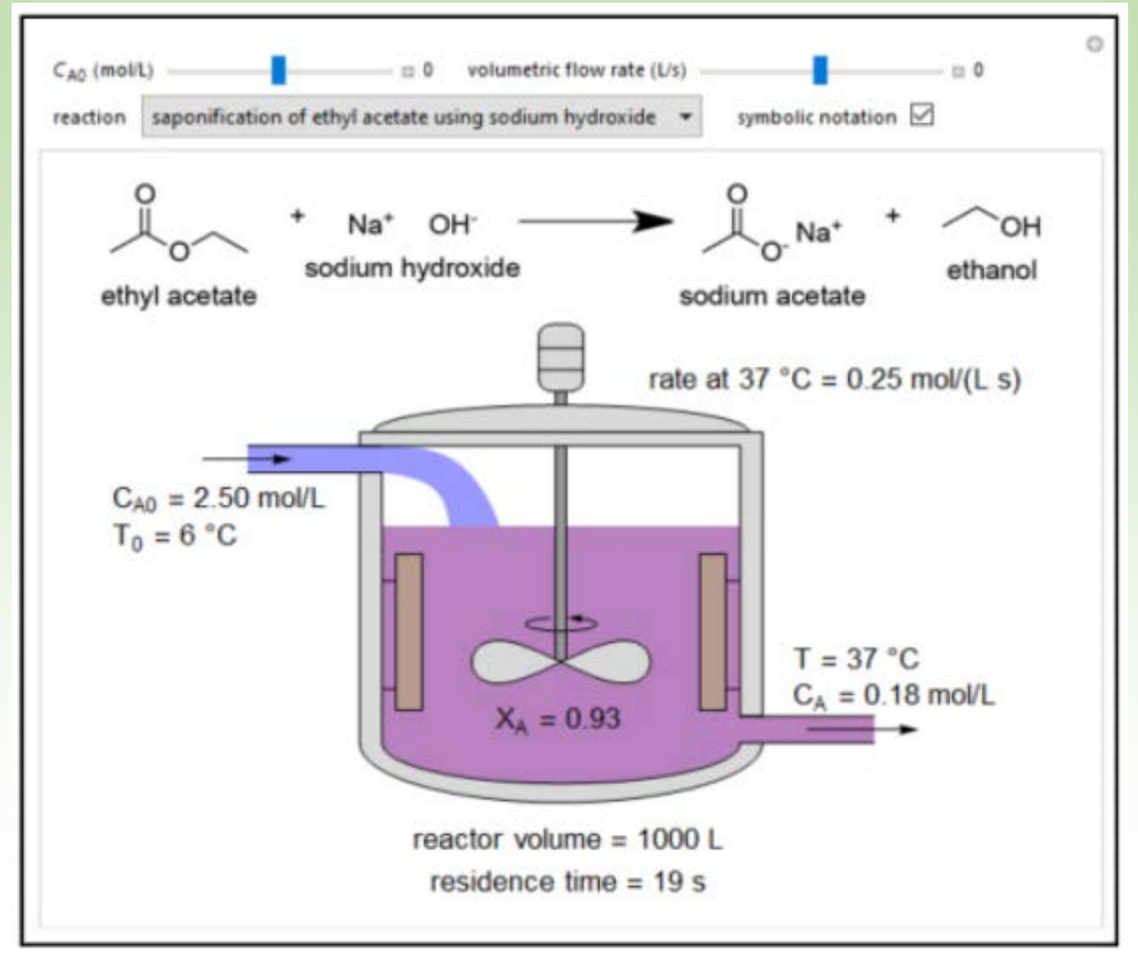
Teaching Advanced Design Concepts Using MATLAB Applications

Jorge E. Gatica

Department of Chemical and Biomedical Engineering
Washkewicz College of Engineering



INTRODUCTION

Exothermic chemical reactions are common in the Chemical Processing Industry (CPI). Effective and safe design of these processes often requires cooling for temperature control strategies. When the energy generated by the chemical reaction exceeds the ability of heat removal, a process referred to as “thermal runaway” ensues. A reactor runaway is characterized by an exponential increase in the rate of heat generation, temperature, and pressure. Pressure build-up is typically observed during a runaway due to an increasing vapor pressure of liquid components and by the production of non- condensable gases. if pressure build-up exceeds the design pressure of the unit or safety layers, an industrial disaster follows. Besides the loss of reactor units due to an uncontrolled conversion process, a runaway reaction may lead to severe damages, thermal explosion, injuries, environmental impacts, and in cases loss of lives.

