Reaction Engineering and Design

Safety Module 1: *T2 Laboratories Explosion*†

This module is based on Example 13-6 in both

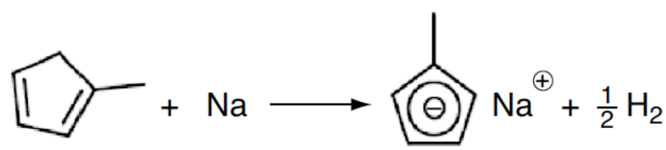
[1] H. S. Fogler, *Elements of Chemical Reaction Engineering*, 6th ed. Pearson, 2020.

[2] H. S. Fogler, *Essentials of Chemical Reaction Engineering*, 2nd ed. Prentice Hall, 2017.

Problem Statement: T2 Laboratories manufactured a fuel additive, methylcyclopentadienyl manganese tricarbonyl (MCMT), in a 2,450-gallon, high-pressure batch reactor utilizing a three-step batch process.

Aerial photograph of T2 taken December 20, 2007. (Courtesy of Chemical Safety Board.)

The first step in the process is the liquid-phase metalation reaction between methylcyclopentadiene (MCP) and sodium in a solvent of diethylene glycol dimethyl ether (diglyme) to produce sodium methylcyclopentadiene and hydrogen gas:



(1)

Hydrogen immediately comes out of the solution and is vented at the top in the gas head space.

What Happened

On December 19, 2007, when the reactor reached a temperature of 455.4 K (360°F), the process operator could not initiate the flow of cooling water to the cooling jacket. Thus, the expected cooling of the reactor was not available and the temperature in the reactor continued to rise. The pressure also increased as hydrogen continued to be produced at an increased rate, to the point that the reactor's pressure control valve system on the 1-inch diameter hydrogen venting stream could no longer maintain the operating pressure at 50 psig (4.4 atm). As the temperature continued to increase further, a previously unknown exothermic reaction of the diglyme solvent that was catalyzed by sodium accelerated rapidly.

† This example was coauthored by Professors Ronald J. Willey, Northeastern University, Michael B. Cutlip, University of Connecticut, and H. Scott Fogler, University of Michigan, and published in Process Safety Progress, 30, 1 (2011).

$$CH_3 - O - CH_2 - CH_2 - O - CH_2 - CH_2O - CH_3 \xrightarrow[Na]{} 3H_2 + misc(l) \& (s) \tag{2}$$

This reaction produced even more hydrogen, causing the pressure to rise even faster, eventually causing the rupture disk which was set at 28.2 atm absolute (400 psig), to break, in the 4-inch diameter relief line of H_2. Even with the relief line open, the rate of production of H_2 was now far greater than the rate of venting, causing the pressure to continue to increase to the point that it ruptured the reactor vessel initiating a horrific explosion. The T2 plant was completely leveled and four personnel lives were lost. Surrounding businesses were heavily damaged and additional injuries were sustained.

The model equations and the parameters are given in Example 13-6 of the chemical reaction engineering textbook listed above.

Watch the Video: *(https://www.youtube.com/watch?v=C561PCq5E1g/)*

Incident Report Available At: *(https://www.csb.gov/file.aspx?DocumentId=5661)*

(a) It is important that chemical engineers have an understanding of what the accident was, why it happened and how it could have been prevented in order ensure similar accidents may be prevented. Applying a safety algorithm to the accident will help achieve this goal. In order to become familiar with a strategy for accident awareness and prevention, view the Chemical Safety Board video on the T2 Laboratories explosion and fill out the following algorithm. See definitions on the last page. If necessary, view the incident report.

Safety Analysis of the Incident

Activity: ____

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Hazard: ____

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Incident: ____

Initiating Event: ____

Preventative Actions and Safeguards: ____

____

Contingency Plan/ Mitigating Actions: ____

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Lessons Learned: ____

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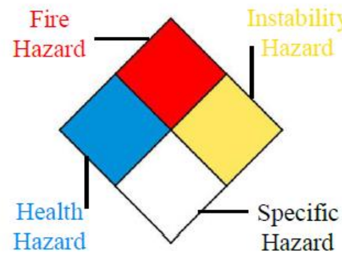
(b) Go to the Living Example Problems (LEPs) for chapter 13 (*http://www.umich.edu/~elements/6e/13chap/live.html*). Load Wolfram/Polymath for Example 13-6 and run the simulation for the case where the reactor cooling fails to work (UA = 0). Use

Wolfram/Polymath to vary parameters and then plot and analyze the reactor temperature and the head-space pressure as a function of time along with the reactant concentrations similar to that shown in Figure E13-6.3(c) of **[1], [2].**

(c) How can this accident be used to prevent future accidents?

