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BRIDGING THE GAP BETWEEN THEORY AND PRACTICE IN PROCESS SAFETY ENGINEERING: SIMULATION-BASED LEARNING FOR THERMAL RUNAWAY REACTIONS

Milan Protić[1], Milan Gocić[2], Ana Bijelić[3], Miomir Raos[4]

Abstract: One of the pressing issues in educating new generations of engineers is bridging the gap between theory and practice. This is particularly important in process safety engineering, where future engineers are expected to work in real industrial facilities, often facing life-threatening conditions that require immediate action. Performing process safety simulations allows students to explore different "what if" scenarios in the safety of a classroom environment. This study presents a detailed methodology for modeling thermal runaway behavior, using the esterification of acetic anhydride with methanol as a case study. This highly exothermic reaction, is simulated under adiabatic conditions to represent a cooling system failure scenario. The methodology was validated by comparing the simulated temperature profile with experimental data from previous studies, showing strong agreement, particularly in predicting the reaction's steady-state temperature. This methodology can be applied to other exothermic reactions, making it a versatile resource for improving process safety in chemical manufacturing.

Key words: Runaway reactions, Modeling, Safety, AVEVA Process simulation, Python, Esterification, Exothermic reactions

1. INTRODUCTION

Thermal runaway is defined by a continuous escalation in heat generation, where an exothermic reaction produces heat faster than it can be removed by the surroundings [1]. This leads to a rapid, uncontrolled increase in temperature, which in turn accelerates the reaction rate, further heat production, and a rise in pressure. The pressure increase is typically driven by the vaporization or decomposition of reaction components [1]. Contributing factors to thermal runaway include incorrect kinetic evaluations, excessive reagent feed rates, impurities, inadequate mixing, and failures in cooling or stirring systems, along with human errors [2]. Given the significant role runaway reactions play in industrial accidents, the development of predictive models is crucial for anticipating such events and enhancing process safety.

While simulation studies are valuable in this context, many existing works lack clarity in presenting modeling details, and reproducibility remains a challenge. More transparent explanations and accessible descriptions of the underlying equations are necessary to improve the utility of these studies. In light of this, the present work aims to provide a detailed, step-by-step methodology for performing thermal runaway calculations.

As an example, the esterification of acetic anhydride with methanol is used, as this reaction is commonly used in studies of thermal runaway phenomena [3]. This esterification reaction produces methyl acetate and acetic acid, both of which are widely used in various industries: methyl acetate serves as a solvent in the production of coatings, cellulose-based materials, plasticizers, lacquers, and ink resins, while acetic acid is a key raw material in the synthesis of pharmaceuticals, dyes, pesticides, and other organic chemicals [3]. The esterification of acetic anhydride with methanol is highly exothermic, with a reaction enthalpy of *ca.* -70 kJ/mol [3], indicating that the reaction can lead to a rapid temperature rise if not properly controlled. Insufficient heat removal can cause the reaction mixture to overheat, potentially resulting in hazardous situations such as reactor over-pressurization or the decomposition of reactants and products that may lead to unwanted events.

In this work, we focus on modeling thermal runaway using the esterification of acetic anhydride with methanol as an example, under adiabatic conditions. The adiabatic mode simulates a reactor cooling system failure, representing a critical safety scenario.

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2. METHODOLOGY

The esterification reaction of acetic anhydride with methanol could be represented as follows:

$(CH_3CO)_2O + CH_3OH \rightarrow CH_3COOCH_3 + CH_3COOH$

The reaction is generally second-order, first-order with respect to each reactant.

In AVEVA Process simulation software, this reaction can be simulated using the Conversion Reactors (CNVR) and the Reaction Generator Tool, as shown in Fig. 1.