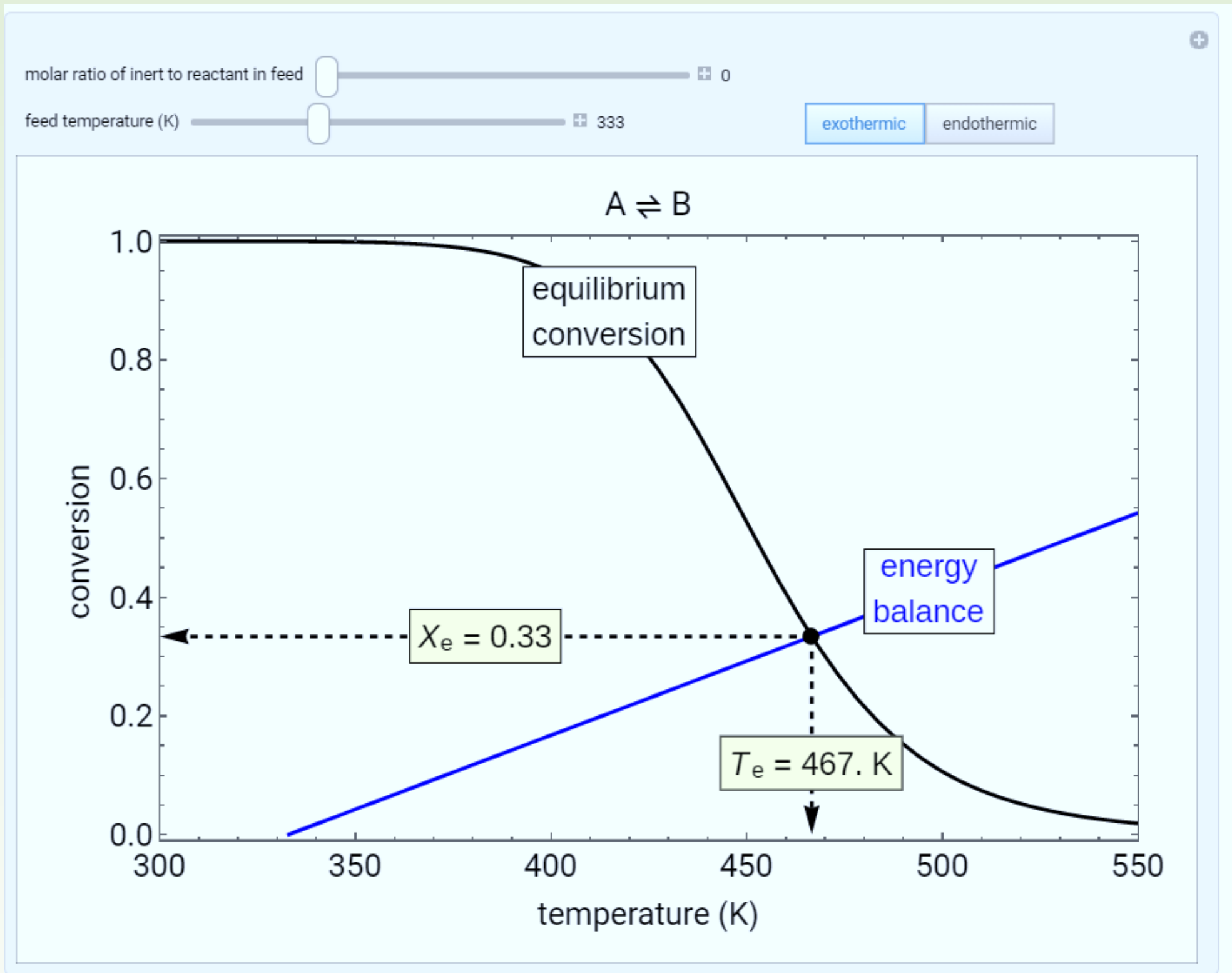
OBJECTIVES

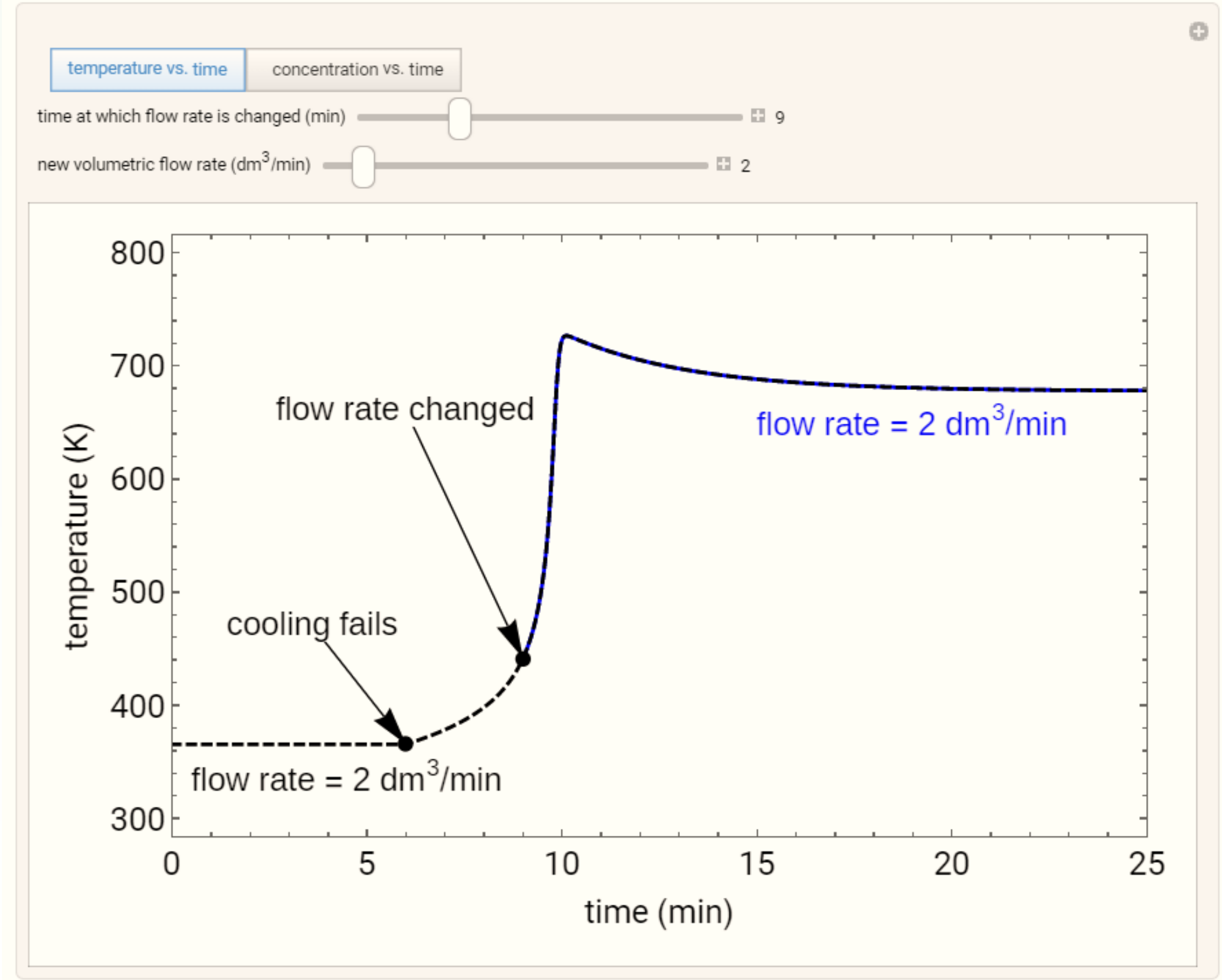
A Chemical Reactor Thermal Runaway condition is the result of a complex interaction between reactor design variables. The detailed solution of equations governing this phenomenon requires advanced (graduate-level) background.

