# Mathematical Prediction of Thermal Runaway Conditions of Ammonium Nitrate Decomposition

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Abstract - The reason behind the runaway decomposition of ammonium nitrate has been studied mathematically. This work aims to determine the root cause of an explosion of ammonium nitrate (AN) during storage. All the data needed for chemical kinetics were taken from Zhe Han's experimental studies. M.M. Khader introduced a new method, the Picard Pade method, which was utilized to solve mathematical models in the current study, and the results were well validated by Zhe Han's experimental work. By splitting the temperature curve into three zones based on the variation in slope with time, the impact of different combinations on temperature increase has been studied and described in depth. With numerical solutions, the effect of ammonium nitrate concentration, decomposition, and formation of nitrogen oxide on the runaway reaction has been well illustrated. Within the scope of the mixture compositions, the mixture with controllable temperature rise is a 44-13.69-9.38-10.93-22 and the mixture with uncontrollable temperature rise is 50-10.69-6.38-16.93-16. The computational tool used to solve the mathematical model in this work is MATLAB.

*Index Terms* - Mathematical, MATLAB, Picard Pade, Runaway, Ammonium Nitrate, Nitrogen oxide.

#### I. INTRODUCTION

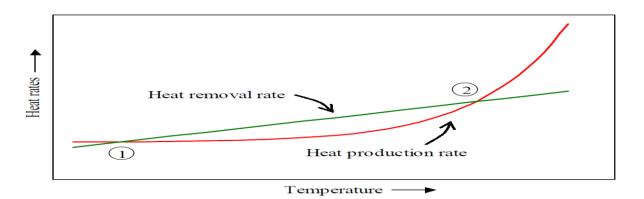
Ammonium nitrate (AN) is a common fertiliser as well as an cataclysmic (destructive) material [1]. It's an premium source of nitrogen as a fertilizers. It is combined with fuel oil to produce Ammonium nitrate fuel oil (ANFO) as an explosive [2]. At room temperature, AN is not accounted as flammable or combustible chemical. [2,3]. It is a powerful oxidizing agent which can explode under certain conditions such as high temperatures, impurities, and confinement [4]. Explosion, fire-related (as an oxidant), and self-sustained decomposition (SSD) are the danger types [2] connected with AN. In this explosion, 270 tons [6] of AN were involved. In this explosion 15 people were killed and more than 250 were injured. [7]. On September 21, 1921, in Oppau, Germany, a 450-ton AN explosion resulted in the deaths of 561 people [8]. The disaster was thought to have been caused by contamination [8]. On April 16, 1947, another AN explosion occurred in Texas City, Texas, killing 581 people. This fire resulted in the release of 2300 tonnes of AN [3]. The Toulouse

catastrophe, which involved 300 tonnes of AN and resulted in 30 deaths, occurred on September 21, 2001 in France [9]. The root cause of the problem was revealed to be chloride contamination. The terrorist assault in Oklahoma City [10] on April 19, 1995, which killed 168 persons, raised awareness of the hazards of AN. The thermal decomposition of AN has been studied in the literature using Differential Scanning Calorimetry (DSC) [11], Accelerating Rate Calorimetry (ARC) [12], and the Setaram C80 Heat Flux Calorimeter (C80) [13]. Due to various testing methods and equipment accuracy, there are some slight differences in the data obtained from the literature.

According to Semenov, the thermal explosion hypothesis provides the foundation for understanding a runaway reaction. The competition between heat generation by an exothermic reaction and heat removal from the reaction mass to, for, the cooling jacket [15] is the subject of this theory. According to Arrhenius, heat generation is proportional to temperature, while heat removal is proportional to temperature (see Fig. 1)

When the rate of heat production equals that of heat removal, a steady state is established [15] which will be true for both intersection temperatures and the ambient temperatures (see Fig. 1). This plot shows the degree of control over the heat production rate. Because the slope of the heat removal line is greater than the slope of the heat production curve at intersection (1), a minor deviation from this steady-state results in an automated return to its origin. As a result, intersection (1) represents a stable operating point where an exothermic reaction is in control. Intersection (2), on the other hand, illustrates an unstable operating point. If a temperature deviation occurs, the original operating conditions will never be restored. The steady-state of intersection (1) will be found if the temperature decreases. The rate of heat generation will always surpass the rate of heat removal in the event of an increase. This will result in an unimpeded self-acceleration of the reaction rate and, as a result, an increase in of heat production, which is known as a runaway reaction [17].