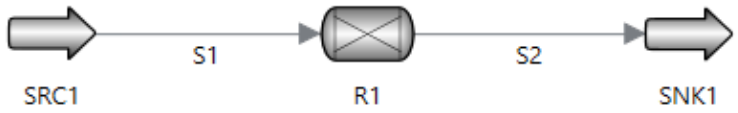

Fig. 1- Esterification reaction in a CNVR (AVEVA Process simulation)

Theoretically, data on temperature and pressure rates can be automatically generated if a trend model is introduced in the AVEVA Process simulation canvas. However, our primary interest here is to go through the calculation process step by step, with a thorough explanation.

To calculate the rate of temperature (dT/dt) and pressure (dP/dt) change for a second-order chemical reaction in an adiabatic reactor, first thing is setting up and solving the mass and energy balance equations. It is very important to account for the reaction kinetics and thermodynamics under adiabatic conditions. In the derivation, the following assumptions were used:

- due to the adiabatic nature of the reaction, there is no heat exchange with the surroundings;
- the gases evolved during the reaction behave as perfect gases;
- the reactor operates at constant volume.

For a second-order reaction the reaction rate is given by the equation:

$$-\frac{dn_A}{dt} = rV = kn_A^2/V$$

where n_A is the number of moles of substance A, r is the rate of reaction per unit volume, V is the reactor volume and k is the rate constant. The negative sign indicates that A is being consumed as the reaction progresses. Reaction rate is temperature-dependent. It can be calculated using Arrhenius equation:

$$k = k_0 \exp\left(-\frac{E_a}{RT}\right)$$

where k_0 is the pre-exponential factor, E_a is the activation energy, R is the gas constant and T is the absolute temperature. Now, it is important to introduce the conversion X of reactant A and differential equation for mass balance. Conversion X can be defined as:

$$X = \frac{n_{A,0} - n_A}{\mathrm{n_{A,0}}}$$

where $n_{A,0}$ is the initial number of moles of A. Differential equation for mass balance is defined by:

$$\frac{dX}{dt} = \frac{k(1-X)^2 n_{A,0}}{V}$$

Since the assumption is that the system is adiabatic, there is no heat exchange with the surroundings, the heat generated (or absorbed) by the reaction raises (or lowers) the temperature. This can be encoded in equation as follows:

$$n_{\text{total}} C_p \frac{dT}{dt} = -\Delta H_{\text{rxn}} \frac{dn_A}{dt}$$

where n_{total} is the total number of moles, C_p is the molar heat capacity at constant pressure and ΔH_{rxn} is the heat of reaction (negative sign for exothermic reactions).

Finally, pressure rate $\frac{dp}{dt}$ can becalculated using the perfect gas law:

$$pV = n_{\text{total}} RT$$

After differentiating with respect to time, we obtain:

$$\frac{dp}{dt} = \frac{R}{V}\left(n_{\text{total}} \frac{dT}{dt} + T \frac{dn_{\text{total}}}{dt}\right)$$

Using the stoichiometry $\frac{dn_{\text{total}}}{dt}$ can be represented as

$$\frac{dn_{\text{total}}}{dt} = n_{A,0}(\nu - 1)\frac{dX}{dt}$$

where ν is the stoichiometric coefficient of products per mole of A reacted.

The three differential equations that accurately capture the dynamics of conversion rate, temperature rate, and pressure rate for a second-order reaction in an adiabatic reactor under the assumptions that there is no heat exchange (adiabatic conditions), that gasses behave as ideal gases, and that are volume of the reactor constant, are summarized in the table below (Table 1). Solving these equations simultaneously allows us to track how the conversion, temperature, and pressure in the reactor evolve over time.

Table 1. - Summary of Differential Equations

Type of differential equation	**Form of equation**
Conversion rate	$\frac{dX}{dt} = \frac{k(1-X)^2 n_{A,0}}{V}$
Temperature rate	$n_{\text{total}} C_p \frac{dT}{dt} = \Delta H_{\text{rxn}} \frac{k n_A^2}{V}$
Pressure rate	$\frac{dP}{dt} = \frac{R}{V}\left(n_{\text{total}} \frac{dT}{dt} + T n_{A,0}(\nu - 1)\frac{dX}{dt}\right)$

3. RESULTS

To validate our approach and ensure the accuracy of our methodology, we compared the modeled data with experimental data obtained by Duh et al. [4]. In their research, the authors utilized reaction calorimetry (RC) to investigate the exothermic esterification reaction of acetic anhydride with methanol. The experiments were carried out using a 2 dm³ Mettler RC1 AP01 glass reactor under different operating conditions: isothermal, temperature-programmed, and adiabatic. For our study, we focused exclusively on the adiabatic mode, as it replicates the safety scenario of a reactor experiencing cooling system failure. A summary of the key experimental data, essential for our calculations, obtained by Duh et al. [4] are provided in Table 2.