(d) What would have happened if the solvent did not decompose?

(e) Review the information in the NFPA Diamond tutorial. After reviewing the information, visit the CAMEO Chemicals website and fill out the blank NFPA Diamond to the right for hydrogen.

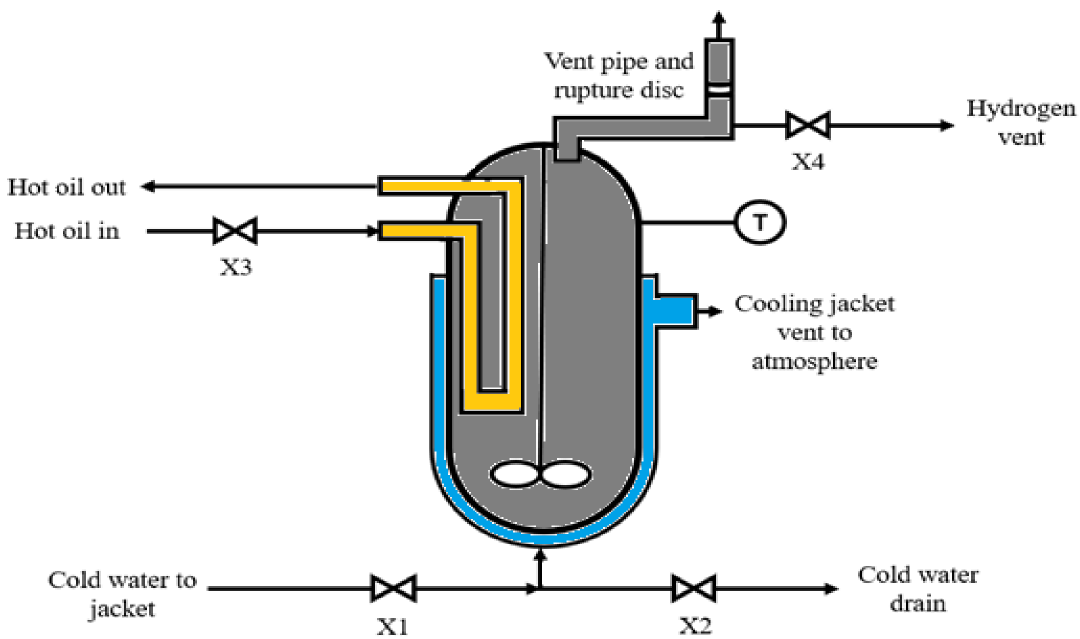


Parts (f)-(h) are based on industry practices used to assess process safety. For more information on process safety and its importance in chemical engineering, please visit the University of Michigan SafeChE website here. *It is recommended that professors only assign 1-2 of the following parts due to the similar nature of the questions.*

(f) Review the information in the BowTie diagram tutorial. After reviewing the information, create a BowTie diagram for the explosion at T2 Laboratories.

(g) A HAZOP study is structured analysis of process design to identify potential vulnerabilities in a facility. Review the background on how to conduct a HAZOP study here before completing one for the following system. It is important to note that not all guidewords and parameters will be relevant for different systems. Some information is given here for guidance:

System to consider: The batch reactor and its connected valves



The inlet of water to the cooling jacket is controlled by valve X1 and the drain from the cooling jacket is controlled by valve X2. The hot oil flow is controlled by valve X3 and the hydrogen vent is controlled by the pressure control valve X4. The temperature is measured using the temperature sensor T.

Process parameters to consider: Level, Flow Rate of Cooling Water, Temperature, Pressure, Closing of Oil Input Valve X3, Composition

(i) Fill out the HAZOP chart as shown in the tutorial. Some other information has been filled out here for you.

Guideword + Parameter = Deviation	Causes	Consequences	Safeguards	Recommendations
More Level	Charging more feed in the batch reactor			
Less/No Flow Rate of cooling water to the jacket				
More (Higher) Temperature	Failure of cooling system			
	High amount of reactants which increases the heat release			
More (Higher) Pressure				
Later closing of hot oil input valve	Failure of control system leading to late closure of valve X3			
Other composition				

(ii) When conducting a HAZOP, you will often find combinations of guidewords and parameters that describe a possible situation for the system that is not hazardous. For the given process parameters, give an example, explain why the situation is not hazardous, and describe another consequence that could occur. *HINT: Consider process efficiency*

(iii) Write a short conclusion on some takeaways from completing a HAZOP for this system and recommendations you would make.