The main objective of this teaching resource is to provide undergraduate students with a tool they can use to examine the effect of different variables on reactor performance and safety.

The MATLAB programming environment has the flexibility of adding portability to applications (apps) through intuitive graphical user interfaces (GUI)..

Two illustrations of applications developed by LeanChemE (www.learncheme.com) are shown below, these applications were developed using Mathematica (Wolfram CDF Player). At CSU we use MATLAB App Builder (Mathworks, Inc.)

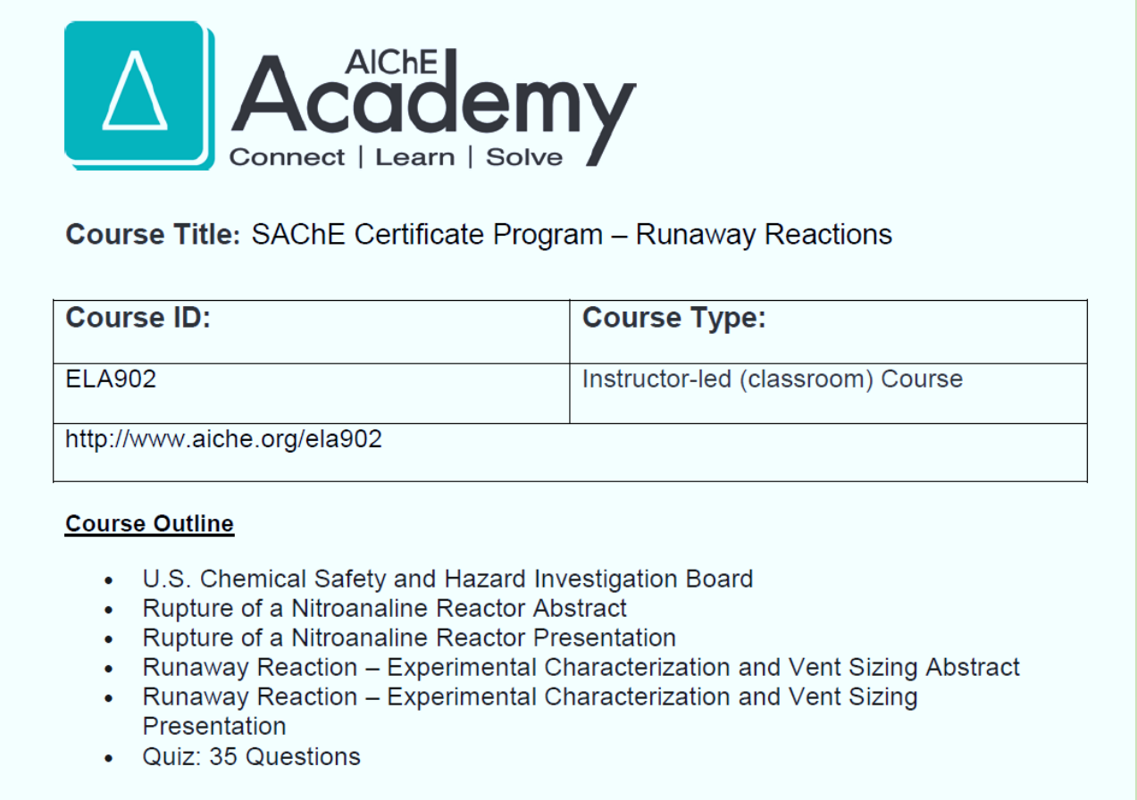




FORMULATING THE TEACHING MODULE

The student will complete a special assignment focusing on the Investigation, Presentation, and Analysis of an Industrial Accident stemming from a “Runaway Reactor.” This assignment includes:

- Completion of the Safety and Chemical Engineering Education (SAChE) Process Safety Certificate “Runaway Reactions”
- Description of an Industrial Accident caused by this type of event
- Analysis of the Design flaws leading to the Accident
- Presentation (before their peers) of the Reactor Thermal Runaway incident
- Submitting a Final Report



AIChE Academy
Connect | Learn | Solve

Course Title: SAChE Certificate Program – Runaway Reactions

Course ID:	**Course Type:**
ELA902	Instructor-led (classroom) Course
http://www.aiche.org/ela902	

Course Outline

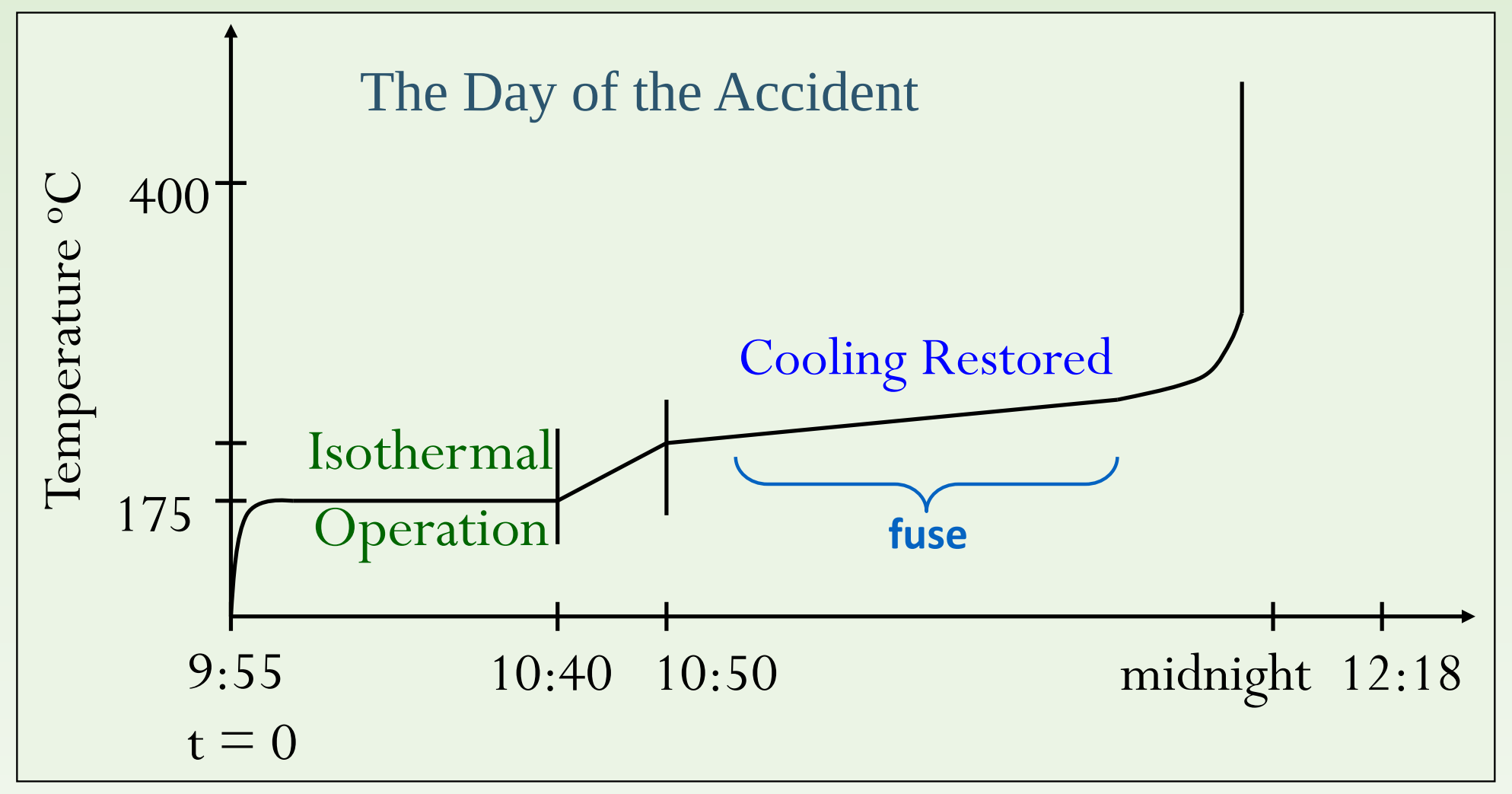
- U.S. Chemical Safety and Hazard Investigation Board
- Rupture of a Nitroanaline Reactor Abstract
- Rupture of a Nitroanaline Reactor Presentation
- Runaway Reaction – Experimental Characterization and Vent Sizing Abstract
- Runaway Reaction – Experimental Characterization and Vent Sizing Presentation
- Quiz: 35 Questions