Table 2. - Key experimental data [4] for the verification of the proposed methodology.

Parameter	Value	Parameter	Value
Mass of methanol (m_{M})	16 g	Concentration of methanol (c_M)	0.6946 mol L^{-1}
Mass of acetic anhydride (m_{A})	756 g	Concentration of acetic anhydride (c_A)	10.298 mol L^{-1}
Heat of reaction (ΔH_{rxn})	-70000 $Jmol^{-1}$	Pre-exponential factor (k_0)	3.6×10^7 L mol^{-1} s^{-1}
Initial temperature (T_0)	293.15 K	Activation energy (E_a)	72600 J mol^{-1}
Specific Heat Capacity ($C_{p,\mathrm{M}}$)	2.53 $Jg^{-1}K^{-1}$	Specific Heat Capacity ($C_{p,\mathrm{A}}$)	1.72 J g^{-1} K^{-1}

3.1. Temperature change in the reactor

Since the concentration of acetic anhydride (c_{A}) is much greater than the concentration of methanol (c_{M}), the acetic anhydride concentration remains nearly constant throughout the reaction ($c_{\mathrm{A},0}$). Thus, we can apply the pseudo-first-order approximation:

$$\text{reaction rate} = -\frac{dc_{\mathrm{M}}}{dt} = k'c_{\mathrm{M}}$$

where: $k' = k(T)c_{\mathrm{A},0}$ and $c_{\mathrm{A},0}$ is concentration of acetic anhydride on the onset of reaction.

Temperature change per conversion (dT/dX) for adiabatic conditions can be calculated as follows:

$$\frac{dT}{dX} = \frac{(-\Delta H_{\mathrm{rxn}})n_{\mathrm{M}}}{C_{p,\mathrm{total}}}$$

After substituting the known parameters, the temperature change per conversion is given by:

$$\frac{dT}{dX} \approx 26.075\,\mathrm{K}$$

Now, we can define the temperature in the reactor at any given moment after the onset of the reaction:

$$T = T_0 + \frac{dT}{dX}X = T_0 + 26.075X$$

Conversion X can be calculated as follows:

$$X = \frac{c_{\mathrm{M},0} - c_M}{c_{\mathrm{M},0}}$$

where $c_{\mathrm{M},0}$ is concentration of methanol on the onset of reaction.

Hence, rate law in terms of X is:

$$\frac{dX}{dt} = \frac{1}{c_{\mathrm{M},0}}\left(-\frac{dc_{\mathrm{M}}}{dt}\right) = k'(1-X)$$

Now, the rate constant, as a function of X, can be expressed as follows:

$$k(T) = k_0\exp\left(-\frac{E_a}{R(T_0 + 26.075X)}\right)$$

Finally, differential equation for conversion can be written as follows:

$$\frac{dX}{dt} = k_0 c_{\mathrm{A},0}\exp\left(-\frac{E_a}{R(T_0 + 26.075X)}\right)(1-X)$$

These equations are nonlinear and coupled. An embedded Runge-Kutta method of order 5 [5] was used to solve the set of differential equations. The method was implemented in Python using the solve_ivp function. Obtained results are shown on Fig. 2.