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**Fig.1.** Diagram of heat flow. The rate of heat generation by chemical reactions and the rate of heat removal through cooling.

Zhe Han's experimental work [16] investigated the thermal decomposition of Ammonium nitrate and found the reasons for the initiation of thermal runaway conditions during the reaction. This work mentions the governing chemical equations for converting ammonium nitrate to nitrogen, oxygen, water, and nitrogen oxide [18,19, 22]. The kinetics data required in resolving the Mathematical model was taken from Zhe Han's work.

#### II.Methodology: 2.1 The fundamentals of chemical reactions

According to violent exothermal reactions, this work primarily entails the end-temperature predictions for reactions in which exothermal effects begin to dominate the reaction, which may cause decomposition to accelerate, leading to explosive behavior of NH<sub>4</sub>NO<sub>3</sub>. In the literature, various decomposition mechanisms of Ammonium nitrate have been reported, with popularly accepted reactions being summarised here. At low temperatures, an endothermic reversible reaction can occur (i.e., around 170  $^{\circ}$ C). It is declared that when melted Ammonium Nitrate is vaporised, ammonia and nitric acid are formed, which could start the disintegration of Ammonium Nitrate through the following radical reactions. [11, 15, 25, and 25] (Eqs. 1-4):

 $\begin{array}{ll} NH_4NO_3 \leftrightarrow NH_3 + HNO_3 & \Delta H = 176 \text{ kJ/mol} & (1) \\ NH_2NO_2 \rightarrow N_2O + 2H_2O & \Delta H = -59 \text{kJmol}^{-1} & (2) \\ NH_4NO_3 \rightarrow 2N_2 + NO + 2H2O; & \Delta H = 257 \text{ kJ mol}^{-1} & (3) \\ NH_4NO_3 \rightarrow 3/4 N_2 + 1/2NO_2 + 2H_2O; & \Delta H = 944 \text{ kJ mol}^{-1} & (4) \\ There will be an explosive decomposition if the material is suddenly heated up. [23] \\ 2NH_4NO_3 \rightarrow N_2 + O_2 + 4H_2O; & \Delta H = 1057 \text{ kJ mol}^{-1} & (5) \end{array}$ 

According to violent exothermal reactions, exothermal effects begin to dominate the reaction, causing an acceleration of decomposition and potentially explosive behaviour (15, 19, 22) (Eqs. 5):

$$\mathrm{NH}_4\mathrm{NO}_3 \longrightarrow \mathrm{N}_2 + 0.5\mathrm{O}_{2}_{+}2\mathrm{H}_2\mathrm{O} \tag{6}$$

This explains why heating AN in confined, enclosed places can result in explosions (15). The following reaction predominates at higher temperatures, and it decomposes into Nitrogen, Oxygen, and water.

## 2.2 Mathematical Modelling of the selected chemical reactions

For predicting thermal runaway conditions, A mathematical model was developed that included mass and energy conservation.

#### **2.2.2 Reaction Kinetics**

Ammonium nitrate decomposition and nitrogen oxide (NO) formation occur simultaneously. Ammonium nitrate (AN) decomposition is an exothermic reaction, whereas nitrogen formation is an endothermic reaction. The following are the reactions [18, 19, 22]:

$$\begin{array}{ccc} NH_4NO_3 \rightarrow N_2 + 0.5O_2 + 2H_2O & -----(7) \\ O_2 + N_2 \rightarrow 2NO & -----(8) \end{array}$$

The following are the reaction rate equations:

 $\begin{array}{c} R_{AN} = K_0 \; exp^{(-E_1/RT)} \left[ \begin{array}{c} C_{AN} \end{array} \right] & ---(9) \quad [19] \\ K_0 = 4.55 x 10^7 \; s^{-1} \; \ E_1 = 102.6 \; kJ/ \; mol \; Hrxn = -118.86 \; kJ/mol \end{array}$ 

$$\begin{array}{ll} R_{\rm NO} = K \, exp^{(-E_2/RT)} \left[ \begin{array}{c} C_{\rm N2} \end{array} \right] \left[ C_{\rm O2} \right] & ----(10) & [18] \\ K_0 = 1.32 x 10^{10} \, {\rm s}^{-1} \, E_1 = 545 \, {\rm kJ/\,mol} & {\rm Hrxn} = 90.4 {\rm kJ/mol} \end{array}$$

### 2.2.3 Mathematical Modelling of the selected chemical reactions

On the selected reaction, the chemical species NH<sub>4</sub>NO<sub>3</sub>, N<sub>2</sub>, O<sub>2</sub>, H<sub>2</sub>O, and NO have an impact. Ordinary Differential Equations were used to create a mathematical model based on these chemical compounds. Zhe Han's [15] experimental work was used to derive the boundary conditions. T.Urbanzki's [18, 27, 29] work provided the chemical kinetic values for NO, while the data for the reaction were taken from Zhe Han's [15]. Using the following governing equation, based on the heat of formation and bond association enthalpies, the heat of reaction for the chemical reaction was calculated.

 $(\Delta h)_{\text{rxn.}} = (\Delta h)_{\text{react.}} - (\Delta h)_{\text{prod.}}$ 

Various Ammonium Nitrate decomposition mechanisms have been reported in the literature, with the most widely approved reactions listed above (9, 10) [11, 14, 15, 26]. At low temperatures, an endothermic reversible reaction can occur (i.e., around 170°C). It is thought that when melted Ammonium Nitrate is vaporised, ammonia and nitric acid are formed, which could start the degradation of Ammonium Nitrate through the following reaction [2,3,4]  $\Delta$ H= 176 kJ mol<sup>-</sup>

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1. Exothermic irreversible reactions occur at higher temperatures (between 170 and 280 degrees Celsius), and the  $\Delta$ H value drops to -59 kJ mol-1, then to  $\Delta$ H=-257 kJ mol-1, and finally to  $\Delta$ H =-944 kJ mol-1. When a material is suddenly heated,, an explosive decomposition ( $\Delta$ H =-1057 kJ mol-1) occurs, raising the temperature and causing a thermal runaway scenario. According to the literature [16, 20], the formation of oxygen, nitrogen, water vapour, and nitrogen oxide (NO) has the greatest impact on reactions. The current research aimed to determine the best compositions of these five chemical species in the reaction mixture, ensuing to see how their concentration affects the temperature at that specific time.

The rate of reaction for both reactions are as follows [17]:

$$R_{AN} = alpha \times [u] \tag{12}$$

$$R_{NO} = beta \times [v] \times [w] \quad ^{0.5} \qquad (13)$$

The concentrations of chemical substances in the specified chemical reactions were calculated using the formulae below [17].

$$\frac{du}{dt} = -R_{AN}$$
(14)  

$$\frac{dv}{dt} = R_{AN} - R_{NO}$$
(15)  

$$\frac{dw}{dt} = R_{AN} - R_{NO}$$
(16)  

$$\frac{dy}{dt} = R_{AN}$$
(17)  

$$\frac{ds}{dt} = R_{NO}$$
(18)

#### Notations

u = Ammonium Nitrate Concentration ([C<sub>AN</sub>]).

 $v = Nitrogen concentration ([C_N]).$ 

 $w = Oxygen Concentration ([C_0]).$ 

y= Water Concentration ([C H20]).

s = Nitrogen oxide Concentration ([C<sub>NO</sub>]).

 $R_{AN}$  = Reaction rate of the exothermic reaction (Ammonium Nitrate).