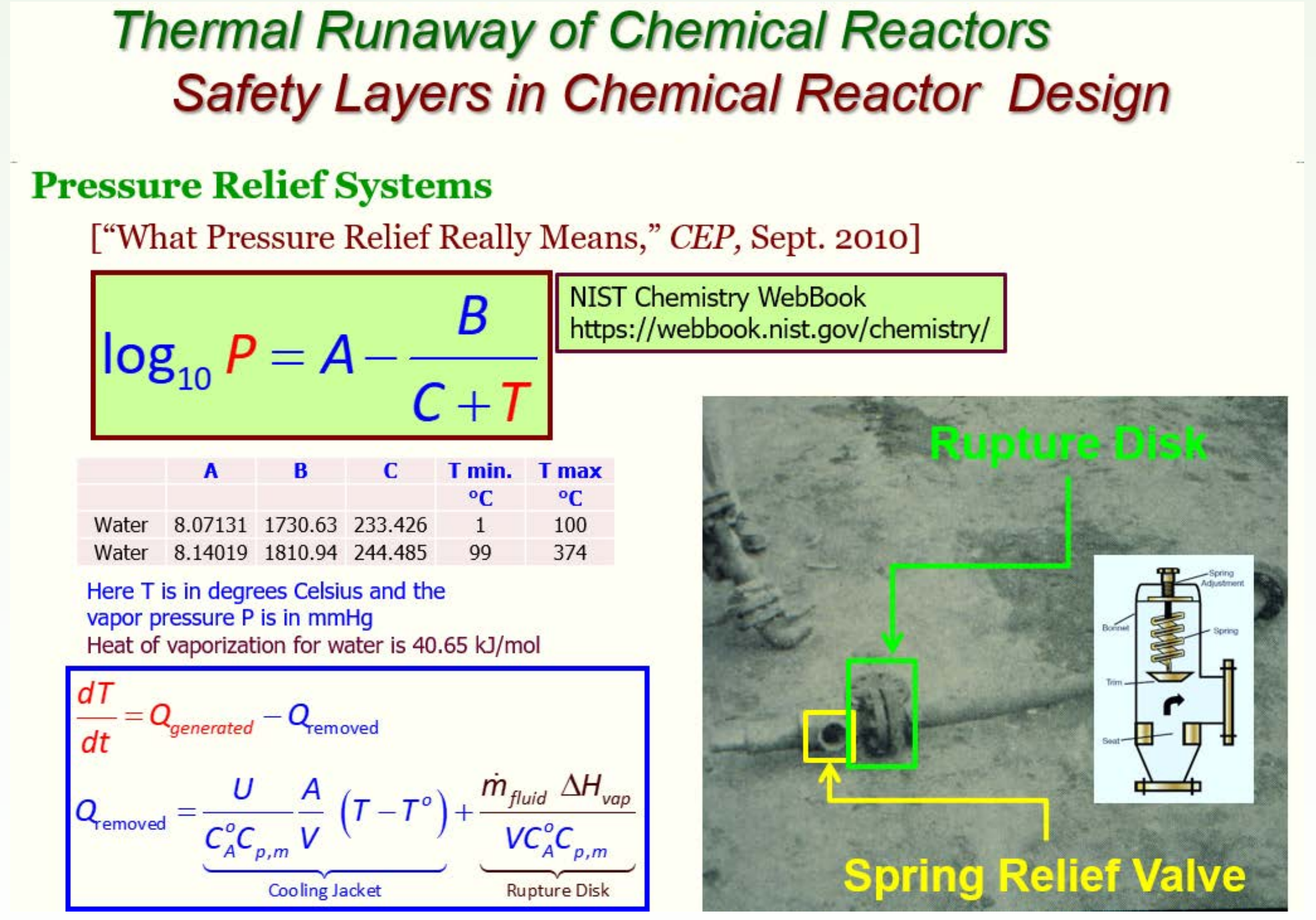
CASE STUDY

August 1969 at 12:18 AM a reactor inside a two-story building at a Monsanto Plant (in Sauget, Illinois) exploded. The blast was due to a reactor rupture - a reactor used in the synthesis of ortho-nitroaniline from orthonitrochlorobenzene (abbreviated as ONCB) and ammonia.

There were only 4 men inside the building at the time of the accident. All four miraculously survived. One man was disabled 6 months. The others lost a total of 10 days. One witness described the explosion as something like a tornado or four or five freight trains hurling at you. Another recalled hearing a hissing sound, followed by the explosion, followed by the loss of his shoes, which were blown off in the blast. “If you can imagine what hell is like, you have a rough idea how it was.” This was a quote from one of the 4 workmen at the scene when the accident occurred. The East St. Louis City hall, located 3 miles north, had one window broken, and residents were awakened from their sleep in Belleville a community located 10 miles southwest of St. Louis.

