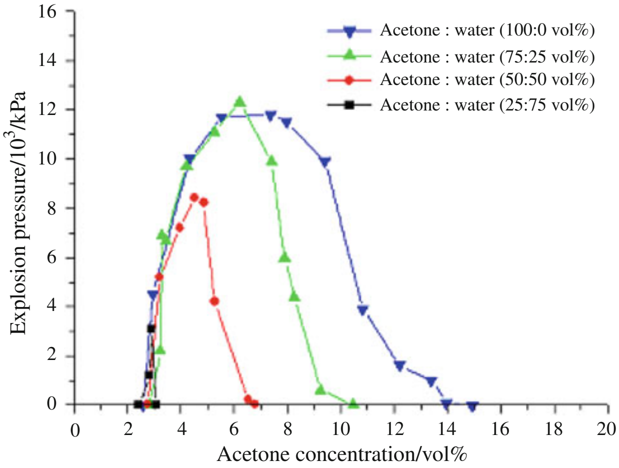


Fig. 5 Explosion pressure versus acetone$_{(aq)}$ with four vapor mixed ratios at 150 °C, 202 kPa and 21 vol.% oxygen [27, 28]

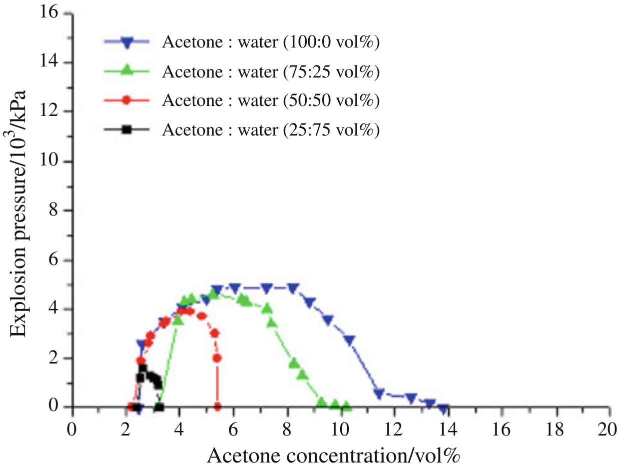


Fig. 6 Explosion pressure versus acetone$_{(aq)}$ with four vapor mixed ratios at 200 °C, 101 kPa and 21 vol.% oxygen [27]

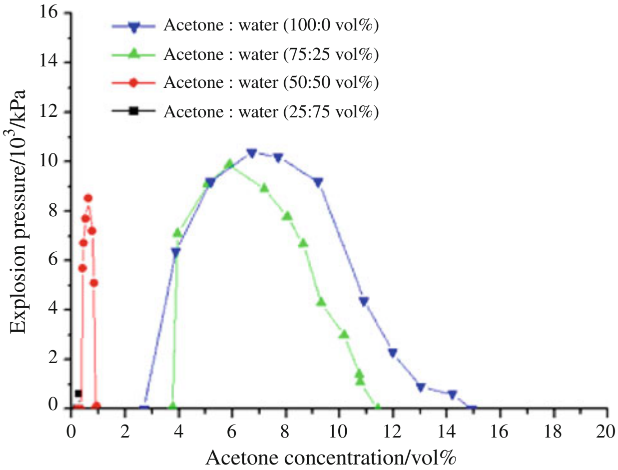


Fig. 7 Explosion pressure versus acetone$_{(aq)}$ with four vapor mixed ratios at 200 °C, 202 kPa and 21 vol.% oxygen [27]

Table 5 Explosion limits (LEL, UEL) and P_{max} for different steam/acetone mixed ratios at 150 °C, 101 kPa and 21 vol.% oxygen [27–29]

Steam/acetone mixing concentration/vol.%	LEL/vol.%	UEL/vol.%	P_{max}/kPa
75/25	2.49	2.80	2,600
50/50	2.38	4.35	4,400
25/75	3.76	9.78	5,100
0/100	2.69	12.80	5,600

enhanced up to 75/25 vol.% acetone and steam mixing sample condition, the LEL and UEL became 2.49 and 2.80 vol.%, and its P_{max} went down to 2,600 kPa from the highest one, 5,600 kPa. Therefore, the P_{max} dropped off and the explosion range narrowed, so that the fire and explosion hazard degree was lessened and lessened further, best showing the steam inert effect by far. From those tests, it was realized that "inert steam" adoption would be a great practical procedure for avoiding flammability losses to a process safety control system, and bring an economic benefit.