 $R_{\text{NO}}\text{=}$  Reaction rate of the endothermic reaction (Nitrogen oxide)

Alpha = Rate constant for the exothermic reaction (Ammonium Nitrate)..

beta = Rate constant for the endothermic reaction (Nitrogen oxide).

 $(\Delta H)_{rxn.}$  = reaction enthalpy.

 $(\Delta H)_{react.} = Reactant enthalpies.$ 

 $(\Delta H)_{\text{prod.}} = \text{Product enthalpies.}$ 

#### 2.2.3 Energy Conservation

The exothermic nature of reactions, particularly those in which the heat of the reaction is the main cause for increase in heat energy because it is vast and the temperature rises rapidly. Another source for increase in heat energy is chemical species high concentration and high heat of reaction will cause an increase in end temperature.

In the results section of this paper, the risky and safe combinations of the mixture have been reported.

The equation that governs the development of heat as a result of the reaction is given below [17, 27].

$$\frac{dT}{dt} = (R_{AN} \times (\Delta h)_{AN} + R_{NO} \times (\Delta h)_{NO}) / (\rho \times C_P)$$
(19)

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#### Notations

 $\frac{dT}{dt}$  - Temperature Change (T) with time (t).

 $(\Delta H)_{AN}$  - Heat of Reaction for an exothermic reaction (Ammonium Nitrate).

 $(\Delta H)_{NO}$  . Heat of Reaction for an endothermic reaction (Nitrogen oxide).

 $\rho$  - Mixture Density.

C<sub>P</sub> - Mixture Specific heat at constant pressure.

Using a PICARD-PADE method, these equations have now been solved in order to determine temperature growth and predict thermal runaway.

#### 2.3 Solution for the Mathematical model:

#### 2.3.1 The Picard-Pade Method:

In this method, the Picard Iteration series will be an function of 'Time' f(t).. We have selected '8' as the order to truncate the series, giving us the Picard Iteration series up to ' $t^7$ '. The Picard Iteration method uses a many iterations to obtain the series are '6. The Picard Iteration series is truncated for the order of '8' and then applied to solve the truncated series using the Pade approximation [16, 17].

The Pade approximation to the function's value is a rational fraction approximation. [16, 17]. The Pade approximation is written like this:

$$P[n/m](t) = \frac{\sum_{0}^{n} Pn \times t^{n}}{1 + \sum_{1}^{m} Qm \times t^{n} m}$$
(20)

The polynomials by degrees 'n' and 'm' are represented by P and Q, respectively.

Choosing the optimal values for n and m to produce the best approximation is an important step while this technique. The desired thermal profile's shape can be used to determine the degrees of numerator and denominator to use. 'n>m' is the most suited criterion for this work.

The Picard Iteration method [17] was used to solve the system of differential equations 14 to 18, which were formulated as follows.

$$u_{i+1} = u(0) + \int_0^{t} [-R_{AN}] dt$$
(21)

$$v_{i+1} = v(0) + \int_0^t [R_{AN} - R_{NO}] dt$$
(22)

$$w_{i+1} = w(0) + \int_0^t [-R_{AN} - R_{NO}] dt$$
(23)

$$y_{i+1} = y(0) + \int_0^t R_{AN} dt$$
 (24)

$$s_{i+1} = s(0) + \int_0^t R_{NO} dt$$
 (25)

$$T_{i+1} = T(0) + \int_0^t (R_{AN} (\Delta h)_{AN} + R_{NO} (\Delta h)_{NO}) / (\rho C_p) dt \quad (26)$$
Notations

Notations

 $R_{AN} = alpha \times u_i$  $R_{NO} = beta \times v_i \times w_i$ 

T (0) is the initial temperature, and u (0), v (0), w (0), y (0), s (0) are the chemical compounds' initial concentration values at the start of the reaction. The initial temperature T(0) has been set to  $80^{\circ}$ C in this work because the at that temperature, the reaction is more likely to begin. In general, the reagent Ammonium Nitrate based on equation (9) and Nitrogen and Oxygen in equation (10) a concentration is maintained, each of the two constituent reactions will increase the concentration of any of the species by the same amount as the reactants in the

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reaction mixture. Individual species proportions, such as  $NH_4NO_3$ ,  $N_2$ ,  $O_2$ ,  $H_2O$ , and NO, can be varied within a set proportion limits [17].