IMPLEMENTATION and DEMONSTRATION





Thermal Runaway of Chemical Reactors
Safety Layers in Chemical Reactor Design

Pressure Relief Systems

[“What Pressure Relief Really Means,” *CEP*, Sept. 2010]

$$\log_{10} P = A - \frac{B}{C+T}$$

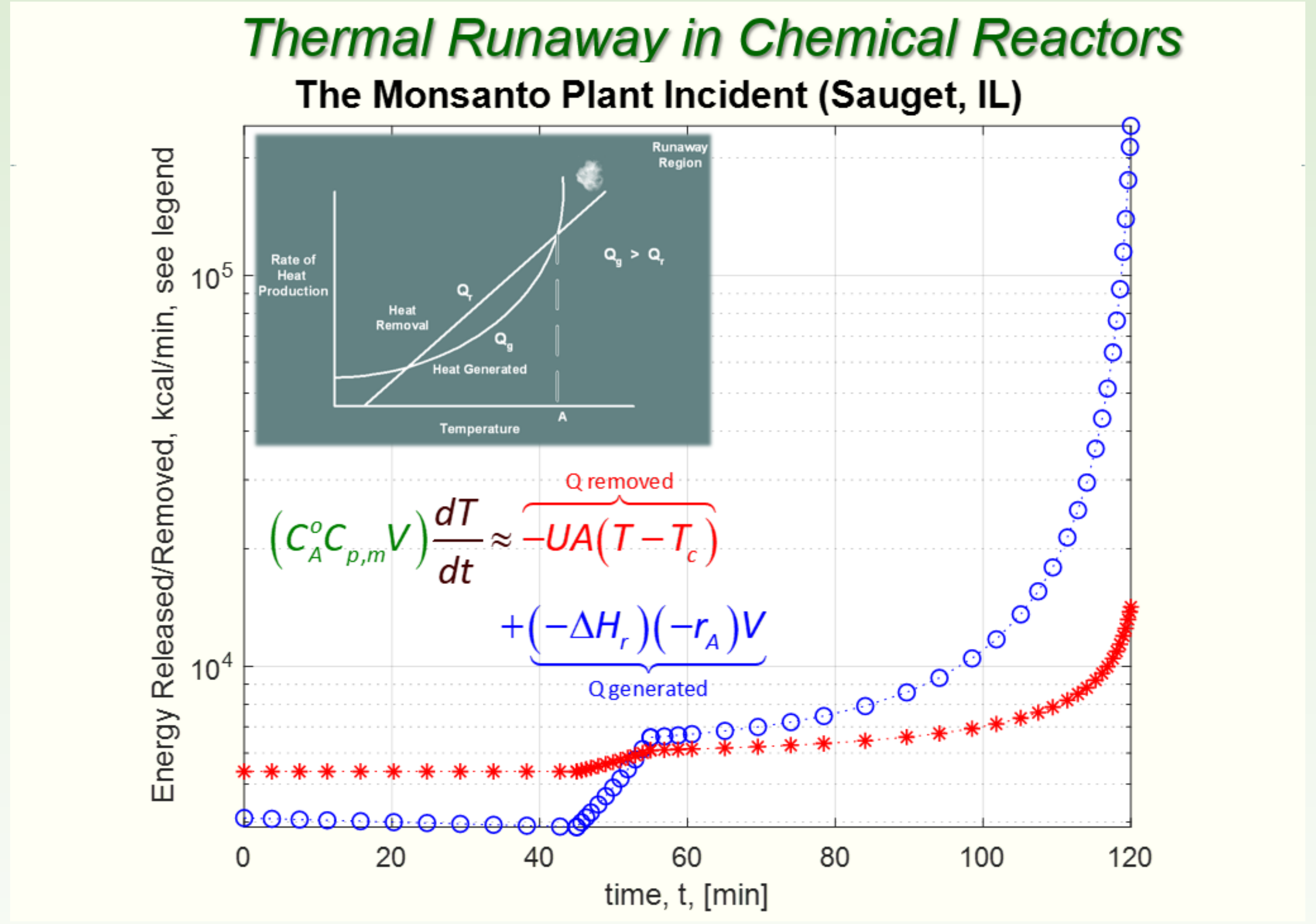
NIST Chemistry WebBook
https://webbook.nist.gov/chemistry/

	A	B	C	T min. °C	T max °C
Water	8.07131	1730.63	233.426	1	100
Water	8.14019	1810.94	244.485	99	374

Here T is in degrees Celsius and the vapor pressure P is in mmHg
Heat of vaporization for water is 40.65 kJ/mol

$$\frac{dT}{dt} = Q_{generated} - Q_{removed}$$

$$Q_{removed} = \underbrace{\frac{U}{C_A^o C_{p,m}} \frac{A}{V} \left(T - T^o\right)}_{\text{Cooling Jacket}} + \underbrace{\frac{\dot{m}_{fluid}\, \Delta H_{vap}}{V C_A^o C_{p,m}}}_{\text{Rupture Disk}}$$

