
FOUNDATIONS OF SPIRITUAL AND PHYSICAL SAFETY WITH CHEMICAL PROCESSES

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1 Introduction

Learning Outcomes

- Become familiar with the course setup and topics
- Understand what you are asked to do to complete the course
- Understand where the course content is: (Learning Suite, Website, Book)
- Understand the importance of being physically and spiritually safe

Reading

- [Safety in Jesus Christ Introduction](#)
- Foundations of Spiritual and Physical Safety: with Chemical Processes by Clint Guymon:
 - Preface
 - Chapter 1: Spiritual and Physical Safety Framework
- [Becoming Men and Women of Integrity](#)

1.1 Stewardship and Safety in Jesus Christ

Jesus Christ taught us to love one another (John 13:34-35) and to care for our bodies as they are temples (1 Corinthians 6:19-20). As stewards of our physical and spiritual well-being, we have a responsibility to ensure safety in all aspects of our lives. This course explores the principles of safety from both spiritual and physical perspectives, emphasizing the importance of ethical decision-making and risk management.

The course is divided up into five modules:

- Module 1: Spiritual Safety and Ethics
- Module 2: Understanding Harm and Risk
- Module 3: Systematic Hazards Analysis
- Module 4: Critical Process Safety Information
- Module 5: Safeguards & Regulations

1.2 Course Materials

- Learning Suite,
 - Please be patient, Learning Suite will be updated throughout the semester
- This Course GitHub Website,
 - Please be patient, this website will be updated throughout the semester
- Foundations of Spiritual and Physical Safety: with Chemical Processes by Clint Guymon
- Other helpful texts:

- The Book of Mormon
- The Bible
- Chemical Process Safety by Daniel Crowl and Joseph Louvar
- What Went Wrong? Case Histories of Process Plant Disasters and How They Could Have Been Avoided by T. Kletz

1.3 Work Expectations

- Lectures (3x's per week),
- Quizzes (In class, 3x's per week based on the reading material),
- Classwork (In class, 0-2x's per week),
- Reading material (prior to each class,)
- Homework (3x per week),
- Mid-term Exams (2-3),
- Final Exam
- Projects
 - Book review,
 - Safety and Ethics Evaluation (analysis, team writeup, and presentation)

1.4 Class Organizations

- Class Groups
- Project Groups

1.5 Course Grades

- Quizzes
 - 5 lowest scores dropped
- Classwork
- Homework
- Exams
 - Midterms
 - Final
- Projects
 - Book Review
 - Safety or Ethics Evaluation

1.6 Chemical Engineering Career Outlook

Hopefully from the above you can see that BYU chemical engineers are unique and in demand. The skills you will learn in this class will help you to be successful in your career.

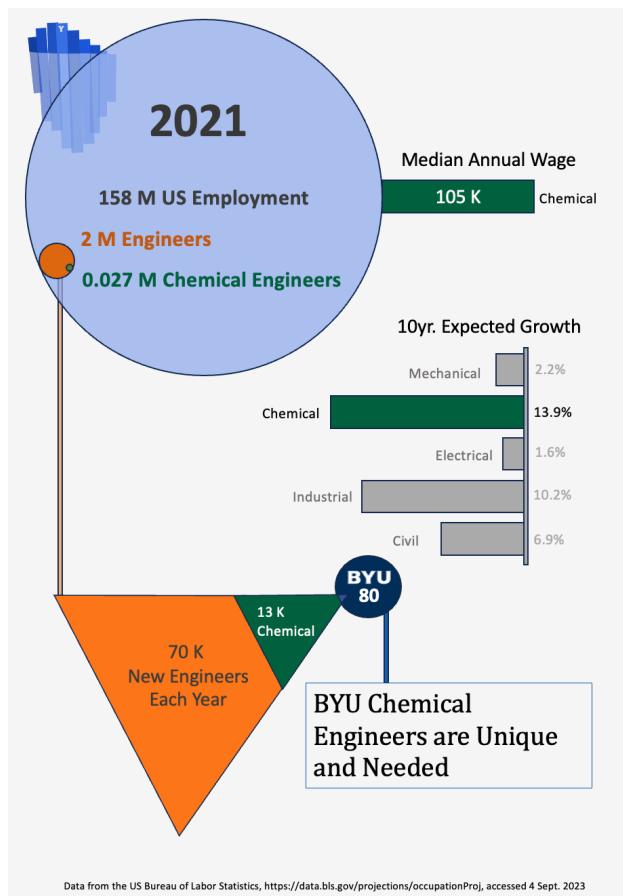


Figure 1: Chemical engineering has a strong career outlook.

1.7 Current Worldwide Problems in Engineering

Chemical Engineers are poised to help in each of these areas:

- Energy
 - Worldwide energy demands are growing
 - We need to use fossil fuels more efficiently and capture more of the biproducts
 - [Energy.gov](#)
 - [Deseret News Article on Potential Energy Crisis](#)
 - Fry, Memmott, Baxter, Rappleye, Wheeler, and Lignell
- Chemical Production
 - We can continue to improve chemical production processes
 - [Chemical and Engineering News](#)
 - Argyle, Hedengren, Knotts, Nickerson, Seo, Tree, Wilding
- Health
 - We need to improve health care delivery and care
 - [World Health Organization](#)
 - Bundy, Pitt, and Lewis

- Water
 - We need to improve water treatment, distribution, and conservation.
 - [World Health Organization](#)
- Transportation - How do we better move people and goods around the world?
- Environment - How do we efficiently continue improving our environment?
 - Plastics production and waste handling and reuse needs improvement.
 - [Environmental Protection Agency](#)
- Security - How do we continue to adapt and peacefully protect people from threats?
- Exploration, Food, and more...

You are the engineers that will work to improve societies' and individuals' quality of life around the world. Importantly, you can also help gather Israel and prepare the world for the second coming of Jesus Christ.

Action Items

Ask God to help you learn and implement principles to be physically and spiritual safe at home and at work.

2 Spiritual Safety and Ethics

Learning Outcomes

- Understand the importance of integrity
- Identify different ethics approaches
- Review the Code of Ethics of the American Institute of Chemical Engineers
- Identify principles of the gospel of Jesus Christ that relate to living a life of integrity and ethics in Chemical Engineering
- Identify the influence of the Holy Ghost and how to heed the prophets invitation to be able to live by truth in an increasingly turbulent world
- Identify common justifications for unethical behavior
- Identify experiences of the prophets in the scriptures regarding ethics and integrity

Reading

- Foundations of Spiritual and Physical Safety: with Chemical Processes; Chapter 2, Sections 1-2.
- [The Living Christ](#)
- [The Family: A Proclamation to the World](#)
- [Daniel 6](#)
- [Alma 14](#)

The world needs ethical people, people with integrity. There is no effective societal relationships be it financial, political, or personal without them built on a foundation of trust. Trust requires integrity or ethics. We can contribute significantly to the world simply by living with integrity and helping others to do the same.

Note

This section of the course is not intended to be an in-depth review of ethics. Rather, it is a brief introduction. There is a whole fields of ethics in disciplines of medicine, finance, and business for example. The purpose of this section is to introduce you to the topic of ethics in chemical engineering and to help you understand how the gospel of Jesus Christ can help us live a life of integrity.

2.1 Integrity

Tad Callister spoke on the importance of integrity on "Becoming Men and Women of Integrity." Elder Tad Callister defines integrity as **a state of purity in mind and heart, devoid of deceit, excuses, rationalizations, or any misrepresentation of facts**. It entails absolute honesty with oneself, God, and fellow human beings. It involves making **decisions based on eternal implications** and necessitates disclosing the complete truth without any alibis or excuses. Furthermore, integrity demands **keeping covenants and commitments**, even in inconvenient times, and being internally driven, not governed by the presence of others. He urges listeners to embrace integrity

not out of obligation but out of genuine desire, highlighting the Lord's acceptance of those who strive to live with integrity.

2.2 Ethics Approaches

Ethics Approach: Utilitarianism

- The greatest good for the greatest number of people
- The ends might justify the means
- The needs of the many outweigh the needs of the few

Ethics Approach: Deontology (Duty)

- Universal moral laws that can be applied to everyone
- Doing the right thing is more important than the outcome
- Double effect: the outcome of an action can be good or bad, but the action itself should be good (torture is bad, even if it is used to save lives)

Ethics Approach: Virtue Ethics

- Focuses on the character of the person
- Actions judged on if a virtuous person would do them
- Virtues include: honesty, courage, compassion, generosity, fidelity, integrity, fairness, self-control, and prudence

Ethics Approach: Contractarianism

- It is unethical to break a contract
- Contracts can form the backbone of society

Example of Jesus Christ by Words of Prophets

- First and Second Great Commandments
- Keep the 10 commandments
- Make and keep covenants with God through authorized ordinances

- Seek for and follow the guidance of the Holy Ghost
- Individuals are expected to apply the principles of the gospel of Jesus Christ to their own lives and make their own decisions
- We will be accountable for our own decisions and actions

2.3 BYU Honor Code

Some Honor Code Commitments

Sections of the BYU Honor Code are given below. I have emphasized some of the wording.

- Represent the **Savior Jesus Christ**, the Church, and the Church Educational System.
- Preserve an inspiring environment, without distraction or disruption, where covenants are kept in a spirit of unity so the **Holy Ghost can teach truth**.
- Live a **chaste and virtuous life**.
- Abstain from alcoholic beverages, tobacco, tea, coffee, vaping, marijuana, and other substance abuse.
- **Participate** regularly in Church services
- **Respect** others
- Obey the **law**.
- **Encourage others** in their commitment to comply with the Honor Code.

The above are only some of the commitments of the BYU Honor Code.

See Also

[BYU Honor Code](#)

2.4 AIChE Code of Ethics

Some AIChE Code of Ethics Principles

Sections of the AIChE Code of Ethics are given below. I have emphasized some of the wording.

- Hold paramount the **safety, health and welfare** of the public and protect the environment in performance of their professional duties.
- **Accept responsibility** for their actions, seek and heed critical review of their work, and offer objective criticism of the work of others.
- Act in professional matters for each employer or client as faithful agents or trustees, **avoiding conflicts of interest** and never breaching confidentiality.
- Perform professional services only in areas of their competence.
- Build their professional reputations on the **merits** of their services.
- Continue their professional development throughout their careers, and provide opportunities for the professional development of those under their supervision.

The above are only some of the expectations when upholding the AIChE code of ethics.

See Also

[AIChE Website](#)

2.5 Commonly Used Justifications for Unethical Behavior

2.5.1 2 Nephi 28:8-11

And there shall also be many which shall say ... fear God—he will **justify** in committing a little sin; yea, lie a little, take the advantage of one because of his words, dig a pit for thy neighbor; there is gno harm in this; and do all these things, for tomorrow we die; and if it so be that we are guilty, God will beat us with a few stripes, and at last we shall be saved in the kingdom of God.

Yea, and there shall be many which shall teach after this manner, false and vain and foolish doctrines, and shall be puffed up in their hearts, and shall seek deep to **hide** their counsels from the Lord; and their works shall be in the dark.

And the blood of the saints shall cry from the ground against them.

Yea, they have ... gone out of the away; they have become corrupted.

Justifications

- Lost revenue
- Lost position
- Lost reputation
- Revenge or sense of justice
- Minimization of harm
- Disagreement on what is ethical
- Misunderstanding of the law or of truth
- Ignorance
- Subordinate following orders or directives
- Rights over responsibility
 - Korihor (Alma 30:27)

2.6 Moral Relativism

Moral Relativism

Moral Relativism is the belief that there are no absolute truths. It is the belief that what is right or wrong is relative to the individual or the situation. It is the belief that there is no objective truth. It is the belief that there is no God. Often, 'moral dilemmas' are used to justify moral relativism in the sense that there may not be an obvious right or wrong answer.