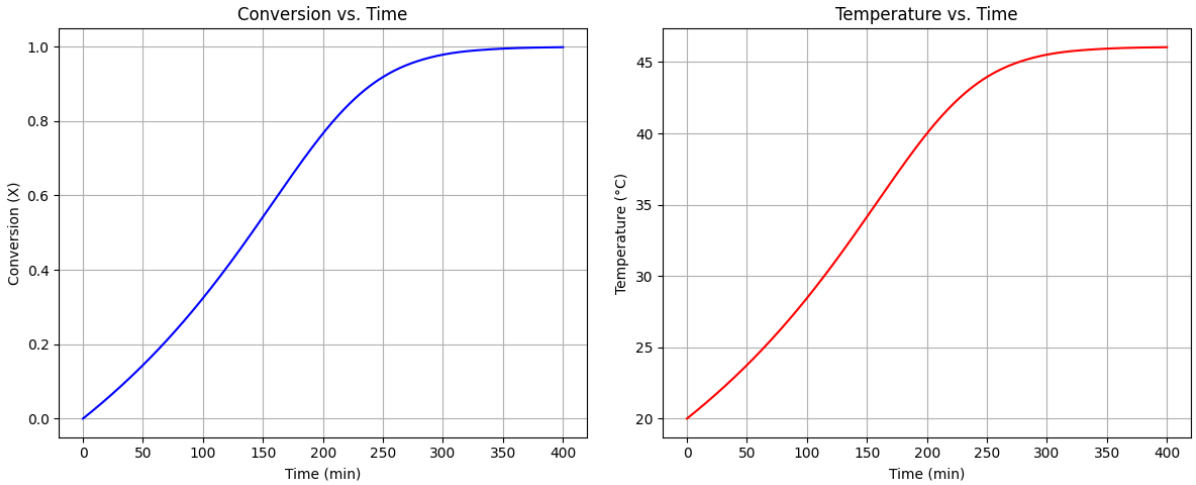

Fig. 2 - Conversion and Temperature in reactor as function of time

3.2. Pressure change in the reactor

In liquid-phase reactions, pressure changes are usually negligible because liquids are nearly incompressible, and there is minimal volume change. However, in a closed system where the temperature increases significantly (as in an adiabatic reaction), the vapor pressures of volatile components can increase, leading to a rise in the total pressure inside the reactor. Vapor pressure increases exponentially with temperature.

To calculate the pressure rate in the reactor (dP/dt) the Antoine equation was used to determine vapor pressures as functions of temperature. According to Dalton's law, the total pressure in the reactor was calculated as the sum of the partial pressures of the vaporized components and any initial pressure. The rate of pressure change was determined based on the rate of temperature change and the dependence of vapor pressure on temperature, using the chain rule:

$$\frac{dP}{dt} = \frac{dP}{dT} \cdot \frac{dT}{dt}$$

Hence, the change in pressure in the reactor from the onset of the reaction is shown in Fig. 3.