Heat of reactions and kinetic constants [18, 19] for exothermic reactions, the activation energy Ea= 102.6 KJ/mol the value of pre-exponential factor A=4.55x107 1/sec at 300 °C and  $(\Delta h)_{NO}$ = 90.4kJ/mol have been considered as alpha = 2.11×10<sup>2</sup> and  $(\Delta h)_{AN}$  = -118.86 kJ/mol respectively.

We obtained a series in 't' by solving the above equations. The Pade approximation method [16, 17] now use the truncated equation. Determining the values of polynomials in the numerator and denominator, i.e. P(t) and Q(t) values, is the issue in the Pade approximation approach. The degree has been set to n=5 and m=2, which meets the criteria set out in Zhe Han's [1] paper, thermal profile (n>m). The equation's total order n+m is a possible representation.

For the mixture with the combination 44-13.69-9.38-10.93-22 , after 6 iterations of the Picard iteration method  $T_6$  (t) with P[4/3], the Pade approximation for Temperature is [17].

### $P[4/3] = \frac{20+10.37t+7.8856*10^{-4}t^2 - 2.535910^{-6}t^3 + 0.00006t^4}{2} (27)$

 $P[4/3] = \frac{1-0.0211t+2.2260*10^{-4}t^2-6.326*10^{-7}t^3}{1-0.0211t+2.2260*10^{-4}t^2-6.326*10^{-7}t^3}$  (27) Similarly, we derived the Pade approximation P [5/3] values for the u<sub>5</sub> (t), v<sub>5</sub> (t), w<sub>5</sub> (t), y<sub>5</sub> (t), and s<sub>5</sub> (t) and iterated for 250 seconds as the reaction occurs for 250 seconds. Temperature, Concentration, and Time graphs have been drawn in the selected interval.

In this work, the software application MATLAB is utilised to solve the chosen chemical system.

#### **III. RESULTS & DISCUSSIONS**

For analysis, the three types of mixtures were considered. The different mixtures is taken as  $NH_4NO_3+N_2+O_2+H_2O+NO$  are taken as 50%-10.69%+ 6.38%+16.93%+16%, 47%-12.69%+8.38%+11.93%+20% and 44%-13.69%+9.38%+10.93%+22%.

The rise in temperature was obtained using NH<sub>4</sub>NO<sub>3</sub> at 50 %, Nitrogen at 10.69%, oxygen at 6.38%, and water vapour at 16.93% and, Nitrogen oxide at 16% (see Fig. 2). We assumed that the five concentrations add up to one, and that each of the two constituent reactions adds to the concentration of any of the species exactly at the expense of matching amounts of the reactants [16, 17]. The temperature profiles are divided into three distinct regions: Initial rapid increasing temperature phase 1 i.e. onset temperature T<sub>onset</sub>, this phase have been described in our previous work [15]., during exothermic reaction rapidly increasing temperature phase 2 i.e. Maximum Temperature T<sub>max</sub> and initiation of the oxidation reaction i.e. endothermic reaction, final rapid increasing temperature phase-3 due to the reaction mixture undergoes complete oxidation reaction i.e. Temperature when Reaction Complete T<sub>f</sub>.