2.7 Book of Mormon Counsel

Book of Mormon

"While society in general may believe that moral relativism is a sign of progress, the Book of Mormon contains examples and teachings that warn us of the dangers of replacing God's commandments with our own relative moral standards." [Daniel Belnap](#)

2.8 The Holy Ghost

"In coming days, it will not be possible to survive spiritually without the guiding, directing, comforting and constant influence of the Holy Ghost"

- President Russell M. Nelson

The Spirit speaketh the truth and lieth not. Wherefore, it speaketh of things as they really are, and of things as they really will be; wherefore, these things are manifested unto us plainly, for the salvation of our souls. (Jacob 4:13)

2.9 Scriptural Examples of Ethics and Integrity

Biblical Examples

- Daniel and the lion's den
- Shadrach, Meshach, and Abednego
- Joseph and Potiphar's wife

Nephite Examples

- Nephi and Laban
- Abinadi and King Noah
- Alma and Amulek
- Moroni and Pahoran

See Also

For further information see Aaron Miller's book titled *The Business Ethics Field Guide: The Essential Companion to Leading Your Career and Your Company to Greatness*, 2016. There's also a BYU course PHIL 213 that is taught frequently. There are many other very helpful resources on ethics and the gospel.

3 Ethics Approaches

Learning Outcomes

- Gain experience in applying ethics approaches to moral dilemmas

Reading

- Foundations of Spiritual and Physical Safety: with Chemical Processes; Chapter 2, Sections 4-6.

3.1 Additional Ethics Resources and Activities

Ethics decisions are made with respect to the principles to which you are committed. If someone is not committed to a specific principle set, it is easier to make unethical decisions with one or more justifications or rationalizations.

It is best to commit to a set of principles prior to the time when you are faced with an ethical decision.

Ethics Approach Step 1

Define

Carefully determine the root dilemma to be resolved. What is the real problem? It is common for ethical dilemmas to be convoluted combinations of many issues and it is tempting to hastily jump in and try to solve the problem. When we do, we often focus on the wrong problem and end up exacerbating the entire situation. Often dilemmas are nothing more than a lack of communication.

Proper definition requires some sleuth work as the relevant data are gathered, the history of the situation is traced, the layers of “who said what and when” are peeled away, and the real dilemma is brought to light. Patience is also required. It is easy to jump to conclusions based on one person’s opinion or on less than all the data. Contractual, legal, and ethical obligations and commitments must be included as part of the definition.

Ethics Approach Step 2

Consider and Analyze

Consider possible actions and then forecast the outcome. This is something like a chess game since there are multiple possible outcomes for a given action depending upon the reactions of others. A good chess player looks multiple moves ahead to anticipate outcomes, and this same mentality is valuable in considering actions to resolve an ethical dilemma. Use the clear principles of the Gospel of Jesus Christ and consider the possible courses of action from each possible course of action. The above ethics principles can be helpful. What actions would be suggested by each ethics theory? The outcomes that need to be considered include the impact on others including the public, co-workers, and family. It is helpful to organize your analysis in a flowsheet that traces actions and outcomes.

Ethics Approach Step 3
Plan

With the results of your analysis, it is time to select and plan your strategy. As you plan and prepare to put your plan into action, seek the guidance of the Spirit. Your plan will usually be a process involving several or many steps rather than a one-step action. Some steps may involve data gathering, and some will be dependent upon the intermediate responses and reactions of others. A good plan will produce inner peace—it will let you sleep at night.

Ethics Approach Step 4
Seek Confirmation

After you have done your homework and decided on a plan, you should seek divine approbation. (See D&C Section 9.) If this does not come, then more homework is most likely needed (Items 1, 2, and 3 above.) When you have this approval, then it is time to put the plan into action.

Ethics Approach Step 5
Act

Do it. Carry out your plan, being cautious and flexible as events unfold. Stick to your principles, but be humble and willing to admit your own failings and culpability

Ethics Approach Step 6
Reflect

Each time we go through the process of dilemma resolution, we should learn about ourselves and others. Take the time to digest the lessons learned so that your wisdom can increase in preparation for the next time. It helps to take some notes or make entries in a journal

3.2 Some Ethics Case Examples

- Chernobyl Firefighters
- Military Agreement of (Mission, Reactor, Ship, then Crew)
- Limited Information results in Bad Decision
- The Challenger Disaster
- Personal Story: Home Purchase

- Sulfanilamide Delayed Release
- The 1971 Ford Pinto
- Censorship

4 On Becoming

Learning Outcomes

- Understand the opportunity to decide to become like God

Reading

- Foundations of Spiritual and Physical Safety: with Chemical Processes; Chapter 2, Sections 3 and 7.

The “Becoming” concept; aligning professional life with spiritual values (e.g., covenants, service); connection to safety culture.

5 Human Body Systems

Learning Outcomes

- Be able to name the different systems in the body

Reading

- Foundations of Spiritual and Physical Safety: with Chemical Processes; Chapter 3, Sections 1-2 (Chemical Lethality).

This section provides an overview of human body systems and toxicology, which are essential for understanding how injuries occur. It covers the anatomy and physiology of major body systems, as well as the principles of toxicology, including dose-response relationships and exposure routes.

5.1 Toxicology

6 Physical Injury Modes

Learning Outcomes

- Be able to identify ways we can be injured

Reading

- Foundations of Spiritual and Physical Safety: with Chemical Processes; Chapter 3, Sections 2 (Heat/Overpressure) & 4

Heat flux and burns; Overpressure and blast injuries; case studies

7 Risk Ranking

Learning Outcomes

- Process Safety Management (PSM) Introduction
- Be able to use the Risk Matrix to rank risks

Reading

- Foundations of Spiritual and Physical Safety: with Chemical Processes; Chapter 4, Sections 1-2

7.1 Criticality of Process Safety

Hopefully in the last discussion we began to establish that process safety is a critical part of manufacturing. But when and how do we systematically go about responsibly managing risks and preventing accidents? We need tools to estimate risks for specific scenarios or actions, and we need tools to reduce those risks.

7.2 Risk Tolerance

Our tolerance for risk varies widely between individuals and organizations. How do we determine what is an acceptable risk? How do we determine what is an unacceptable risk? How do we determine what is a tolerable risk? How do we determine what is a negligible risk?

What risks do you voluntarily accept everyday?

- Getting struck by lightning?
- Getting hit by a meteorite?
- Getting in a car accident?
- Slipping on ice?
- Getting skin cancer?
- Getting the flu?

What involuntary risks do you accept frequently?

- Eating lead in your food?
- Eating salmonella in your food?
- Breathing in particulate matter?
- Getting drafted into the military?

What spiritual risks do you accept?

- Being exposed to damaging images?

- Being exposed to damaging philosophies?
- Consuming content that is not edifying?

How does your risk tolerance outside of work compare to your risk tolerance at work?

Note

As an industry consultant who performed many hazards analyses on explosive operations, we typically estimated the risks for a given hazard subjectively using the risk matrix shown below. About 1% of the time, for the most consequential hazards, we would quantify the risks using a more rigorous method. That more rigorous method is called Quantitative Risk Assessment (QRA). QRA is a topic to be discussed later in the course.

7.3 Risk Matrix

		RISK ASSESSMENT MATRIX			
		Catastrophic (1)	Critical (2)	Marginal (3)	Negligible (4)
PROBABILITY	Frequent (A)	High	High	Serious	Medium
	Probable (B)	High	High	Serious	Medium
	Occasional (C)	High	Serious	Medium	Low
	Remote (D)	Serious	Medium	Medium	Low
	Improbable (E)	Medium	Medium	Medium	Low
	Eliminated (F)	Eliminated			

Figure 2: Qualitative Risk Matrix

Risk is estimated by both the severity and its event probability or frequency. Usually the severity is listed first and the event probability is listed second. For example, getting hit by lightning would be catastrophic (death or a 1) but that event probability is very low (improbably, E), so that hazard rank would be 1E for most locations you're in. What ranking would you give the following physical events?

- Getting in a car accident driving to and from work over a 35 mile commute in a city?
- Getting in a car accident driving to and from work over a 35 mile commute in a rural area?
- Breaking your arm while playing frisbee?
- Getting burned by your stove while cooking?
- Getting burned eating hot pizza?
- Getting killed as an arborist cutting down 50 foot trees with a chain saw while being secured with a plastic rope?

Spiritual Risk Rankings What about a risk rating for \textbf{spiritual events}? Physical injury is straightforward like scratches and scrapes to broken bones or loss of sight to death. Spiritual injury is not as straight forward and it's difficult to recognize sometimes. For that reason, we'll primarily focus on physical risks. However, we can define spiritual harm as being separated from God if we fail to keep His commandments. Some activities are not edifying and participating in those may not immediately lead to committing a mistake or sin. However, small acts of setting aside God can result in spiritual or emotional trauma. In that light, could you ranking the following events?

- Not reading your scriptures for a day? (What emotional or spiritual harm would result, corresponding to a severity, and instead of a frequency, how probable is it that you would be harmed to that severity)
- Not reading your scriptures for a week?
- Viewing pornography?
- Lying to your spouse?
- Lying to your boss?

Important

The overall risk assessment based on the severity and frequency are ranked from eliminated, to low, medium, serious, and high. That overall risk is labeled by a color as well in the risk matrix above.

The risk acceptance level in the defense or energetics manufacturing industry was acceptable in the medium range (marked yellow and roughly equivalent to an employee getting injured in driving to and from work). If risks are in the medium range (colored orange), recommendations (engineering or administrative controls) were given to reduce the event probability or the event severity. If risks were in the red or high category, operations could not be performed without mitigating steps to substantially lower that risk.

7.4 OSHA 29 CFR PSM Elements

Compliance to the standard is required for those operations meeting the Threshold Quantities values for different listed chemicals but these principles are applied in other scenarios to reduce risks.



Figure 3: OSHA PSM Elements

- Employee Participation
- **Process Safety Information**
- **Process Hazards Analysis**

- Operating Procedures
- Training
- Contractors
- Pre-Startup Safety Review
- Mechanical Integrity
- Hot Work Permits
- Management of Change
- Incident Investigation
- Emergency Planning and Response
- Audits
- Trade Secrets

7.4.1

8 Quantitative Assessment

Learning Outcomes

- Be able to use the poisson distribution to estimate the probability of an event

Reading

- Foundations of Spiritual and Physical Safety: with Chemical Processes; Chapter 4, Sections 3-4

When quantifying the risk from a specific failure mode, it can be important to understand several event likelihoods or probabilities such as:

- probability of the event occurring in a given time period (or given number of cycles)
- probability of a given energy level being exceeded (such as an energy level that would cause a failure) during that event
- probability that given the energy level is exceeded, that the failure mode or failure outcome will occur
- probability that an individual or group of individuals will be exposed to the event
- etc.

Perhaps a simple example is the probability of breaking a hip after age 65. You'd include the probability of falling down as one impetus and perhaps a bike crash as another and then for each of those you'd have the probability of a break given the event occurred. We are part of such calculations as we pay insurance premiums. Actuarial science is the discipline that deals with the quantification of risk using probabilities.

In the discussion here, we will focus on quantitatively estimating event probabilities, or the probability an event will occur in a given time period.

8.1 Event Probability from Poisson Distribution

There are many statistical distributions including the normal distribution, chi squared, exponential, etc. that can be used to model event probabilities. One of the most common distributions used in reliability engineering is the Poisson distribution. The Poisson distribution is often used to model the number of events that occur in a fixed interval of time or space. The probability of observing k events in a given time period is given by the Poisson probability mass function:

$$P(k) = \frac{\lambda^k e^{-\lambda}}{k!} \quad (1)$$

where λ is the rate of occurrences.

In the treatment here, we will create a λ' prime that is the rate per unit time and we will also only care that k or the number of events is greater than or equal to 1. This is because we are interested in the probability of at least one event occurring in a given time period. As such, the following is true of the probability estimate:

$$P = 1 - e^{-\lambda' t} \quad P = 1 - e^{-\mu t} \quad (2)$$

where the second equation is how it is given in Crowl and Louvar's Chemical Process Safety 4th edition.