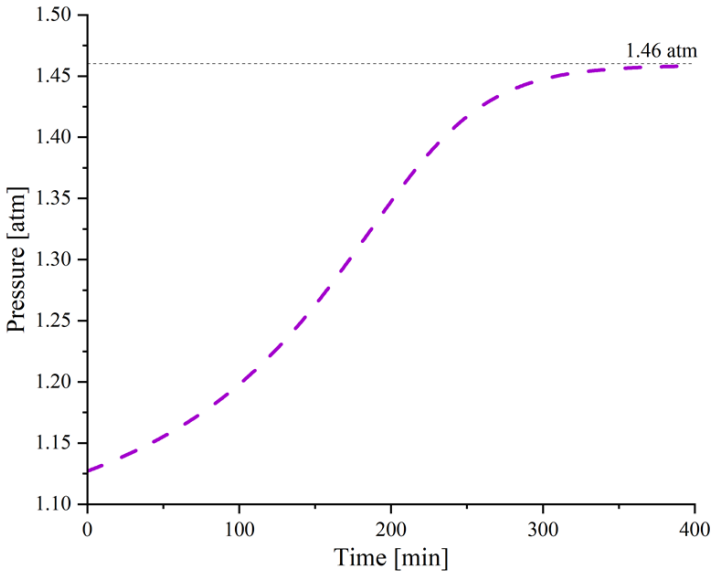

Fig.3 - Pressure change in the reactor as a function of time

The pressure is shown to increase from an initial value of approximately 1.1 atm and approaches a final value of ca. 1.5 atm. The pressure rises gradually over time, which is consistent with the progress of the reaction. As the esterification reaction proceeds, volatile components are produced, increasing the total vapor pressure in the system. The initial rate of pressure increase is relatively slowly. This may be attributed to the reaction starting with a lower conversion rate, where the production of volatile components is still limited. The temperature in the reactor is also likely lower during this stage, resulting in lower vapor pressures. The pressure rise accelerates during this period, reaching a steeper slope. This corresponds to the phase where the reaction is more active, with higher conversion rates and increased production of volatile substances. The temperature increase observed in the Fig. 2 likely contributes to this pressure buildup, as vapor pressure is temperature-dependent. As the reaction nears completion, the rate of pressure increase slows down, and the curve begins to flatten out, approaching a final equilibrium pressure of 1.46 atm. This suggests that the production of volatile components has been stabilized, and the system is reaching a steady state. The nearly constant pressure at the end indicates that the esterification reaction is essentially complete. The final pressure of 1.46 atm is a result of the equilibrium established between the vapor phase and the remaining liquid phase components. This value depends on the extent of reaction completion, the volatility of the products, and the temperature within the reactor.

4. RESULTS

The obtained results considering the temperature change over time were compared with the experimental data and the data obtained by simulation by Duh et al. [4] (Fig. 4).

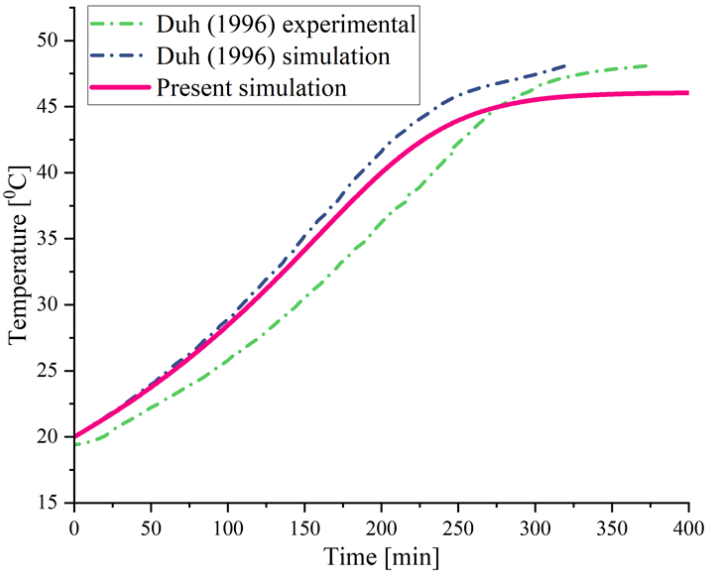

Fig.4 - Comparative results for the temperature change in the reactor as a function of time

The figure shows comparative results for the temperature change in the reactor over time during the esterification of acetic anhydride with methanol. All three curves exhibit a similar trend, with temperature increasing over time, indicating the progress of the exothermic esterification reaction. The temperature rises rapidly in the initial stages, then gradually levels off as the reaction reaches completion. The simulation results by Duh et al. [4], closely follow the experimental data, with some deviations. The experimental data show a slightly lower temperature rise at certain points, which could be due to experimental uncertainties or factors not fully accounted for, such as heat loss or non-ideal mixing. The present simulation aligns more closely with Duh et al. [4] simulation results than with the experimental data, especially at the higher temperature range and later stages of the reaction. However, there is a slight deviation in the initial temperature rise, where the present simulation predicts a more gradual increase compared to the data obtained by Duh et al. [4]. All curves converge to a final temperature around 45°C, indicating that the models accurately predict the endpoint of the reaction. This consistency across different simulations and experimental data supports the validity of the model for steady-state temperature prediction.