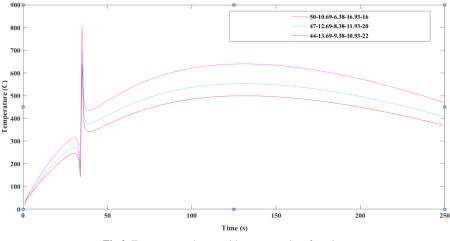


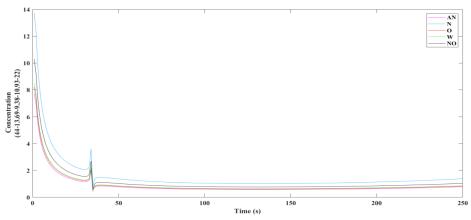
Fig.2. Temperature change with respect to time for mixtures
Table I

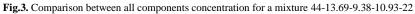
Observations based on the results.			
Mixture proportions	PHASE-I	PHASE-II	PHASE-III
in %ge's	(Onset	(Maxiumum	(Temperature at Recation
	Temperature $(T_0)$ )	Temperature( $T_{max}$ ))	Complete (T <sub>f</sub> ))
50-10.69-6.38-	Temp = 310.5 °C	Temp = 805.7°C	Temp =470 °C
16.93-16	Time = $31 \text{ sec}$	Time = 35sec	Time = $250 \text{ sec}$
47-12.69-8.38-	Temp = 269.1 °C	Temp = 701.1 °C	Temp=406 °C
11.93-20	Time = $29 \text{ sec}$	Time = $35 \text{ sec}$	Time = $250 \text{ sec}$
44-13.69-9.38-	Temp = 243.8 °C	$Temp = 637^{\circ}C$	Temp = $368 ^{\circ}\text{C}$
10.93-22	Time = $29 \text{ sec}$	Time = 35sec	Time = 250sec

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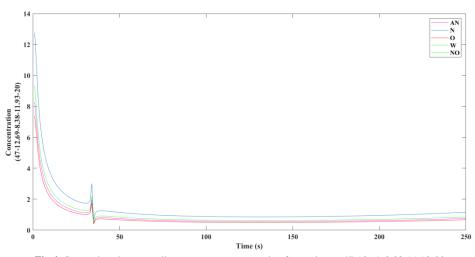


Fig.4. Comparison between all components concentration for a mixture 47-12.69-8.38-11.93-20

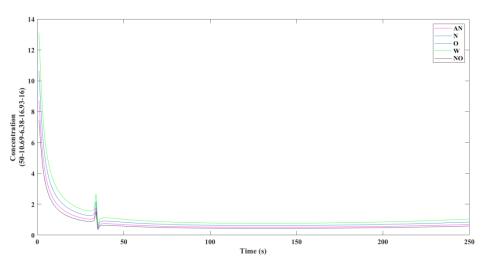


Fig.5. Comparison between all components concentration for a mixture 50%-10.69%-6.38%-16.93-16

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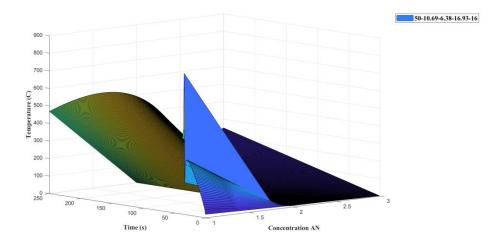


Fig.6. Temperature change with respect to time and AN concentration for a mixture 50%-10.69%-6.38%-16.93-16

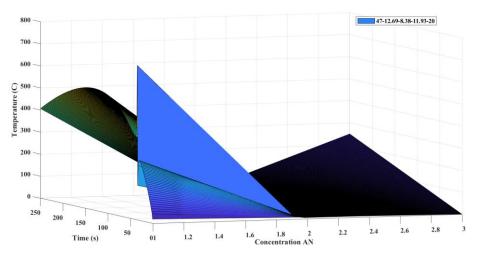


Fig.7. Temperature change with respect to time and AN concentration for a mixture 47-12.69-8.38-11.93-20

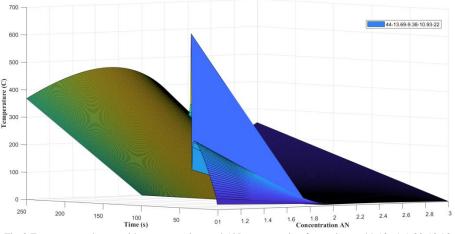


Fig-8 Temperature change with respect to time and AN concentration for a mixture 44-13.69-9.38-10.93-22

#### 3.1 Discussion

When compared to the other two compositions, the 50%-10.69%+ 6.38%+16.93%+16%, mixture shows faster temperature growth in phase-1 and phase-2 takes place at a higher temperature of around T<sub>max</sub>=805.7°C (see Fig. 2). While 47%-12.69%+8.38%+11.93%+20% takes less than 40 seconds

to reach 600°C, 44%-13.69%+ 9.38%+10.93%+22% requires more than 40 seconds.