Event Probability

Poisson Distribution

$$P = \frac{\lambda^k e^{-\lambda}}{k!}$$



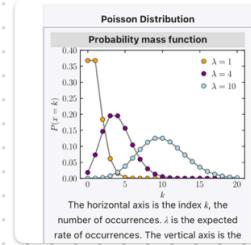
λ is the rate of occurrences
 k is the # of occurrences/events
 The probability of 1 or more events
 is $P = 1 - e^{-\lambda} (k=0)$

Here the rate of occurrences/events is
 1 event in a given time frame.

If we incorporate that time then

$$P(\text{at least 1 event}) = 1 - e^{-\lambda \cdot t}$$

As time increases, the probability of at least one event occurring increases to 1 or certainty, there will be at least one event. And conversely, short time yields a probability vanishingly small.



credit wikipedia

Figure 4: Poisson Distribution Discussion

8.2 Multiple Event Probability Estimates

For clarity, the example shown above has a mean time between failures ($1/\mu$) of 6000 seconds, 100 minutes, or 1.67 hours. The probability of a failure occurring in 1 second is $1.67e-4$ which is very close to $\mu = 1.67e-4$. However for longer times like 1 month, the probability of failure is very close to 1 but μ is 432 failures expected per month. Don't confuse μ or the failure rate with P , the probability of failure in a given time period.

```
import numpy as np
P = 1 - np.exp(-1/6000*1)
print(f'The probability of failure in 1 second is {P:.8f}, which is approximately equal to mu = {1/6000}')

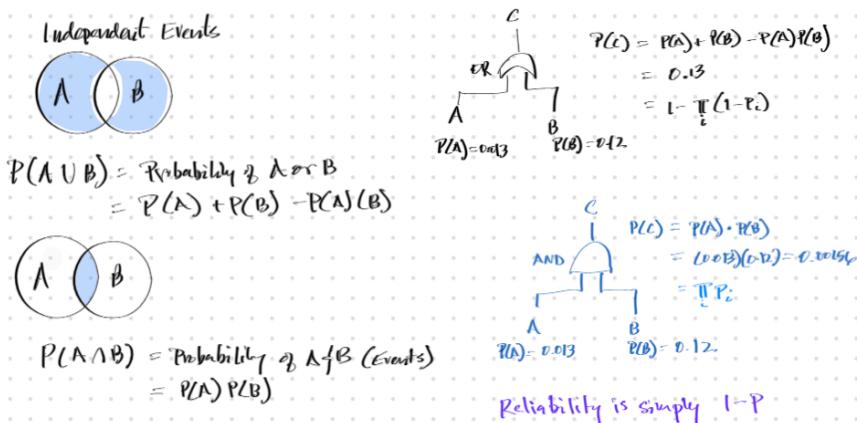
The probability of failure in 1 second is 0.00016665, which is approximately equal to mu = 0.00016667

mu = 1/100*60*24*30 # rate per month
P = 1 - np.exp(-mu*1)
print(f'The probability of failure in 1 month is {P:.3f}, which is not equal to mu = {mu:.0f}'')

The probability of failure in 1 month is 1.000, which is not equal to mu = 432
```

Important

Please be very familiar with Examples 12-1 and 12-2 in Crowl and Louvar's Chemical Process Safety 4th

**N O T E .**

The above P values indicate a probability of failure within a given time frame. This P value is different from μ or λ that is the average failure rate.

For example, the average rate of dropping a glass while carrying it for 2 min might be $1/50$.

thus $\mu = \frac{1}{50} = \frac{0.01 \text{ faults}}{2 \text{ min}} \text{ or } \frac{1.2 \text{ faults}}{2 \text{ hrs}}$

However, the probability of dropping the glass in 2 hours is not 1.2 (probabilities can range between 0-1) but is $1 - e^{-\lambda t} = 1 - e^{-1.2} = 0.679$

* dropping at least once

Warning: Common Error is to confuse P with μ

Figure 5: And Or Probability Discussion

edition. Those examples are great in helping you work with reliability, probability, failure rates and mean time between failures for and and or systems.

8.3 Monte-Carlo

Monte-Carlo methods can be used when there are more complex scenarios in terms of interactions between events, dependencies, etc. In this case, the probability of an event occurring is estimated by simulating the scenario many times and counting the number of times the event occurs. The probability is then estimated as the number of times the event occurs divided by the total number of simulations.

Example Monte-Carlo Simulation

```
#import needed packages
import numpy as np
import matplotlib.pyplot as plt

# Number of random numbers to generate
N = int(1e4)
```

MONTE-CARLO INTRO

Monte Carlo uses a computer to make many random events "occur" and then the user simply uses contributing calculations to obtain the probability of an overall event

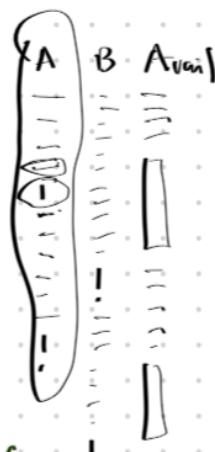
Example: Event A occurs at a MTBF of 0.75 unit time.

Event B occurs at a MTBF of 2 unit time.
Unit time could be a minute, day, year, etc.

MONTE CARLO DISCRETE STEPS

- Obtain the probabilities of at least one event occurring in unit time for both Event A & Event B. The unit time should be the same for both.

$$P_{A,B} = 1 - e^{-\frac{1}{MTBF_{A,B}} \cdot 1 \text{ unit time}}$$



- Generate N random #s from the uniform distribution = unit

- Determine if an event "occurred" from the following:

```
For each in unit:
    if each < PA:
        return 1
    else:
        return 0
```

- Generate an Event A array accordingly as well as an Event B array

- Determine if 1 or both events occurred at each index. The total count of that or A / AND D can be used to estimate a combined probability simply by summing & dividing by N

- The MTBF for the A OR 1 AND condition can then be found from

$$MTBF = \frac{1}{P_{A,B}} \text{ unit time}$$

```
MTBF_A = 1 # mean time between failures, unit time for Event A
muA = 1/MTBF_A # average events per unit time for A
1 -np.exp( -muA) # probability of at least one event in unit time (poisson process)
```

0.6321205588285577

```
muA*np.exp( -muA) # probability of exactly one event in unit time (poisson process)
```

0.36787944117144233

```
unif = np.random.uniform(0, 1, N) # generate N random numbers between 0 and 1
# 1 if event, 0 if no event, where the if statement is the Monte Carlo approach
eventA = [1 if x < 1 -np.exp( -muA) else 0 for x in unif]
```

Each entry in that list is an “event” over a duration of unit time and it can either be a failure or a success.

```
pA = sum(eventA)/len(eventA) # fraction of time with at least one event, probability of event in time unif
```

0.6369

```
#determine the average rate of events per unit time
-np.log(1 -pA)
```

1.013077000561847

```
# now let's do the same thing for a Poisson process with a second 'event'
unif = np.random.uniform(0,1,N) #generate new random numbers
MTBF_B = 2 # mean time between failures
muB = 1/MTBF_B # average events per unit time
eventB = [ 1 if x < 1 -np.exp( -muB) else 0 for x in unif ]
```

```
# now consider eventA and eventB as two independent Poisson processes in an OR gate
eventAorB = [min(1,sum([a,b])) for a,b in zip(eventA, eventB)]
```

```
pAorB = sum(eventAorB)/len(eventAorB) # fraction of time with at least one event
pAorB
```

0.7773

```
#combination of the two events for the average rate of events per unit time (mu)
-np.log(1 -pAorB)
```

1.5019297047188152

```
# now consider eventA and eventB as two independent Poisson processes in an AND gate
eventAandB = [a*b for a,b in zip(eventA, eventB)]
pAandB = sum(eventAandB)/len(eventAandB) # fraction of time with at least one event
pAandB
```

0.2523

```
#Calculation of the probability of A and B occurring at the same time (product of the two probabilities)
pab = (1 -np.exp( -muB))*(1 -np.exp( -muA))
pab
```

0.2487200592643541

```
#combination of the two events for the average rate of events per unit time (mu) from simulation  
-np.log(1 -pAandB)  
  
0.29075345097626715  
  
#combination of the two events for the average rate of events per unit time (mu) from product of probab  
-np.log(1 -pab)  
  
0.28597693937029134
```

9 Inherent Safety Principles

Learning Outcomes

- Be able to identify the difference between different inherent safety approaches
- Be able to identify key components of each inherent safety approach

Reading

- Foundations of Spiritual and Physical Safety: with Chemical Processes; Chapter 5, Sections 1

9.1 Process Safety

9.1.1 Safety Culture

How important is safety to you and those around you? What does process safety mean? What does it mean to your company? Are you willing to work for a company that does not value safety? Is it true that a company that does not value safety does not value you?

Ultimately, we are responsible for our safety, both physical and spiritual. We'll talk about many accidents in the course. For example, a few days ago, the Los Angeles Times reported about Zuko Carrasco, who was paralyzed while leading people on a trust fall. He blames himself as he was the last to descend when what he thought he heard was "on belay" but his belayer was not yet ready. He jumped and fell 40 feet and was paralyzed from the waist down. He had safely completed that activity many times before.

9.1.2 Voluntary and Involuntary Risk

Most are much more comfortable assuming voluntary versus involuntary risk. As a chemical engineer, how will you mitigate those two types of risk? Undoubtedly, a chemical engineer will work under voluntary risk and be on the front lines of helping to reduce involuntary risk to the public.

9.1.3 Safety Metrics

You say you're safe...prove it. Some safety metrics are training hours, near misses, number of lost time accidents, etc.

9.1.4 Accident Statistics

Accident statistics are used to help us understand the risks we face. They are also used to help us understand the effectiveness of our safety programs.

9.1.5 Safety Triangle

9.1.6 OSHA Recordable

Employers with more than 10 employees are required to keep a record of serious work-related injuries and illnesses. This is called the OSHA 300 log. It is required by the Occupational Safety and Health Administration (OSHA) which has legal authority to enforce workplace safety laws. Recordable injuries and illnesses are:

- Any work-related fatality.



Figure 7: Safety Triangle showing that reducing the incidents of lower consequence events can reduce the quantity of higher consequence events.

- Any work-related injury or illness that results in loss of consciousness, days away from work, restricted work, or transfer to another job.
- Any work-related injury or illness requiring medical treatment beyond first aid.
- Any work-related diagnosed case of cancer, chronic irreversible diseases, fractured or cracked bones or teeth, and punctured eardrums.
- There are also special recording criteria for work-related cases involving: needlesticks and sharps injuries; medical removal; hearing loss; and tuberculosis.

Consequences from OSHA violations can be severe in addition to the injury and illness suffered by the employee. Consequence of an OSHA recordable incident could include: increased scrutiny from OSHA, potential fines and penalties, higher workers' compensation costs, negative impact on company reputation, decreased employee morale, and increased insurance premiums; essentially, an OSHA recordable incident shows employees were unnecessarily harmed which can lead to significant financial repercussions.

10 Hazards Analysis

Learning Outcomes

- Be able to complete several hazard analysis steps

Reading

- Foundations of Spiritual and Physical Safety: with Chemical Processes; Chapter 5, Sections 2 (Intro)

10.1 Effective Hazards Analysis Steps

Hazard Identification and Evaluation with Risk Analysis and Assessment

1. Define the process

This step can involve collecting documentation such as a process flow diagram (PFD), piping and instrumentation diagram (P&ID), operating procedure and other relevant information. It is also important to gather information about the process, such as the materials used, and the operating conditions among other things.

2. Identify the hazards analysis method to use

Hazards analysis methods include HAZOP, FMEA, and fault tree analysis (FTA). The choice of method will depend on the specific process and the goals of the analysis.