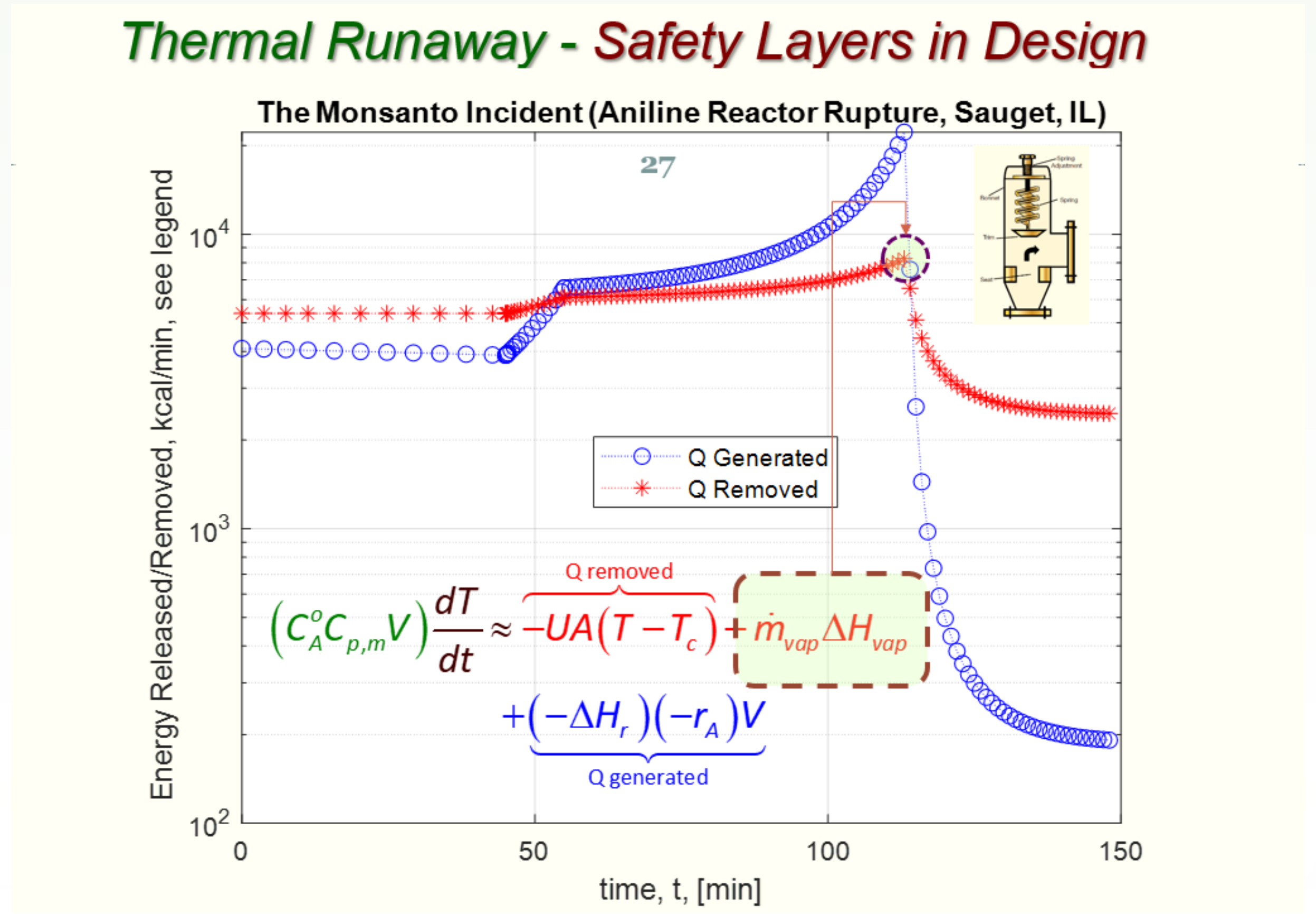


Thermal Runaway in Chemical Reactors

The Monsanto Plant Incident (Sauget, IL)

$$\left(C_A^o C_{p,m} V\right)\frac{dT}{dt} \approx \overbrace{-UA\left(T - T_c\right)}^{\text{Q removed}} \underbrace{+\left(-\Delta H_r\right)\left(-r_A\right)V}_{\text{Q generated}}$$

We note that the pressure-safety-relief disk should have ruptured when the critical (rupture) pressure (~ 700 psi) but did not and the temperature continued to rise. If the disk had ruptured, at 700 psi we know from fluid mechanics that the maximum mass flow rate, , out of the 2-in. orifice to the atmosphere (1 atm) would have been 830 kg/min at the time of rupture.