(h) A Layers of Protection Analysis (LOPA) is a semi-quantitative study to identify available safeguards and determine if the safeguards sufficiently protect against a given risk.

Review the background on how to conduct a LOPA study here before filling the table out for the system described in this module. Some information is given for guidance:

- Assume that the plant can only accept a moderate risk
- The explosion at T2 Labratories resulted in 4 fatalities and significant damage to the plant

LOPA Study for T2 Labs Explosion		
Initiating Event	Cause:	Cooling water failure
	Consequence:	High temperature and pressure inside the reactor that can lead to rupture and explosion
	FOIE:	
IPL(s)	Description of IPL_1, IPL_2, ...	Rupture Disk
	$PFD = PFD_1 \times PFD_2 \times ...$	
MCF	MCF = FOIE x PFD	
	Category of MCF:	
Severity	Impact:	Multiple fatalities and extensive plant damage
	Category:	
Risk	Type of risk:	
	Acceptable / Unacceptable?	
If risk evaluated above is unacceptable, please continue below:		
Proposed IPL(s) (P-IPL(s))	Description of P-IPL_1, P-IPL_2, ...	
	P-PFD = P-PFD_1 x P-PFD_2 x ...	
MCF	MCF = FOIE x PFD x P-PFD	
	Category of MCF:	
Risk	Type of risk:	
	Acceptable / Unacceptable?	

(i) Describe what was the most unsettling to you about the incident.

Wolfram

Click here to download Wolfram CDF Player for free.
Click here to view CDF installation tutorial.
Click here to download Wolfram code for this module.

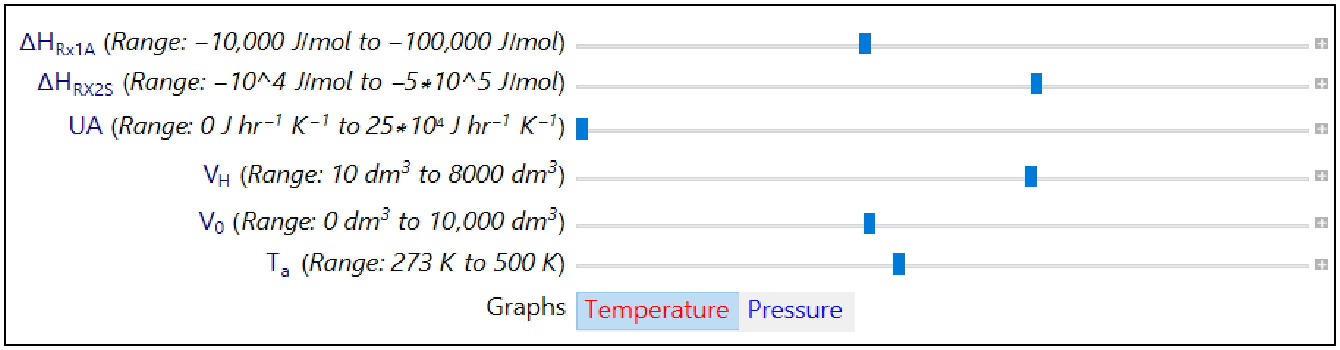


Figure 1.1 Wolfram sliders.

Sample output graph:

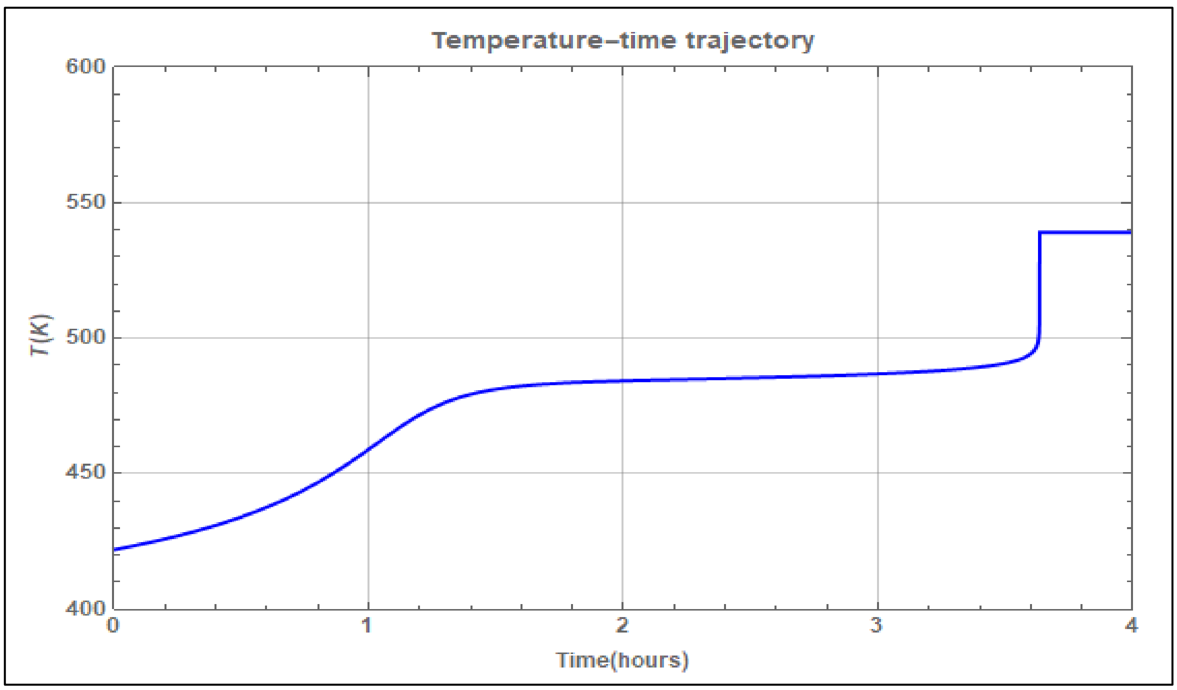


Figure 1.2 Temperature of the reactor with time.

(i) What is the minimum value of UA such that there would be no decomposition of the diglyme solvent? Assume coolant supply is working and the diglyme solvent begins to decompose at T = 490K.

(ii) Find a value of the heat of reaction for the secondary reaction of diglyme (ΔH_{RX2S}), below which no explosion would have occurred. This is referring to reaction (2) above.

(iii) Write a set of conclusions after you have varied all the parameter values.

Definitions

Activity: The process, situation, or activity for which risk to people, property or the environment is being evaluated.

Hazard: A chemical or physical characteristic that has the potential to cause damage to people, property, or the environment.

Incident: What happened? Description of the event or sum of the events along with the steps that lead to one or more undesirable consequences, such as harm to people, damage to property, harm to the environment, or asset/business losses.

Initiating Event: The event that triggers the incident, (e.g., failure of equipment, instrumentation, human actions, flammable release, etc.). Could also include precursor events, (e.g., no flow from pump, valve closed, inadvertent human action, ignition). The root cause of the sum events in causing the incident.

Preventative Actions and Safeguards: Steps that can be taken to prevent the initiating event from occurring and becoming an incident that causes damage to people, property, or the environment. Brainstorm all problems that could go wrong and then actions that could be taken to prevent them from occurring.

Contingency Plan/ Mitigating Actions: These actions occur after the initiating event. They are steps that reduce or mitigate the incident after the preventative action fails and the initiating event occurred.

Lessons Learned: What we have learned and can pass on to others that can prevent similar incidents from occurring

BowTie Diagram: A qualitative hazard analysis tool through which potential problems and consequences associated with a hazard are studied through a pictorial representation. Necessary preventive and mitigating barriers are determined to reduce the process safety risk.

Hazard and Operability Study (HAZOP): A qualitative hazard analysis tool that uses a set of guide words to determine whether deviations from design or operating intent can lead to undesirable consequences. The existing safeguards are evaluated and if required, actions are recommended to mitigate the consequences.

Layer of Protection Analysis (LOPA): A semi-quantitative study that determines initiating event frequency, consequence severity, and likelihood of failure of independent protection layers (IPLs) to calculate the risk of a scenario. If the existing risk is intolerable, then additional IPLs are suggested to bring down risk to an acceptable level.

Table 1.1 Nomenclature

Symbol	Description	SI Unit
P	Reactor pressure	Pa
T	Reactor temperature	K
ΔH_{Rx1A}	Heat of reaction for Reaction 1	$J.mol^{-1}$
ΔH_{RX2S}	Heat of reaction for Reaction 2	$J.mol^{-1}$
UA	Overall heat transfer coefficient multiplied by heat transfer area (for reactor-cooling jacket system)	$J.s^{-1}.K^{-1}$
V_0	Volume of reactor in the liquid	m^3
V_H	Volume of head space	m^3
T_a	Temperature of water in cooling jacket	K
Q_g	Heat generated in the reactor	W
Q_r	Heat removed from the reactor	W
C_A	Concentration of methylcyclopentadiene	$mol.m^{-3}$
C_B	Concentration of sodium	$mol.m^{-3}$
C_S	Concentration of diglyme	$mol.m^{-3}$