3. Identify the Hazardous Top Level Event and contributing factors with

- a Fault Tree Analysis (FTA)
 - Including deductive and inductive reasoning
- a HAZOP (Hazards and Operability Study)
 - Including guide words and deviations

4. Fill out a Hazards Analysis (HA) Table

For each failure mode (the lower level events in your fault tree analysis), fill out the hazards analysis table including the following information:

- Task description or process step
- Hazard type
- Hazard description
- Event consequence
- Safeguards currently present to mitigate the hazard

- Rank (1A to 5E) for severity and likelihood of the hazard
 - Recommendations to reduce the risk of the hazard
5. Potentially complete a quantitative risk analysis for those hazards with a high risk ranking
6. Incorporate other PSM elements per the OSHA 1910.119 standard

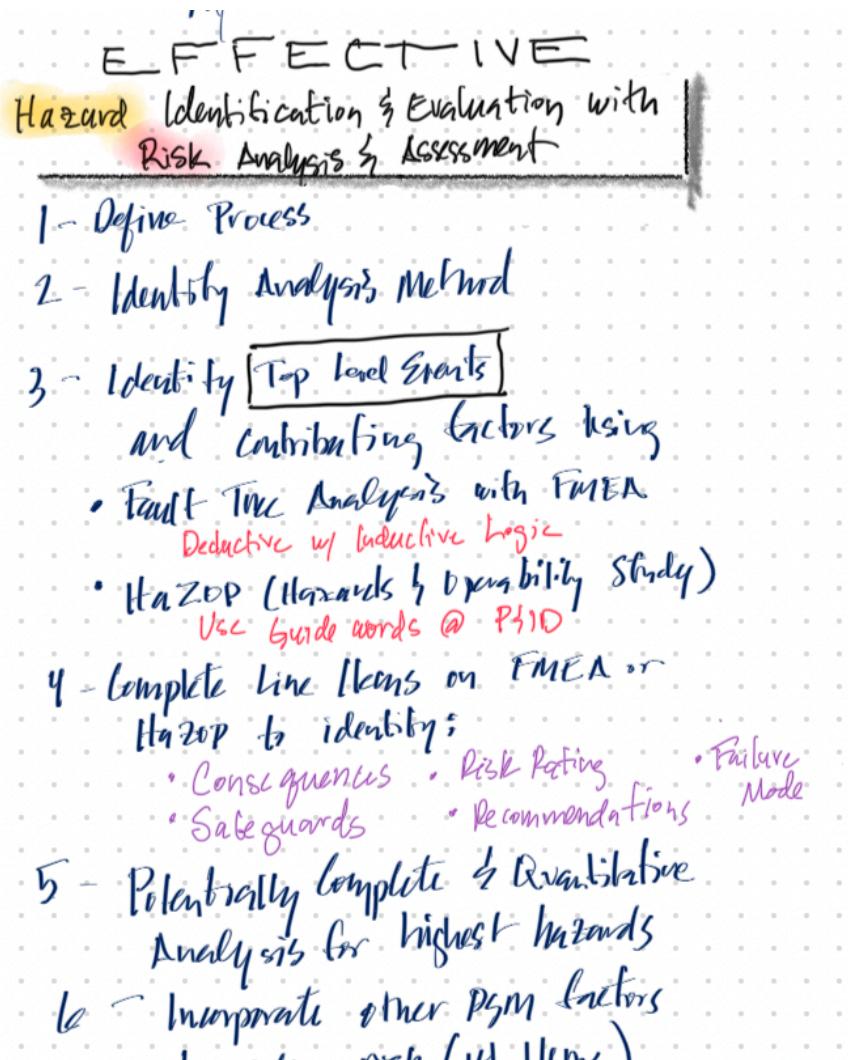


Figure 8: Effective Hazards Analysis Steps

10.2 Recommended Hazards Analysis Methods

The recommended methods for hazards analysis that we used effectively in evaluating explosive, pyrotechnic, and propellant based processes included:

- Fault Tree Analysis (FTA) with deductive and inductive reasoning followed by Failure Mode and Effects Analysis (FMEA) where the HA table is filled out for each failure mode.

- HAZOP (Hazards and Operability Study) with guide words and deviations

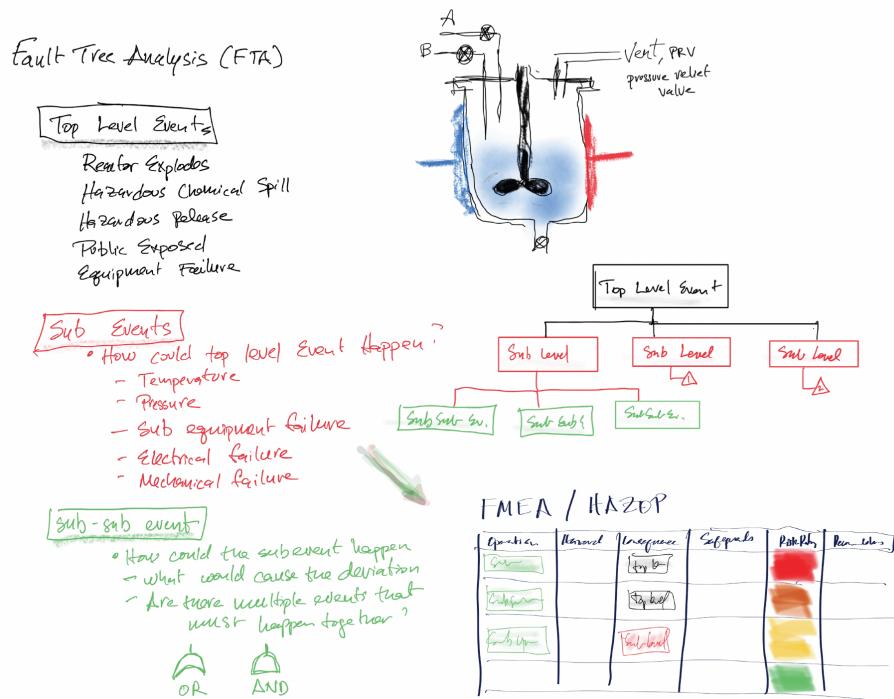


Figure 9: Fault Tree Analysis to Hazards Analysis Table

10.3 When Should you Conduct a Hazards Analysis? As early in the process as feasible.

Many complex processes have been designed and built prior to completion of a hazards analysis (FTA with a FMEA, or HAZOP). This makes integration of engineering controls into the process very difficult or costly or both. Ideally you complete a hazards analysis at the design stage and other stages including:

- Design (a Design Hazards Analysis)
- Construction and Startup
- Operation
- Decommissioning
- Accident Investigation

10.4 Process Safety Information (PSI) is Critical

Process safety information including details of the process, the materials used, and the operating conditions is critical to completing a hazards analysis. We'll talk a lot more about PSI.

Other helpful graphics for hazards analysis and review download pdf: <physical/supportfiles/FTAwRev1.pdf>

NEEDED INFORMATION FOR EFFECTIVE HAZARDS ANALYSIS

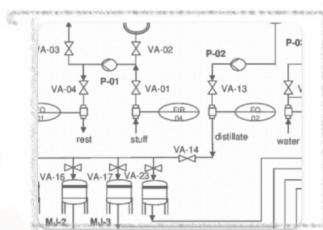
Chemical Information

- Flammability
- Toxicity
- Reactivity



Process Information

- PFD (Process Flow Diagrams)
- P&ID's (Piping & Instrumentation Diagrams)
- Equipment details
- Procedures
 - Start-Up
 - Operation
 - Shut Down



Other Important Info

- Near Miss Details
- Accident History

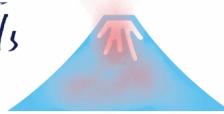


Figure 10: Needed Information for Effective Hazards Analysis

11 Logic and Safety

Learning Objectives

- Learn about critical and creative thinking skills for analysis and evaluation of problems and cause-effect relationships.
- Highlight argument validation and fallacies.
- Learn about the difference between deductive and inductive reasoning.
- Know how deductive and inductive logic apply to hazards analysis

Reading

- Read about deductive reasoning in an article or book.

Logic and critical thinking are skills that can help you to evaluate information and make decisions. We will use these skills to help us systematically consider hazards that could lead to catastrophic events.

11.1 Logic and Critical Thinking

Critical thinking is the ability to think clearly and rationally about what to do or what to believe. It includes the ability to engage in reflective and independent thinking. Someone with critical thinking skills is able to:

- Understand the logical connections between ideas.
- Identify, construct and evaluate arguments.
- Detect inconsistencies and common mistakes in reasoning.
- Solve problems systematically.
- Identify the relevance and importance of ideas.
- Reflect on the justification of one's own beliefs and values.

11.1.1 Deductive Reasoning

Deductive reasoning is a type of logical thinking that starts with a general statement and then applies that statement to a specific case. For example, if we know that all cats have tails, and we know that Fluffy is a cat, then we can deduce that Fluffy has a tail.

A few examples from process safety:

- All flammable materials can be ignited and burn, and we know that gasoline is a flammable material, then we can deduce that gasoline can be ignited and burn.
- Reducing the oxygen concentration in a room will reduce the likelihood of a fire, and we know that the oxygen concentration in a room can be reduced by displacing oxygen with an inert gas, then we can deduce that displacing oxygen with an inert gas will reduce the likelihood of a fire.

- Encouraging cleanliness and holding hand rails contributes to a culture of safety, and we know that a culture of safety reduces the likelihood of accidents, then we can deduce that encouraging cleanliness and holding hand rails reduces the likelihood of accidents.

11.1.2 Deductive Validity

Deductive validity is a property of arguments. An argument is valid if the truth of its premises guarantees the truth of its conclusion. In other words, an argument is valid if the conclusion is true whenever the premises are true. The following argument is valid, because the conclusion must be true, given the premises:

- All humans are mortal.
- Socrates is human.
- Therefore, Socrates is mortal.

11.1.3 Inductive Reasoning

Inductive reasoning is a type of logical thinking that starts with a specific case and then applies that case to a general statement. For example, if we know that Fluffy has a tail, and we know that Fluffy is a cat, then we can induce that all cats have tails.

A process safety example:

- The Bhopal disaster was caused by a chemical incompatibility with water. We can induce that there may be other chemicals that are incompatible with water and could result in severe consequences.

11.1.4 Inductive Force

An inductively forceful argument is one where the truth of the premises makes the conclusion more likely to be true. For example, the following argument is inductively forceful:

- 90% of the people we have interviewed love to play soccer.
- Therefore, the next person we interview will also love to play soccer.

11.1.5 Fallacies

A fallacy is the use of invalid or otherwise faulty reasoning, or “wrong moves” in the construction of an argument. A fallacious argument may be deceptive by appearing to be better than it really is. Some fallacies are committed intentionally to manipulate or persuade by deception, while others are committed unintentionally due to carelessness or ignorance. An example of a fallacy is:

- If you love your country, you will support the war in X.
- You do not support the war in X.
- Therefore, you do not love your country.

Other Examples of Fallacies

- Ad hominem: attacking the person instead of the argument.
- Appeal to authority: using the opinion or position of an authority figure, or institution of authority, in place of an actual argument.
- Appeal to emotion: manipulating an emotional response in place of a valid or compelling argument.

- Appeal to fear: using fear to influence the conclusion.
- Appeal to flattery: using flattery to influence the conclusion.
- Circular reasoning: supporting a statement by repeating it in different words. Similar to affirming the consequent: if A, then B. B, therefore A. Also similar to begging the question: assuming the conclusion in the premise.
- False dilemma: giving two choices when in fact there are three or more.
- Cause and effect: assuming that the effect is related to a cause because the events occur together. Implying causation from correlation.
- Sunk cost: assuming that future events will be affected by past events, which have no bearing on future outcomes.
- Strawman: creating a false or made up scenario and then attacking it. Similar to a red herring: diverting attention from the real issue by focusing instead on an issue having only a surface relevance to the first.
- Tu quoque: avoiding having to engage with criticism by turning it back on the accuser - answering criticism with criticism.
- Wishful thinking: making decisions according to what might be pleasing to imagine, rather than according to evidence or reason.
- Slippery slope: asserting that a relatively small first step inevitably leads to a chain of related events culminating in some significant impact.
- Herd mentality: doing or thinking things because many other people do or think the same. Similar to bandwagon: doing or thinking things because many other people do or think the same.

Example Reasoning from Current Events**Consider and Analyze: Large Fires****Note**

- The earth's temperature is increasing.
- Weather patterns are changing.
- These weather changes are causing an increase in the prevalence of wildfires.
- The fires are causing significant damage and some fatalities.
- To reduce this damage and loss of life, we need to limit the earth's temperature from increasing.