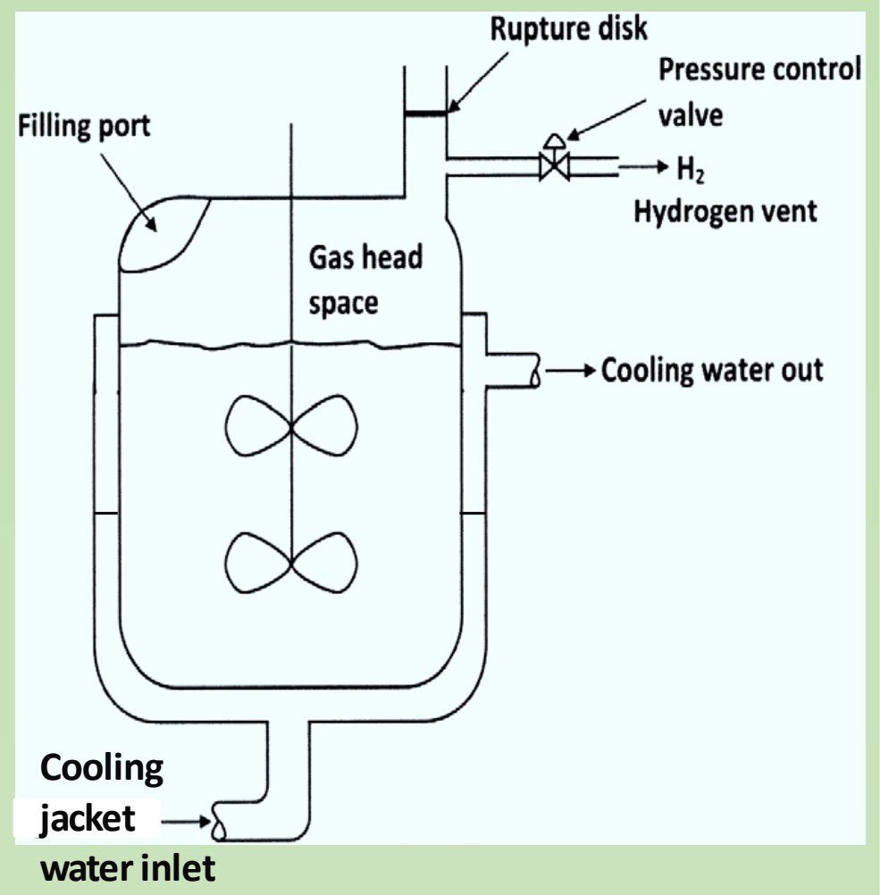


Thermal Runaway - Safety Layers in Design

The Monsanto Incident (Aniline Reactor Rupture, Sauget, IL)

$$\left(C_A^o C_{p,m} V\right)\frac{dT}{dt} \approx \overbrace{-UA\left(T - T_c\right)}^{\text{Q removed}} + \boxed{\dot{m}_{vap}\Delta H_{vap}} \underbrace{+\left(-\Delta H_r\right)\left(-r_A\right)V}_{\text{Q generated}}$$

CONCLUSIONS and FUTURE DEVELOPMENTS



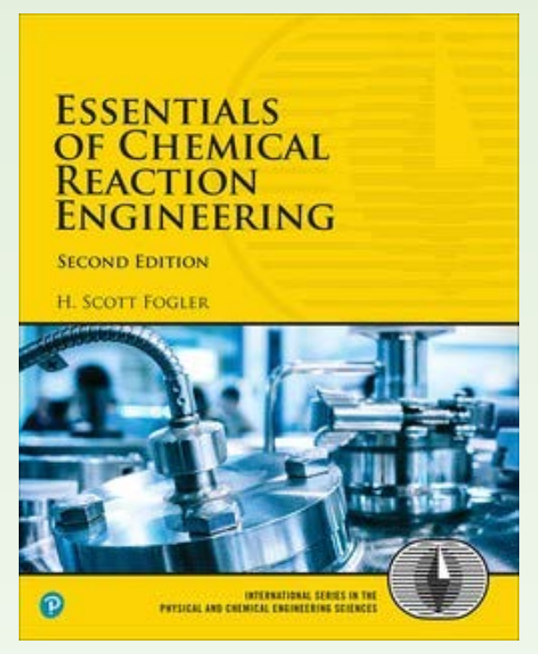
- A MATLAB Application (app) for a thermal runaway case study was successfully developed.
- The app allowed students to examine fundamental reactor design criteria that can have implications in thermal runaway scenarios.
- Students can visualize the importance and effect of fundamental concepts such as (1) cooling capacity design for non-isothermal reactor operation, (2) identification of the “point-of-no-return” condition, (3) evacuation times once the “point-of-no-return” condition is reached, (4) design of pressure-control valves, and (5) design of rupture disks.

Chemical reactors are known to be the key unit in determining the feasibility, marketability, and profitability of most processes involving chemical transformations. This design scenario was selected for several reasons, chief among them were (1) its numerical complexity, (2) programming required to implement a robust numerical solution, and (3) its relevance in the design of a classical unit (typically at the center of any chemical process). Extension to similar design scenarios, and other processing units is planned for next semester.

OPEN ACCESS RESOURCES

The class selected to develop and test the first teaching module was the upper-level junior class: CHE 404 Chemical Reactor Design. This class has enrollments ranging between 40-60 students.

The textbook adopted for this class is a very popular textbook used in the large majority of Chemical Engineering Programs around the world:



“Essentials of Chemical Reaction Engineering”
by H. Scott Fogler (2nd Ed., 2017)
Pearson Higher Education
ISBN: 9780134663906
https://www.pearson.com/us/higher-education/

Suggested Retail Price
$130 (paper), $104 (digital)

The Michael Schwartz Library provides free access though the O’Reilly textbook subscription (www.oreilly.com/library/view/essentials-of-chemical/9780134663906/)

This access provides significant savings for students. The O’Reilly subscription, however, does not include any of the supplementary materials; which motivated the development of these modules.

ACKNOWLEGMENTS

The American Institute of Chemical Engineers (AIChE) provides free membership and access to educational resources to Chemical Engineering majors (www.aiche.org/students/student-leader-resources)

Process Safety Certificates are free of charge for Student members of the American Institute of Chemical Engineers (www.aiche.org/ccps/education)

LeanChemE (www.learncheme.com) , an NSF-supported educational initiative at the Colorado State University (Boulder), provides resources for the development of interactive modules and screencasts for Chemical Reactor Design.

The modules are being developed using the MATLAB Programming Environment (platform supported at CSU)

This project was completed under initiatives sponsored by the CSU Center for Teaching Excellence, and the 2020 Textbook Affordability Program (Michael Schwartz Library).

Support and resources are gratefully acknowledged.