Explosion area

Many explosion disasters that happen in a process or plant generally result from flammable chemicals located inside their explosion limits. Since most flammable liquids are normally stored and handled above their FP, they continuously evolve off vapors when the vapor-air mixture is within the explosion limits [13]. Under this view, the authors carefully transferred the experimental data, LELs and UELs into a concrete scheme, drawing an "explosion area" schematic picture (Fig. 8) based on individual explosion limits of acetone$_{(aq)}$ solutions investigated under 150/200 °C, 101/202 kPa, and 21 O_2 vol.%.

In Fig. 8 [27–29], the explosion area is inside two well-specified boundaries of LEL and UEL. As the authors know, vapor-air mixtures will explode upon encountering an effective ignition source [10]. Hence, this scheme's outcome would be very useful and quite significant for industrial process safety to keep a chemical plant from fire and explosion, discovered at the first time. The authors should carefully avoid setting the concentration of the loaded fuels into this dangerous explosion zone. Furthermore, due to the influence of inert steam, LEL and UEL lines almost intersected at one point at about 3 vol.% of the explosion limit. Once LEL and UEL were integrated into the same goal, it dropped off the LEL boundary, and then withdrew from the explosion zone gradually. At the moment, testing samples neither could be ignited in the 20-L-apparatus nor could the explosion record be detected

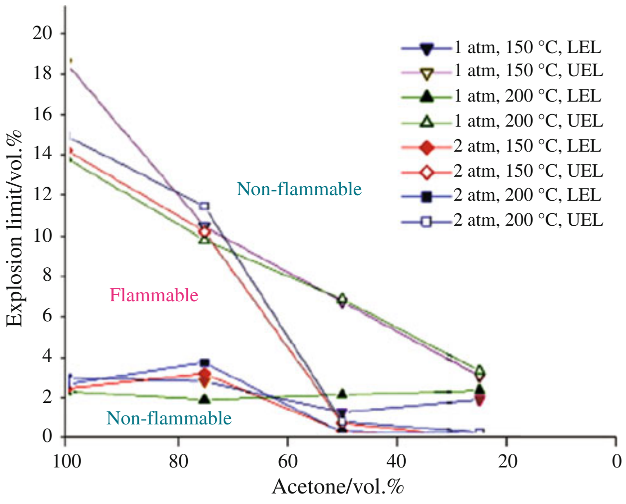


Fig. 8 Explosion area of four different acetone$_{(aq)}$ solutions at 150/200 °C, 101/202 kPa and 21 vol.% oxygen [27–29]

to its computer interface [23] under this simulated operating status. From fire and explosion hazards prevention viewpoint, the results could provide the crucial safety-related parameters to forestall flammability hazards.

As future study, the authors might also test them at elevated initial temperatures and pressures to find the substantial changes in the explosion area, flammability properties, and fire/explosion hazard degree.

Discrete data of experimental results

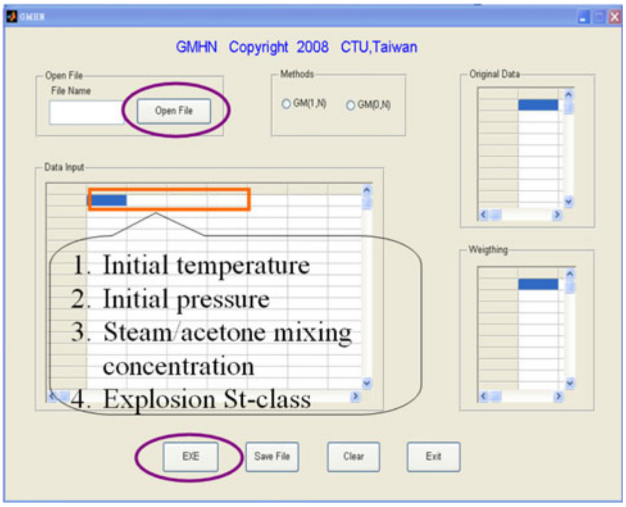
To grade the influence factors in the steam/acetone mixing system, the authors established Table 6 in accordance with the experimental records derived from 20-L-apparatus flammability tests. In Table 6, there are three input and an output data: initial temperatures (150/200 °C), initial pressures (101/202 kPa), different steam/acetone mixed samples (75/25, 50/50, 25/75, and 0/100 vol.%), and explosion class (output data), respectively. The initial temperatures (150/200 °C) became 1 and 2, sequentially. Two initial pressures (1/2 atm) were recorded as 1 and 2, in turn. Four steam/acetone mixing samples with the elevated acetone component (75/25, 50/50, 25/75, and 0/100 vol.%) were changed into 1, 2, 3, and 4 successively. Similarly, the output results of St classes (St 0–3) should be presenting the discrete data, 1, 2, 3, and 4, correspondingly. In Table 6, it was assumed that the greater the value of discrete data was, the higher the hazard of fire and explosion for an influence factor would be. The authors inputted the 16-sets discrete data summarized in Table 6, including the four "input" influence factors and one corresponding "output" result for weighting analysis both by GM(1,*N*) model and GM(0,*N*) model of grey system theory. The results of weighting analysis were generated later and were discussed as follows.