11.2 Perception != Reality

Nuclear risk perception vs reality

Chemical risk perception vs reality

11.2.1 Influence of the Holy Ghost

We should do all we can to learn and determine what is true. We can then ask God if it is true. The Holy Ghost witnesses of truth. It is a feeling of peace and assurance. It is a gift from God that is available to all people. It is a way that God communicates with us. President Nelson has said that:

Quote by President Nelson

in coming days, it will not be possible to survive spiritually without the guiding, directing, comforting, and constant influence of the Holy Ghost.

11.3 Application

Application of logic and reasoning principles to systematic hazards analysis involves both deductive and inductive logic.

12 HAZOP Intro

Learning Outcomes

- Be able to complete a basic HAZOP by applying guide words and documenting failure modes, consequences, and safeguards in a table

Reading

- Foundations of Spiritual and Physical Safety: with Chemical Processes; Chapter 5, Sections 2.1
- HAZOP Analysis: <https://smsenergetics.com/risk-management/process-hazards-analysis/hazop-basis>

12.1 Hazards and Operability Study (HAZOP)

Systematic method of identifying hazards in a process plant using a process flow diagram (PFD) and/ or a piping and instrumentation diagram (P&ID) and guide words.

12.1.1 Process Flow Diagram (PFD)

Example PFD of the Haber-Bosch process from [Haber process](#)

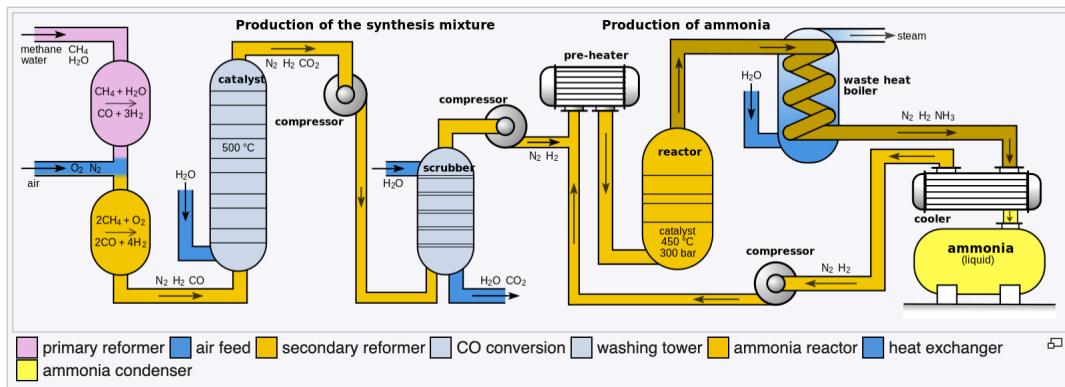


Figure 11: Example Haber Bosch Process PFD

Nodes are judiciously picked at points where the process changes significantly. The nodes are numbered and the node numbers are used in the HAZOP study.

12.1.2 Piping and Instrumentation Diagram (P&ID)

A piping and instrumentation diagram can be very detailed or it can simply denote key process components. Build drawings are for the construction of the plant and can be very detailed. Those diagrams are usually proprietary and so difficult to get an example to show. However, there are public domain examples of P&IDs. The P&ID published here is from a somewhat complex Aspen Plus flowsheet of the Haber-Bosch process. It was published [Spatolisano and Pellegrini \(2023\)](#). The drawing lacks details on instrumentation.

Another example of a piping and instrumentation diagram for an internal combustion scenario is shown in [Kim et al. \(2016\)](#).

This site does a good job of explaining the symbols of PID diagrams and gives a few examples: <https://www.edrawmax.com/pid/>. PID symbols are not standardized, so you may see different symbols used in different diagrams. PID's are very helpful, invaluable, in designing a process plant (Smokeless powder manufacturing in Mulwala, NSW, Australia). The P&ID is a more detailed diagram than the PFD. It shows the process flow, but also shows the instrumentation and control devices.

Similar to the PFD, nodes are judiciously picked at points where the process changes significantly. The nodes are numbered and the node numbers are used in the HAZOP study.

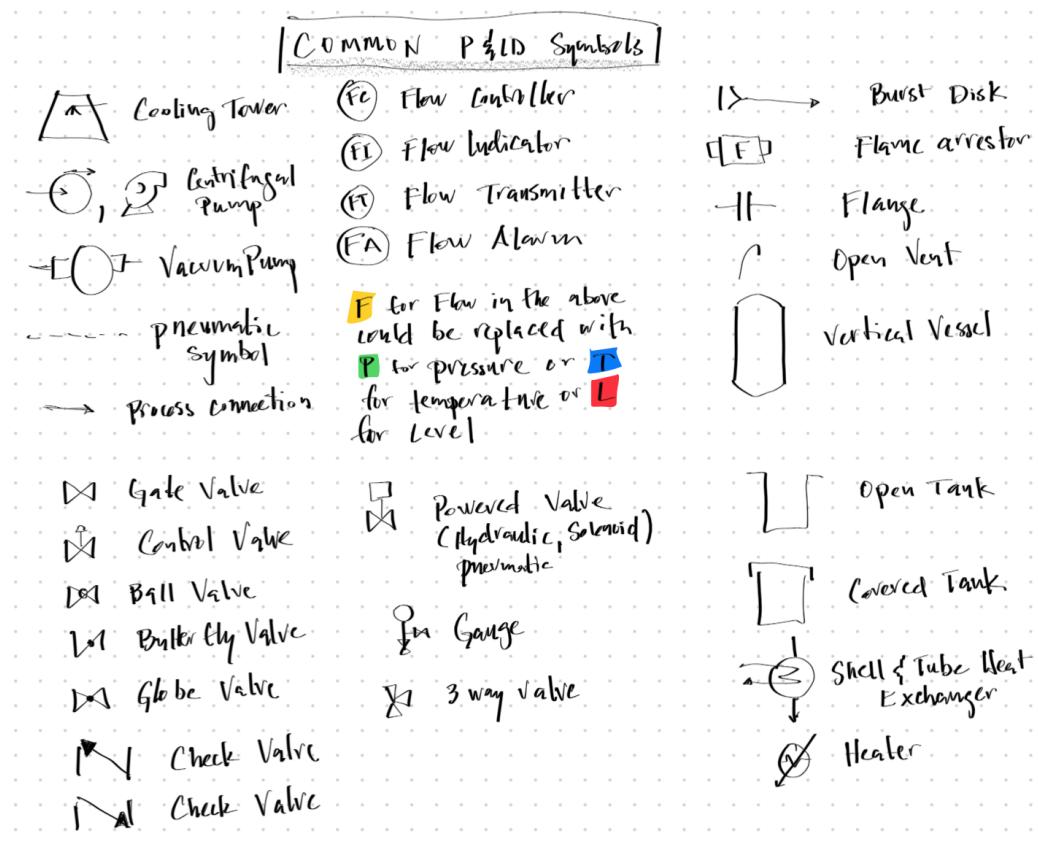


Figure 12: Example PID Symbols

12.1.3 P&ID Activity

Draw a P&ID for a continuous washing machine. Water, soap, and clothing enter the machine and water and soap exit in one stream and wet clothing in another exit stream. The system has water flow control with feedback, soap amount control, and clothing (material) control.

12.1.4 Guide Words

- High, Low, No Flow, Reverse Flow
- High, Low Pressure
- High, Low Temperature

Example P&ID for Simple Process

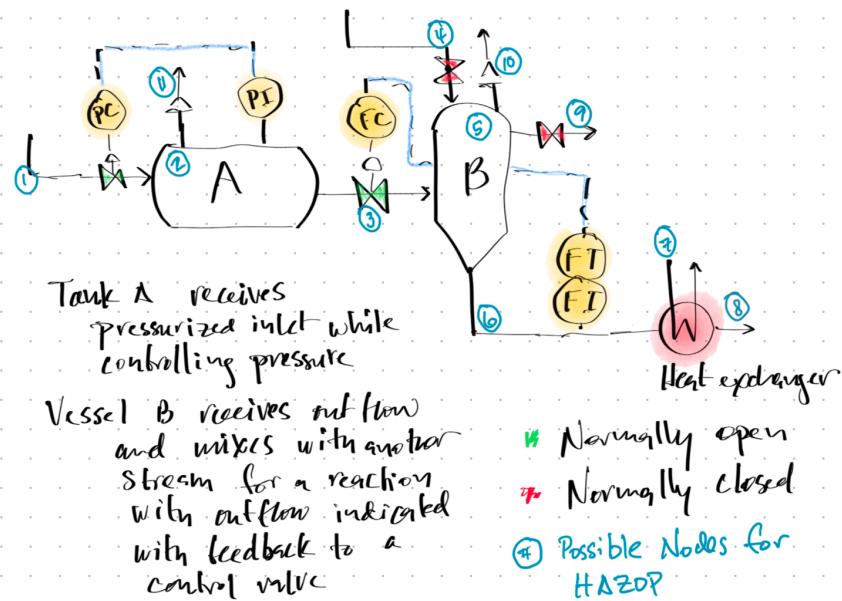


Figure 13: Example P&ID

Continuous Washing Machine Example

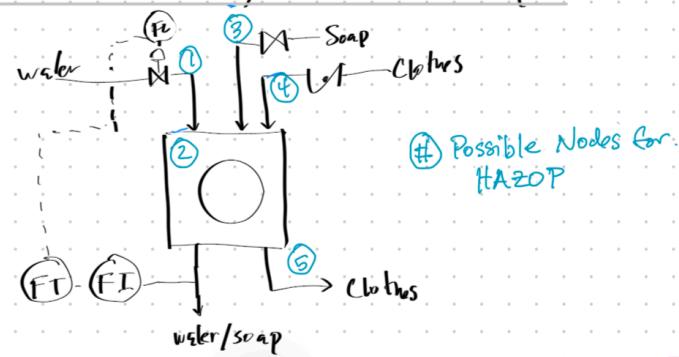


Figure 14: Washing Machine P&ID

- High, Low, No Level
- High, Low Composition
- High, Low Reaction Rate, Side reaction, Reverse reaction
- High, Low, No Power
- Wrong material

12.2 Documentation

Document the HAZOP study in a table. The table should have the following columns:

- Node number/ Operation
- Guide word
- Cause/Hazard
- Consequence
- Safeguard
- Risk Rating
- Recommendation

13 HAZOP Case Study

Learning Outcomes

- Gain practice with completing part of a HAZOP
- Gain knowledge on accident scenarios

Reading

- Foundations of Spiritual and Physical Safety: with Chemical Processes; Chapter 5, Sections 2.1 (Examples)

CSB Investigation of H2S Poisoning in a Pump House in Texas: Aghorn Operating Waterflood Station Hydrogen Sulfide Release

<https://www.csb.gov/aghorn-operating-waterflood-station-hydrogen-sulfide-release-/>

1:50 - 6:50 Event Summary

- Oil and water mixture sits and separates in an initial holding tank
- Water (Produced Water) is pumped out of the bottom to reintroduce into the well then pumped to the suction tank
- Waterflood station or pump house used to pressurize water
- High pressure piston pumps inject water back into the well to allow greater amounts of oil to be recovered
- Pump house occasionally occupied 2x per day
- H2S alarm and critical warning light not functional
- Alarm notification to service personal of an oil level alarm with pump malfunction of some kind
- Personal H2S monitor not brought into pump house by the operator
- Pump plunger had shattered and H2S was released with the water
- Operator was fatally injured by H2S
- Wife also fatally injured by H2S

Download lecture freeform here: [https://github.com/clint-bg/safetyinjc/blob/main/physical/supportfiles/311 HAZOP Case Study.pdf](https://github.com/clint-bg/safetyinjc/blob/main/physical/supportfiles/311%20HAZOP%20Case%20Study.pdf)

14 Fault Tree Analysis

Learning Outcomes

- Be able to complete a basic fault tree analysis with a hazardous top level event

Reading

- Foundations of Spiritual and Physical Safety: with Chemical Processes; Chapter 5, Sections 2.2
- Fault Tree Analysis: [Fault tree analysis](#)
- Job Hazards Analysis Template: <https://uolab.groups.et.byu.net/files/safety/JHATemplate.docx>

Fault tree analysis (FTA) is a top-down, deductive failure analysis in which an undesired state of a system is analyzed using boolean logic to combine a series of lower-level events. This analysis method is used to understand how systems can fail, to identify the best ways to reduce risk, and to estimate event rates of a safety accident or a particular system level (functional) failure.