According to literature [15], reached by the highest temperature reaction is 500-550°C, which will result in an explosion. This shows that the runaway phenomena has already occurred and has reached an uncontrollable stage. The

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lowest temperature is around 250°C-300°C, although it is on a decreasing trend that is controllable and decreases over time.

The temperature development of Ammonium Nitrate decomposition and the formation of Nitrogen Oxide with different composition mixtures is the focus of this study. The main cause of a runaway phenomenon during Ammonium Nitrate decomposition, according to the literature is a rise in the reagent's mixture (AN) [15]. If we look attentively at the plots above, we can see that they all follow the same trend. As indicated in the graph above, we tested temperature changes with various mixtures. The first three plots represent the temperature change caused by the reagent combination change shown in Fig-2. The three graphs show how temperature changes in response to changes in the mixture. The temperature, as can be seen, follows a pattern in these plots. When it executes the initial reaction stage, the slope decreases, but the sudden increase is due to the exothermic reaction, and there will be some decrease due to the endothermic reaction, i.e. oxidation reaction [15].

In Fig. 2, the temperature profile along the reaction time is equivalent to the temperature at the first section of the reaction time zone [22, 24]. Because the reaction is highly exothermic, a temperature jump is seen, indicating that Ammonium Nitrate decomposition generates a significant amount of heat. The temperature then decreases consistently along the reaction time zone as the rate of Ammonium Nitrate disintegration decreases and nitrogen oxide production, which is an endothermic process, occurs [15]. Because of the endothermic reaction, the rate of NO slowed, causing the temperature to rise. As the temperature rises, the rate of Ammonium Nitrate decomposition increases, resulting in a low concentration of Ammonium Nitrate in the product.

We can see that the slope changes as we vary the reagent mixture (see Fig. 2). As the percentage of AN in the mixture decreases, the slope decreases. As a result, AN dissociation, in addition to the N and O2 combination, plays a crucial part in raising the temperature. As a result, the increase in the composition of AN reagent will boost temperature growth. The same can be seen in (see Figs. 6, 7, 8) as well.

The third plot in Fig. 2 appears to be nearly identical, but when we compare them with literature, we notice that these two plots differ in increase in slope, with the (see Fig. 2, 6, 7, 8) mixture having a lower slope (see Fig. 2), implying that the temperature increase in 44-13.69-9.38-10.93-22 plot 3 is slower than the other two plots (see Fig. 2). For explanation, if we consider the mixture of the plot 44-13.69-9.38-10.93-22 is lower compared with the other two mixtures. If we observe 50%-10.69%-6.38%-16.93-16 has more slope than 47-12.69-8.38-11.93-20. This suggests that in (see Fig. 2), the Oxidation reaction will have little influence, and the temperature rises gradually to be easily controlled[22].

The next three plots (see Fig. 3, Fig. 4, and Fig. 5) show us a comparison between all components concentration for three mixtures, which indicates the maximum and minimum concentrations are associated to Nitrogen and ammonium nitrate. Unfortunately, the ammonium nitrate concentration at the end of the reactor would not be zero. The reactor should be heated more to complete the decay of ammonium nitrate. [22, 24].