Table 6 List of discrete data of experimental results in this study

Testing pattern/no.	Initial temperature/°C	Initial pressure/kPa	Steam/acetone mixing concentration/vol.%	Explosion class/St
01	1	1	1	2
02	1	1	2	2
03	1	1	3	2
04	1	1	4	1
05	1	2	1	3
06	1	2	2	2
07	1	2	3	2
08	1	2	4	2
09	2	1	1	2
10	2	1	2	2
11	2	1	3	2
12	2	1	4	1
13	2	2	1	3
14	2	2	2	3
15	2	2	3	2
16	2	2	4	2

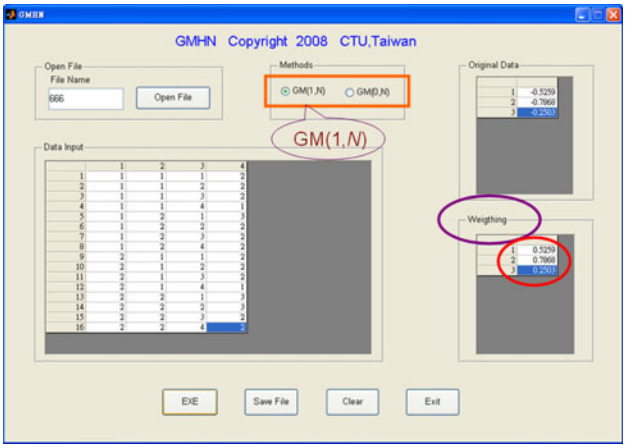
Analysis results by grey GM(h,*N*)

Figure 9 shows the GMHN weighting analysis tool box used for this study [16, 26]. According to the calculation and compared with the significant component of the influence factors by means of grey system theory, the 16-sets weighting analysis values of GM(1,*N*) model and GM(0,*N*) model were displayed in Figs. 10 and 11, respectively. Where both in the "Data Input" table of the two pictures, in the top row, the "numbers 1–4" stand for the four "input" influence factors in this study in turn, which were initial temperature (number 1), initial pressure (number 2), steam/acetone mixing concentration (number 3). The "number 4" represents the corresponding "output" result, i.e., *St* class (number 4). In addition, the "Weighting" column on the right-and-down side there shows the weighting analysis results for the four "input" influence factors, individually. It was found that the influence factor 2, "initial pressure" has the highest influence weighting analysis value not only by GM(1,*N*) model (number 2/0.7868) but also by GM(0,*N*) model (number 2/0.7302). The second factor in GM(1,*N*) was initial temperature (number 1, 0.5259), but in GM(0,*N*) was steam/acetone mixing concentration (number 3, 0.2774). Otherwise, the third one had the contrary situation; it was opposite to the initial temperature (number 1) and the steam/acetone mixing concentration (number 3). The third influence factor was steam/acetone mixing concentration (number 3, 0.2503) in GM(1,*N*) model, whereas in the GM(0,*N*) model it was initial temperature (number 1, 0.1696).



1. Initial temperature
2. Initial pressure
3. Steam/acetone mixing concentration
4. Explosion St-class

Fig. 9 GMHN weighting analysis tool box used for this study [16, 26]



File Name: 666

Methods: ● GM(1,N) ○ GM(0,N)

Data Input

	1	2	3	4
1	1	1	1	2
2	1	1	2	2
3	1	1	3	2
4	1	1	4	1
5	1	2	1	3
6	1	2	2	2
7	1	2	3	2
8	1	2	4	2
9	2	1	1	2
10	2	1	2	2
11	2	1	3	2
12	2	1	4	1
13	2	2	1	3
14	2	2	2	3
15	2	2	3	2
16	2	2	4	2