5. CONCLUSIONS

In this paper, a detailed methodology for calculating pressure and temperature changes during the esterification of acetic anhydride with methanol under adiabatic conditions is presented. This runaway reaction was selected because it has been extensively studied in the literature, and a lot of experimental data are available for verification. The data from Duh et al. [4] where both the simulation and experimental data for this particular esterification process are provided, were used to verify the obtained results.

The agreement between the present simulation and Duh's results [4] indicates that the methodology proposed herein provides a reliable representation of the esterification process, although small discrepancies in the early phase suggest potential improvements in capturing initial reaction kinetics or heat transfer effects. Additionally, the slight discrepancy between the experimental and simulation data highlights the importance of refining models to account for practical phenomena that may not be fully captured by theoretical approaches.

Data for the pressure rise in the reactor were not provided in Duh et al. [4] hence, the obtained results in this study couldn't be validated. However, the obtained results for the pressure rise in the small Toledo RC1 reactor seem realistic. It is important to emphasize that the pressure profile provides insights into the reaction kinetics and system dynamics. The initial slow rise in pressure indicates a controlled start to the reaction, while the steep increase in the intermediate stage reflects the reaction's

peak activity. The leveling off towards the end signifies the approach to equilibrium. These findings are consistent with the temperature profile, where the temperature increase aligns with the reaction's progress and contributes to the corresponding pressure changes.

The verification conducted in this study has paved the way for further research and validation of the model on other reactions for which experimental data are available. Additionally, this approach provides an opportunity for scaling up procedures to industrial reactors. This is particularly important for predicting the consequences of the worst-case scenario (temperature and pressure rise), such as a failure of the cooling system.

To conclude, since thermal runaway reactions are a significant hazard in chemical processing industries due to their potential to cause catastrophic failures, such as explosions, fires, and reactor overpressurization [3], it is crucial to implement rigorous safety measures to prevent and control thermal runaway scenarios. Simulation serves as a powerful tool in the chemical process industry, enhancing the understanding of complex reactions and providing a platform for testing safety measures before implementation. By incorporating simulations into safety protocols for preventing thermal runaway, risk can be better anticipated and managed, ultimately leading to safer operating conditions and reduced likelihood of catastrophic failures. This proactive approach not only enhances the safety of personnel and the environment but also improves operational efficiency by ensuring that processes are well understood and controlled.

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6. REFERENCES

[1] J. A. Barton, and P. F. Nolan, “Incidents in the chemicalindustries due to thermal runaways chemical reactions,” in *Safety of Chemical Batch Reactors and Storage Tanks*, A. Benuzzi, and J. M. Zaldivar (Eds.), Dordrecht, Netherlands: Kluver Academic Publishers, pp. 99-124, 1991.

[2] C. Vianello, E. Salzano, A. Broccanello, A. Manzardo, G. Maschio, “Runaway Reaction for the Esterification of Acetic Anhydride with Methanol Catalyzed by Sulfuric Acid,” *Ind. Eng. Chem. Res.*, vol. 57, no. 12, pp. 4195–4202, 2018. https://doi.org/10.1021/acs.iecr.7b05160

[3] L. Liu, J. Liang, J-c. Jiang, L. Ni, “Investigating the inherent safety designs of typical exothermic reaction processes,” *J. Loss Prev. Process Ind.*, vol. 76, 104586, 2022. https://doi.org/10.1016/j.jlp.2021.104586.

[4] Y.-S. Duh, C.-C. Hsu, C.-S. Kao, S. W. Yu, “Applications of reaction calorimetry in reaction kinetics and thermal hazard evaluation,” *Thermochim. Acta*, vol. 285, no. 1, pp. 67-79, 1996. https://doi.org/10.1016/0040-6031(96)02899-7.

[5] J. R. Dormand, and P. J. Prince, “A family of embedded Runge-Kutta formulae,” *J. Comput. Appl. Math.*, vol. 6, no. 1, pp. 19–26, 1980. https://doi.org/10.1016/0771-050X(80)90013-3.