14.1 1st Example of Fault Tree Analysis (FTA)

14.1.1 Procedure

Communte to work or school avoiding injury from a traffic accident or other hazards.

14.2 2nd Example of Fault Tree Analysis (FTA)

14.2.1 Procedure

A batch reactor is used to complete a reaction needed for the benefit of others. The reactor process has the following processing steps:

1. The reactor is filled with the raw material, a somewhat toxic material.
2. The reactor is heated to the desired temperature (100 F).
3. The reactor is pressurized to the desired pressure (20 psig).
4. Reactant B is slowly added to the reactor. An exothermic reaction occurs and the jacket must begin to cool the reactor to maintain the desired temperature.
5. The reaction proceeds at a given reaction rate at that temperature and pressure until all of the reactant B has been added.
6. The reactor is cooled to room temperature and the product is removed.

14.2.2 Some Hazards

- Product C has a low boiling point and is toxic. If the reactor is not cooled properly, the product will vaporize and escape from the reactor.
- If stirring is not maintained, the reaction will not proceed at the desired rate and the reactor will overheat.
- Reactor is used for multiple products

Figure 17: Image of the batch reactor credit to: <https://www.essentialchemicalindustry.org/processes/chemical-reactors.html>

14.3 Combination of FTA and FMEA:

An accident investigation prior to the accident

Example start on an FTA: (lower left is 'Blades fall off')

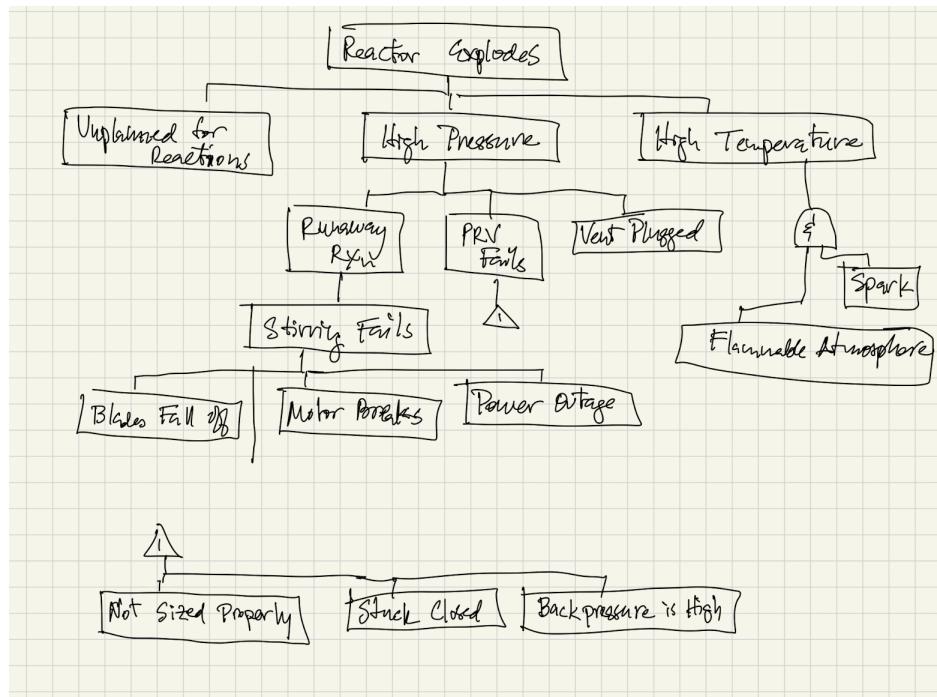


Figure 18: Example Fault Tree Analysis

Example start of the FMEA/ Hazards Analysis



BYU TIPICE

Job Hazards Analysis (JHA)

Title:	Document No.:	Page:
Operator/ Test Individual:	Rev:	Date:

BYU CH EN Job Hazards Analysis						
Task Description	Hazard Type	Hazard Description	Consequence	Safeguards	Rank	Recommendations
Reactor Operation - Stirring	Electrical Failure	Controller Fails from Power Outage	Stirring ceases resulting in a runaway reaction, high pressure, and potential violent reactor explosion	Battery Powered alarm present to indicate power failure Backup power generator present	2D	
Reactor Operation - Stirring	Component Failure	Motor Fails	Stirring ceases resulting in a runaway reaction, high pressure, and potential violent reactor explosion	Alarm present on motor indicating presence of stirring Emergency venting of reactor contents possible	2D	

Figure 19: FMEA Example

FMEA

Clint Guymon

Brigham Young University

1st Jan, 2025

created in  Curvenote

Keywords Spiritual Safety, Process Safety, Chemical Engineering, Risk Assessment

Learning Outcomes

- Be able to complete a basic failure mode and effects analysis

Reading

- Foundations of Spiritual and Physical Safety: with Chemical Processes; Chapter 5, Sections 2.3
- Failure Mode and Effect Analysis: <https://smsenergetics.com/risk-management/process-hazards-analysis/fmea-basis>

1 Process Hazards Key Safety Principles:

- **Replace** the hazardous material or process
- **Reduce the quantity** of hazardous material
- **Reduce the time** the hazardous material is present
- **Reduce the number of people** exposed

2 Key Tools for Safe Operations:

- **Hazards Analysis (HA)** - An incident investigation before the incident (HAZOP, FMEA, FTA, etc.)
- **Process Safety Information (PSI)** - Information about the process and hazards of the materials
- Other **PSM** elements such as Management of Change, Operating Procedures, Training, Pre-Startup Safety Review, Mechanical Integrity, Hot Work Permit, Emergency Planning and Response, Incident Investigation, and Compliance Audits

3 Project Components

- Process Background, Scope, and Details
- Process Flow Diagram (PFD) or Piping and Instrumentation Diagram (P&ID)
- Process Safety Information
- Any Incident Investigation Reports or Details
- Hazards Analysis
- Process Impacts (Ethical, Global, Economic, Environmental, and Societal)
- Documentation

3.1 Process Impacts

Ethical - How does the process impact the ethical standards of the company and the industry? Or What ethical decisions may led to a potential incident? How could those decisions be different, from an ethical standpoint?

Global - How does the process impact the global community? Is there a difference in how the process or incident is viewed in different countries?

Economic - How does the process impact the economy?

Environmental - How does the process and potential incidents impact the environment?

Societal - How does the process impact society? Does it change the attitudes of the public towards the company or industry?

4 Example Analysis - Primary Explosive Material Transfer

4.1 Process Background and Scope

In the defense industry, primary explosives are used in the production of ammunition and other devices. These materials are sensitive to heat, shock, electrostatic discharge (ESD), impact, and friction. The process of transferring these materials from one location to another during processing occurs regularly. One such scenario is the transfer of a small quantity of Compound B from a pass-thru box to a hopper that feeds a press. An operator carries the Compound B in a small jar from the pass-thru box to the hopper. The scope of the analysis is from the time the operator picks up the jar of Compound B to the time the jar is emptied into the hopper.

4.2 Process Flow Diagram

This animated gif shows the process of moving a small quantity of material in a jar from the pass-thru to the the hopper.

4.3 Incident Description

On April 18, 20___, an operator was transferring a small quantity of Compound B from a pass-thru box to a hopper that feeds a press. The operator was wearing a lab coat and gloves. The operator picked up the jar of Compound B from the pass-thru box and was walking towards the hopper when the operator fell. The jar flew towards the hopper and upon impact exploded and caused a fire. The operator was injured and the fire was extinguished by the fire suppression system. The operator was taken to the hospital and treated for burns and lacerations. The operator was released from the hospital the next day.

4.4 Process Safety Information (PSI)

Compound B is a complex of a reactive salt and heavy metals. It is toxic to living organisms and is unstable. It is sensitive to heat, shock, ESD, impact, and friction. It is used in the production of ammunition and other devices. The material is stored in a magazine and during processing, a portion of the storage amount is separated inside a shielded enclosure into a small jar. That jar is then transferred to a hopper that also is shielded. The hopper feeds a press that forms the material into a shape that is used in the production of ammunition.

SDS (Example information for illustrative purposes only)

The SDS for Compound B has the following applicable items:

- **Physical and Chemical Properties** - Compound B is a white powder that is odorless. It is a complex of a reactive salt and heavy metals. It is toxic to living organisms and is unstable. It is sensitive to heat, shock, ESD, impact, and friction.
- **Stability and Reactivity** - Compound B is unstable and is sensitive to heat, shock, ESD, impact, and friction.
- **Toxicological Information** - Compound B is toxic to living organisms.
- **Handling and Storage** - Compound B should be stored in a magazine. During processing, a portion of the storage amount is separated inside a shielded enclosure into a small jar. That jar is then transferred to a hopper that also is shielded.
- **Exposure Controls and Personal Protection** - Operators should wear lab coats and gloves when handling Compound B. Operations should control ESD and avoid impact and friction scenarios.

Small-scale Safety Testing

Safety testing with friction, impact, and ESD devices have shown that the threshold initiation level (a 3.4% chance of ignition) is 30 lbf at 8 feet per second, 10 cm, and 150 mJ, respectively.

Equipment Details

The pass-thru box is a shielded enclosure that has a door on each side. The operator opens the door on one side and places the jar of Compound B inside. The operator then closes the door and opens the door on the other side. The operator then removes the jar of Compound B from the pass-thru box. The hopper is a shielded enclosure that has a door on the top. The operator opens the door and empties the jar of Compound B into the hopper. The operator then closes the door.

Previous Incidents

There have been no previous incidents involving the transfer of Compound B from the pass-thru box to the hopper. However, in a related process, an operator did drop a small quantity of Compound B without incident.

4.5 Hazards Analysis

HAZOP HAZard and OPerability studies are best suited for processes with flowing materials and multiple inter-related steps. A piping and instrumentation diagram (P&ID) is used to identify the process steps and the materials that flow between them. The P&ID is then used to identify the nodes for which the guide words can be applied.

FTA and FMEA A Fault-Tree Analysis (FTA) and a Failure Modes and Effects Analysis (FMEA) are best suited for processes that have fewer steps but can have a myriad of failure modes. These tools are used to identify the failure modes and the effects of those failures, including safeguards, and recommendations. An FTA and FMEA are better suited to this incident scenario than a HAZOP.

4.5.1 Fault Tree

This is a simplified fault tree for the incident scenario. The fault tree shows the top event (Injury during transfer) and the sub events that can initiate Compound B resulting in injury. Just a few of the potential events are given with friction and impact sceanrios.