As temperature increases, ammonium nitrate deterioration happens [24]. As appeared in Figures 3, 4, 5 the initial concentration of AN decreases implies to moderately low rate of mass exchange between just a little amount of AN vapour. As a result, these variables cause AN in the reaction to decay in an unrelated way. In the beginning section of the reactor the grouping of AN clustering decreases, as seen in Figures 3, 4, 5, although there is a gradually reducing pattern in the rest of the reactor. Furthermore, due to the high mass transfer coefficients and high blending rate toward the first part of a reactor, higher AN deterioration occurs in this area.

The concentration profile of Nitrogen Oxide along the reactor is shown in Figures (3, 4 5) as it gradually increases. In addition to causing acid rain, nitrogen oxide is a major pollutant of the environment. Because Nitrogen Oxide is produced in large quantities, mass exchange occurs, and Nitrogen Oxide is transferred. When the concentration of  $N_2$ and  $O_2$  along the reactor rises, the rate of mass transfer of nitrogen oxide generation decreases.

The concentration patterns of  $O_2$ ,  $N_2$ , and  $H_2O$  along the reaction time are illustrated in Figures 3, 4, and 5. The concentration profiles of  $O_2$  and  $N_2$  have the same behaviour in Figures 3, 4, and 5, but are greater in Figures 3 and 4 and less in Figure 5. This trend is attributable to the AN decomposition reaction, in which both of them are produced and then consumed, resulting in NO.  $N_2$  and  $O_2$  are only produced in the initial stages of the reaction due to the rate of AN disintegration is moderately high; nevertheless, when the rate of  $O_2$  and  $N_2$  generation decreases.

Moreover, oxidation of  $N_2$  leads in reduced  $N_2$  and  $O_2$  levels in the reactor's remaining space. In this approach, the  $O_2$  and  $N_2$  groups increase at the beginning of the reaction zone, but subsequently gradually decrease[24]. The concentrations of  $O_2$ and N2 expand in a pattern along the reaction zone, as shown in Figures 3, 4, and 5. As previously stated, the AN decay rate is insignificant, therefore no  $O_2$  and N2 will be generated, and their expanding content will only be associated with mass exchanges. As a result,  $N_2$  and  $O_2$  concentrations would not be zero at the beginning. The amount of  $H_2O$  generated during AN decay is different from the amounts of  $O_2$  and N2. The initial concentration of  $H_2O$  in the first portion of the reaction zone is much greater due to the extensive disintegration of AN in the first part of the reaction zone.

The three plots (see Fig. 6, Fig. 7, and Fig. 8) show us temperature change with respect to time and AN concentration for a three mixture The rapid breakdown of ammonium nitrate results in a greater fall in ammonium nitrate concentration over time. Furthermore, as the temperature rises, the concentration of ammonium nitrate drops. As a result, increasing the temperature will accelerate the conversion of ammonium nitrate. The plots (see Fig. 6, Fig. 7, and Fig. 8) clearly show AN decomposition with time and temperature in the three mixtures. When % of AN increases the temperature increases along with time. It was shown clearly in the three mixtures and the concentration of AN decreases with time. Unlike in the past, there will be a significant difference in the final temperatures (see Fig. 6 to 8). the only difference is that the slopes of (see Fig. 6) are marginally lower than those of (see Fig. 7).

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We can see from these three plots Fig-2 which composition is the most hazardous one and unmanageable, and which composition is the safest and most controllable.

#### **IV. CONCLUSION**

The solutions obtained using the Picard-Pade technique are acceptable and match the values found in the literature. It is evident that as the Ammonium Nitrate Percentage increases, the final temperature rises as well. The slope of the curve is rapidly increasing when the amount of reagents (e.g., AN) increases. This shows that increasing the Ammonium Nitrate content will make the reaction temperature uncontrollable since it will grow at a faster rate. When we examine the plot, we can see thatand the observation from the results Table-1, the dangerous or risky composition will be 50-10.69-6.38-16.93-16. After 40 seconds, the temperature increases at such a rapid rate that it becomes uncontrollable. When we examine the plot, we can see that, the safest mixture is 44-13.69-9.38-10.93-22, which has a decreasing slope, If we look at the plot and the results from Table 1, we could see that the temperature growth produced by this mixture can be controlled.

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