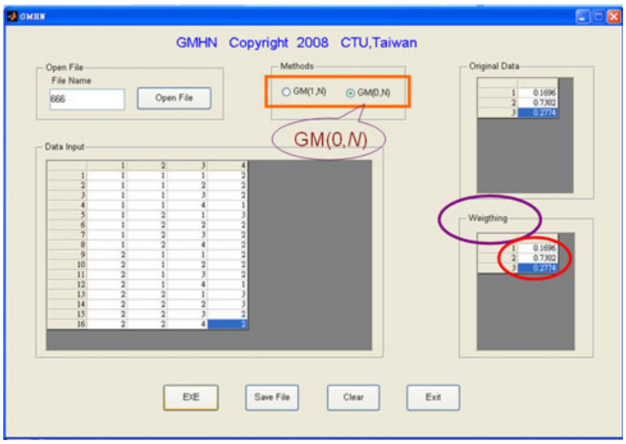
Original Data

1	-0.5259
2	-0.7868
3	-0.2503

Weigthing

1	0.5259
2	0.7868
3	0.2503

Fig. 10 Sixteen-sets weighting analysis values of GM(1,*N*) model used in this study



File Name: 666

Methods: ○ GM(1,N) ● GM(0,N)

Data Input

	1	2	3	4
1	1	1	1	2
2	1	1	2	2
3	1	1	3	2
4	1	1	4	1
5	1	2	1	3
6	1	2	2	2
7	1	2	3	2
8	1	2	4	2
9	2	1	1	2
10	2	1	2	2
11	2	1	3	2
12	2	1	4	1
13	2	2	1	3
14	2	2	2	3
15	2	2	3	2
16	2	2	4	2

Original Data

1	0.1696
2	0.7302
3	0.2774

Weigthing

1	0.1696
2	0.7302
3	0.2774

Fig. 11 Sixteen-sets weighting analysis values of GM(0,*N*) model used in this study

According to the above analysis by grey GM(1,*N*) and GM(0,*N*) model, it was strongly suggest that the manager or plant engineer in such an steam/acetone mixing system should consider controlling the effect of initial reaction pressure first. In addition, the steam/acetone ratio influence factor in this study, demonstrating the influence on inert steam [$H_2O_{(g)}$] to reduce flammability hazard degrees according to the variations of experimentally derived safety-related properties should be considered as well. As for the hazard of initial temperature, it should also be carefully considered for the process safety concern. This study establishes a complete flammability hazard evaluation approach that is combined with an experimentally and theoretically feasible way for fire/explosion prevention and protection. The outcomes would be useful for positive decisions for safety assessment for the relevant practical plants or processes.

Conclusions

- This study proposes a helpful reference with an experimentally and theoretically adequate approach for flammability prevention and protection.
- Several important flammability properties of acetone$_{(aq)}$ solutions (steam/acetone mixing ratios (75/25, 50/50, 25/75, and 0/100 vol.%) at 150, 200 °C, 760, 1520 mmHg, and 21 O_2 vol.%, and the influence on inert steam to loading fuel concentration were found experimentally.
- While augmenting the inert steam, the explosion area and hazard became small and narrow, and so did the flammability characteristics, including P_{max} and $(dP\,dt^{-1})_{max}$ of the tests.
- The influence factor of "initial pressure" has the highest influence weighting analysis value both by GM(1,*N*) (0.7868) and GM(0,*N*) (0.7302) model, indicating it is the most important factor among the other influence factors. Therefore, it was strongly suggest that the manager or plant engineer in such a steam/acetone mixing system should consider controlling the effect of initial reaction pressure first.
- The second influence factor in GM(1,*N*) was initial temperature (number 1, 0.5259), but in GM(0,*N*) was steam/acetone mixing concentration (number 3, 0.2774).
- The third influence factor was steam/acetone mixing concentration (number 3, 0.2503) in GM(1,*N*) model, whereas in GM(0,*N*) model it was initial temperature (number 1, 0.1696).
- The traditional method for investigating the flammability characteristics and hazard was further confirmed by the soft computing methods of the grey system theory approach.

- This study first combined the 20-L-apparatus experimental measurement and grey system theory approach for flammability hazard assessments both experimentally and theoretically.

Recommendations

- Testing with different initial temperatures, or combined with other soft computing methods, such as rough set.
- Establishing a comprehensive model for the explosion limits and MOC in this system or, if not, predicted.
- Changing inert gases (CO_2, N_2), and increasing initial pressure to draw a complete triangular flammability diagram.

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