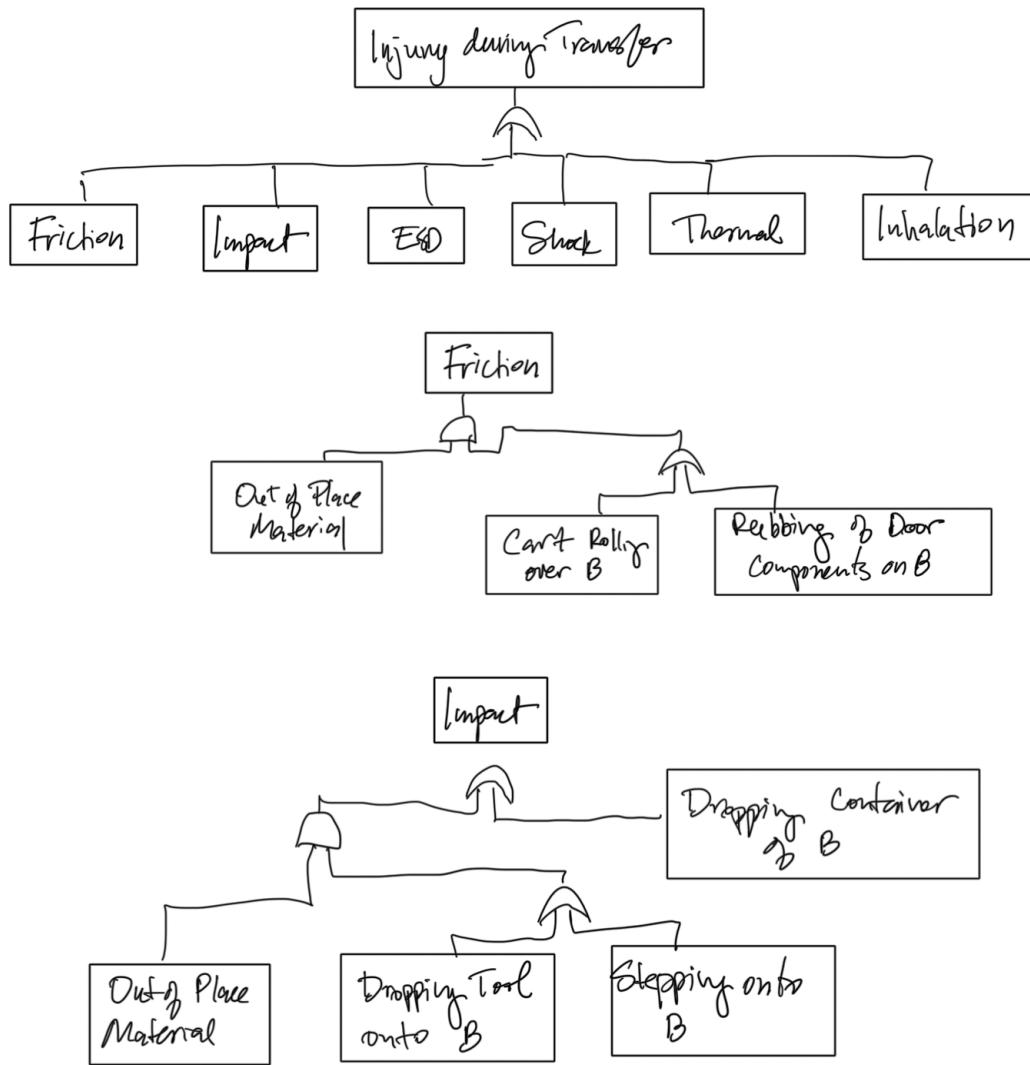


Figure 1: Example Fault Tree Analysis

4.5.2 FMEA

A simplified FMEA of the incident scenario based on the above fault tree is shown below. The FMEA shows the process steps, the failure modes, the effects of those failures, the safeguards, risk rating, and the recommendations.

Step	Failure Mode	Effect	Safeguards	Risk Rating	Recommendations
Pass-thru	Operator opens door with out-of-place material	Ignition and potential injury	Pass-thru metal doors are separated on plastic rollers	3D	Evaluate preventative maintenance measures for cleaning rollers
Pass-thru	Out-of-place material present	Potential ignition and injury	Operator visually inspects pass-thru once a week	3D	Evaluate preventative maintenance measures for cleaning pass-thru
Operator Transfer	Operator drops jar	Ignition of bulk collection of Compound B	Jar is made from hard plastic potentially reducing impact impulse	2C	Use a cart to transfer the jar from the pass-thru to the hopper with the cart under the pass-thru or hopper when the operator lowers or lifts the jar
Pass-thru	ESD discharge to material	Ignition of material with injury		3D	Operator should wear an ESD wrist strap at that station or have conductive shoes. Consider completing an ESD evaluation to quantify ESD hazards
Operator Transfer	A tool is dropped on the contaminated floor	Ignition of material with injury	The floor is cleaned once a week	4D	
More FTA Failure Modes	This list is insufficient. All of the FTA items should be adequately addressed				

4.6 Process Impacts

Ethical - The company has a responsibility to protect its employees from harm. The company should have a robust process safety management system in place to prevent incidents like this from occurring. The company should also have a robust incident investigation process to determine the root cause of the incident and to prevent similar incidents from occurring in the future. Any quantity of explosives material requires compliance with OSHA's Process Safety Management (PSM) requirements.

Global - The incident could have global implications if the company is a global supplier of ammunition or other devices. The company could lose business if the incident is not handled properly. The company could also face

legal action. Specifically, components used to manufacture Compound B is sourced from a country with less than ideal working conditions. The company could consider communicating and aiding the manufacturing country in improving working conditions.

Economic - This incident is not likely to prevent the company from completing the orders it has. However, the company could lose business if the incident is not handled properly. The company could also face legal action. The company could also face fines from OSHA for not having a robust process safety management system in place (if applicable).

Environmental - The incident could have environmental implications if the fire suppression system used to extinguish the fire allowed significant runoff of the Compound B into the environment. The company should have a robust environmental management system in place to capture and treat any flow streams including accident scenarios.

Societal - The incident could have societal implications if the company is a major employer in the area. The company could lose business if the incident is not handled properly, or this incident shows a lack of care for the employees if there is a pattern of incidents.

4.7 Documentation

4.7.1 Presentation

A five minute presentation with up to 30 slides is prepared and delivered with the team members. Since time is so limited, focus on the most important points to convey of the process, previous incidents, specific hazards, specific outcomes, and specific recommendations. You want to convey what should be learned from the process and or incidents with specific details that enforce safety principles.

4.7.2 Memorandum

A memorandum is prepared and delivered that has all of the details as exemplified above but to a fuller extent. Specific requirements including a rubric is given in Learning Suite. An example memorandum might include the following sections:

- **Process Background and Scope** - A detailed description of the process and the scope of the analysis.
- **Process Flow Diagram** - A process flow diagram or piping and instrumentation diagram.
- **Incident Description** - A detailed description of any incidents.
- **Process Safety Information** - A detailed description of the process safety information from multiple sources.
- **Hazards Analysis** - A subsection of the hazards analysis (with the full HA after the report as an addendum or appendix).
- **Process Impacts** - A description of the process impacts to global, economic, environmental, and societal aspects.
- **Recommendations** - A highlight of the critical recommendations from the analysis.
- **Conclusion** - A brief summary of the important points.

15 FMEA Case Study

Learning Outcomes

- Learn more about completing an FMEA from an in-depth example

Reading

- Read about an FMEA example on the CSB website.

Rocket Motor Manufacturing and Pratt and Whitney Space Propulsion in San Jose, CA

Download lecture freeform here: [https://github.com/clint-bg/safetyinjc/blob/main/physical/supportfiles/311_FMEA Case Study.pdf](https://github.com/clint-bg/safetyinjc/blob/main/physical/supportfiles/311_FMEA%20Case%20Study.pdf)

16 DHA and PHA

Learning Outcomes

- Know the difference between a FMEA, HAZOP, and PHA
- Know the difference between a DHA and a PHA

Reading

- Foundations of Spiritual and Physical Safety: with Chemical Processes; Chapter 5, Sections 2.4-3

17 Industrial Hygiene

Learning Outcomes

- Learn the four steps of industrial hygiene
- Evaluate the magnitude of exposures and responses
 - Vapors
 - Dusts
 - Noise
 - Thermal radiation

Reading

- Foundations of Spiritual and Physical Safety: with Chemical Processes; Chapter 6, Section 1
- Foundations of Spiritual and Physical Safety: with Chemical Processes; Chapter 7, Section 1

17.1 Industrial Hygienists

Industrial hygienists are typically part of the safety and health team in a company. They are responsible for identifying, evaluating, and controlling workplace hazards together with workers and management.



Figure 20: Picture of an Industrial Hygienist in a Chemical Plant
<https://images.app.goo.gl/EmTPJxCdSidwUoXQ6>

The four steps of industrial hygiene are:

1. **Anticipation:** Identifying potential hazards before they occur.
2. **Recognition:** Identifying hazards that are present.
3. **Evaluation:** Determining the magnitude of the exposure and the response.
4. **Control:** Implementing measures to control the hazards.

17.1.1 Common Tools used by Industrial Hygienists



Figure 21: Industrial Hygiene Tools

Note

The EH&S department together with Industrial Hygienists work to keep everyone safe. The safety team utilizes Process Safety Management (PSM) to identify and control hazards as we discussed in the previous lectures. However, it is important to remember that safety is everyone's responsibility. Some facilities have thousands of employees and only a few industrial hygienists. It is important to take responsibility for your own safety and work with the safety team.

17.2 Quantifying Exposures

TWA, time-weighted average, is the most common way to quantify exposures. It is the exposure averaged over an 8-hour workday.

17.2.1 Gases and Vapors

Note

Even if the exposure is longer than 8 hours, the TWA is still calculated over an 8-hour workday. For example, if a worker is exposed to a chemical for 12 hours, the TWA is calculated over 8 hours.

$$\text{TWA} = \frac{\sum_{i=1}^n C_i \cdot T_i}{8} = \frac{1}{8} \int_0^8 C(t) dt \quad (3)$$

where C_i is the concentration of the chemical at time i and T_i is the time the concentration is present.

17.2.2 Example Concentration Profile

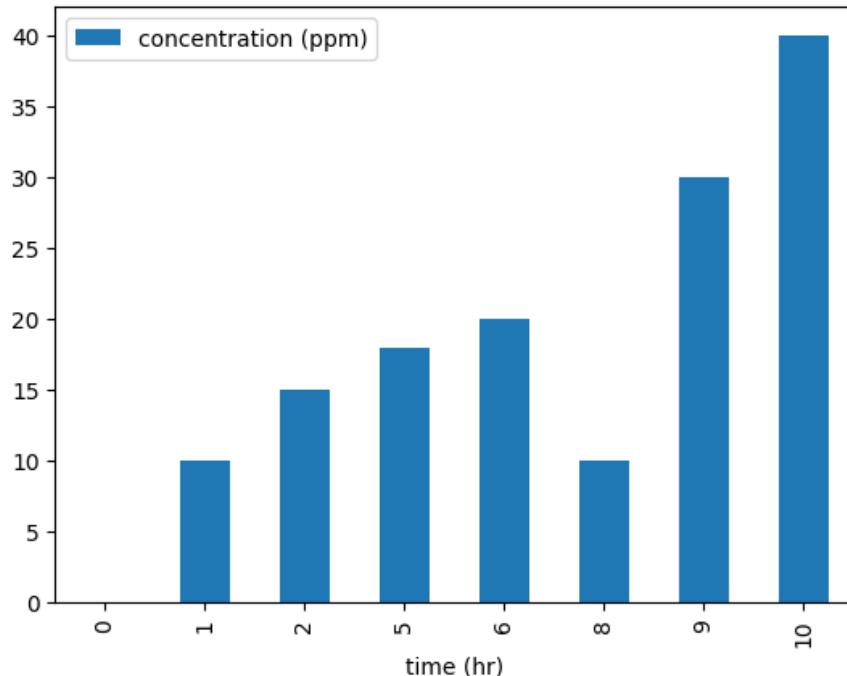
Time (hours)	Concentration (ppm)
0	0
1	10
2	15
5	18
6	20
8	10
9	30
10	40

```

import numpy as np
import matplotlib.pyplot as plt
import pandas as pd

#example discrete concentration profile
data = {'time (hr)': [0, 1, 2, 5, 6, 8, 9, 10],
        'concentration (ppm)': [0,10,15,18,20,10,30,40]}
df = pd.DataFrame(data)
df.plot(x='time (hr)', y='concentration (ppm)', kind = 'bar')
plt.show()

```



```

#TWA Calculation; Method 1 (assume the current measure is the same for the previous interval)
TWA_1 = 0; ti_1 = 0;
#for loop through each time interval
for i in range(1, len(df)):
    #calculate TWA for each interval
    C_i = df['concentration (ppm)'][i]
    t_i = df['time (hr)'][i]
    TWA_1 += C_i*(t_i -ti_1)
    ti_1 = t_i;
print(f'TWA_1 = {TWA_1/8:.1f} ppm')

TWA_1 = 23.6 ppm

#TWA Calculation; Method 2 (use the trapezoidal rule)
TWA_trap = 0;
#for loop through each time interval
for i in range(1, len(df)):
    #calculate TWA for each interval
    C_i = df['concentration (ppm)'][i]
    C_i_1 = df['concentration (ppm)'][i -1]
    t_i = df['time (hr)'][i]

```

```
t_i_1 = df['time (hr)'][i -1]
TWA_trap += (C_i+C_i_1)*(t_i -t_i_1)/2
print(f'TWA_trap = {TWA_trap/8:.1f} ppm')

TWA_trap = 21.4 ppm

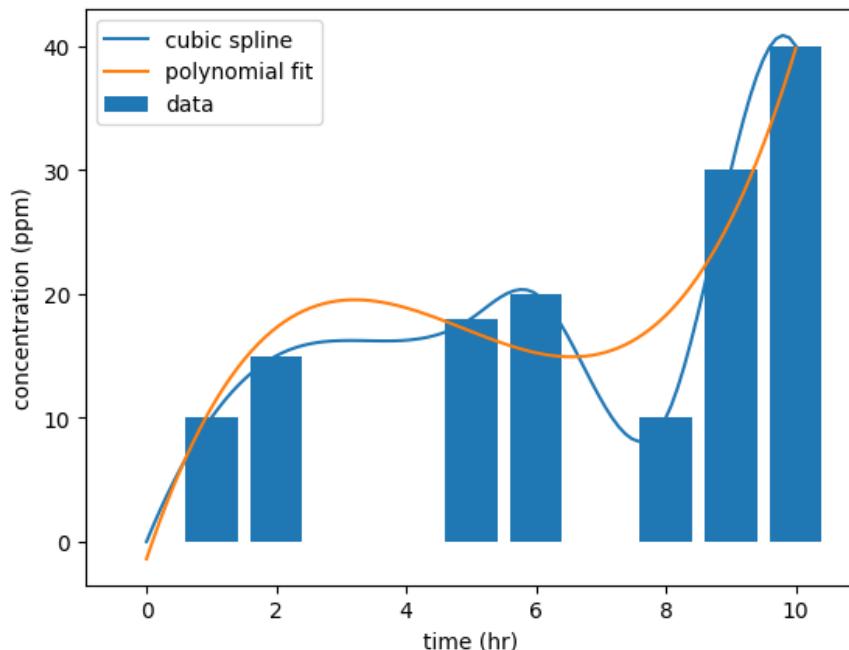
#TWA Calculation; Method 3 (fit a polynomial to the data and integrate with cspline1d_integral)
from scipy.interpolate import CubicSpline
#fit a polynomial to the data
cs = CubicSpline(df['time (hr)'], df['concentration (ppm)'])
#integrate the polynomial with quad
from scipy.integrate import quad
TWA_CSpline, err = quad(cs, 0, 10)
print(f'TWA_CSpline = {TWA_CSpline/8:.1f} ppm')

TWA_CSpline = 21.1 ppm

#fit a polynomial to the data
p = np.polyfit(df['time (hr)'], df['concentration (ppm)'], 3)
#integrate the polynomial
TWA_poly = quad(np.poly1d(p), 0, 10)[0]
print(f'TWA_poly = {TWA_poly/8:.1f} ppm')

TWA_poly = 22.1 ppm

#plot the data and the polynomial fit
t = np.linspace(0, 10, 100)
C = np.poly1d(p)(t)
plt.plot(t, cs(t), label='cubic spline')
plt.plot(t, C, label = 'polynomial fit')
plt.bar(df['time (hr)'], df['concentration (ppm)'], label = 'data')
plt.xlabel('time (hr)')
plt.ylabel('concentration (ppm)')
plt.legend()
plt.show()
```



```
#tabular display of the results
print('Method\tTWA (ppm)')
print(f'1\t{TWA_1/8:.1f}')
print(f'trapezoid\t{TWA_trap/8:.1f}')
print(f'CSpline\t{TWA_CSpline/8:.1f}')
print(f'Polynomial_3\t{TWA_poly/8:.1f}'')
```

Method TWA (ppm)

1 23.6

trapezoid 21.4

CSpline 21.1

Polynomial_3 22.1

Was the worker over exposed? If the TLV-TWA is 20 ppm for the above chemical, then YES, the worker was over exposed.

Consequences of Overexposure

Overexposure to chemicals can cause a variety of health effects. Some chemicals can cause immediate effects such as dizziness, nausea, and headaches. Others can cause long-term effects such as cancer, reproductive issues, and organ damage.

In order to prevent this scenario from happening again, the industrial hygienist would work with the safety team to implement control measures such as increased ventilation and the use of a respirator with a organic vapor cartridge for example.

- Using a respiratory for long periods of time is not ideal

17.2.3 Multiple Gaseous Chemicals

What if there are multiple hazardous vapors present?

Overexposure can be determined by the below equation:

$$\sum_{i=1}^n \frac{C_i}{\text{TLV-TWA}_i} > 1? \quad (4)$$

The TLV-TWA for gaseous mixtures can be found by:

$$\text{TLV-TWA}_{\text{mixture}} = \frac{\sum_{i=1}^n C_i}{\sum_{i=1}^n \frac{C_i}{\text{TLV-TWA}_i}} \quad (5)$$

Note

Once the mixture TLV-TWA is found, determining the exposure can be done using the same equation as before where the sum of the concentrations for each timeframe is summed and divided by 8 hours.

17.2.4 Dusts

Dusts are treated the same way but instead of using ppm, mg/m³ is used.

17.2.5 Noise

Sound pressure level (SPL) is used as an intensity measure. The lowest SPL that can be heard by the human ear is near 2E-5 Pa. Thus in the below equation I_o is 2E-5 Pa.

$$\text{dB} = 10 \log_{10} \left(\frac{I}{I_o} \right) \quad (6)$$

where P is the sound pressure and I is the intensity.

See "Permissible Noise Exposures," [<https://www.osha.gov/laws-regulations/standardnumber/1910/1910.95>] (<https://www.osha.gov/laws-regulations/standardnumber/1910/1910.95>) where you can use the combination rule of $\sum \frac{D_i}{\text{MTA}_i} > 1?$ to determine if the worker is overexposed, where D_i is the duration at the given dB sound level and MTA is the maximum time allowed at that level.

17.2.6 Thermal Radiation

Flames, hot metal surfaces, and other heat sources can cause burns. The heat flux is the amount of heat energy transferred per unit area per unit time. The heat flux is measured in W/m².

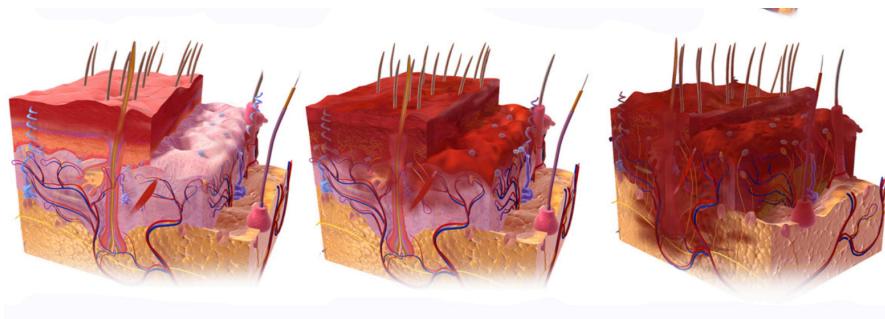


Figure 23: Industrial Hygiene Tools [Image Reference](#)

From Handbook of Chemical Hazards Analysis Procedures (1989), Table 4.2

Heat Radiation Intensity (kW/m ²)	Time for pain (seconds)	Time for 2nd Degree Burn (seconds)
1	115	663
2	45	187
3	27	92
4	18	57
5	13	40
6	11	30
8	7	20
10	5	14
12	4	11

Reference Link

You may have to click the 'reference link' twice to get it to work.

Initial Source

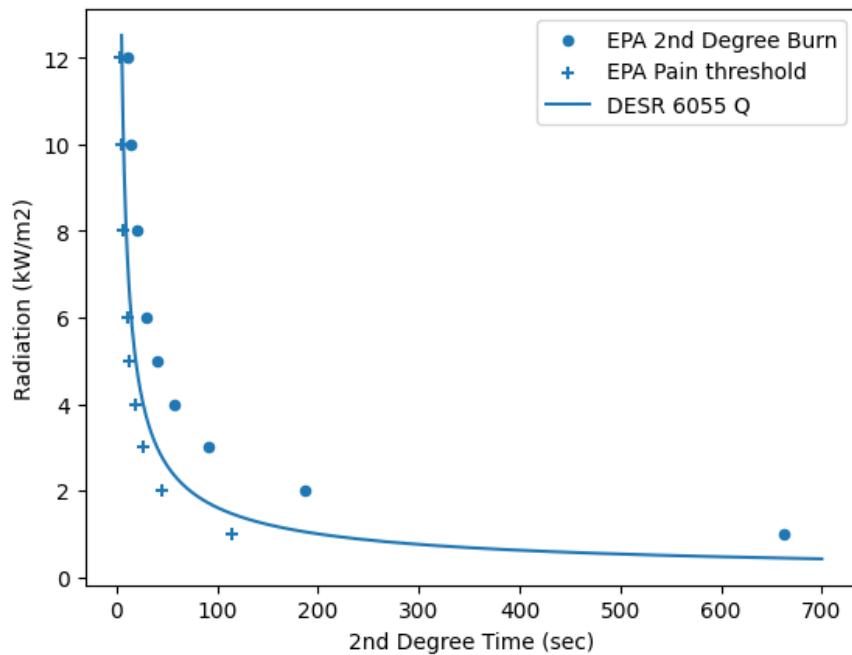
The initial source of the above table is Buettner, K, "Effects of Extreme Heat and Cold on Human Skin, II Surface Temperatures, Pain and Heat Conductivity in Experiments with Radiant Heat," Journal of Applied Physiology, 1951, 3, 703.

```
data = {'Radiation (kW/m2)':[1,2,3,4,5,6,8,10,12],  
       'Pain time (sec)':[115,45,27,18,13,11,7,5,4],  
       '2nd Degree Time (sec)':[663, 187,92,57,40,30,20,14,11]}  
df = pd.DataFrame(data)
```

[DESR 6055.09](#) is the handbook for the Department of Defense and gives the following relationship for heat flux (q, kW/m²) and time,t, before a 2nd degree burn:

$$t = 200 \cdot q^{-1.46} \quad (7)$$

```
#Causitive variable from Probit correlations from death from burning  
time = np.linspace(5, 700, 1000)  
def Q2(t):  
    return (t/200)**(-1/1.46)  
  
df.plot(x='2nd Degree Time (sec)', y='Radiation (kW/m2)', kind = 'scatter', label='EPA 2nd Degree Burn')  
plt.scatter(df['Pain time (sec)'], df['Radiation (kW/m2)'], marker = '+', label = 'EPA Pain threshold')  
plt.plot(time, Q2(time), label = 'DESR 6055 Q')  
plt.legend()  
  
<matplotlib.legend.Legend at 0x16c44ef10>
```



200/60

3.333333333333335

The above plot shows that the relationship used for the military (DESR 6055) is conservative relative to the EPA's Handbook of Chemical Hazards Analysis Procedures. Consider that in full sun, the approximate radiation is 1 kW/m². Would it really take 660 seconds (11 minutes) to get a sunburn that blisters? No, it would take longer indicating that both relationships are conservative.

Estimating thermal flux from a fire The radiation from a fire or fireball decreases with the square of the distance from the fire. The heat flux is given by:

$$q = \frac{P}{4\pi r^2} \quad (8)$$

where P is the power of the fire in watts and r is the distance from the fire in meters.

Thus, if a fire has a power of 1 MW and you are 10 meters away, the heat flux is:

'Your answer here'

How long would you have before a 2nd degree burn?

18 Toxicity

Learning Outcomes

- Learn how toxicants enter and are eliminated from the body.
- Understand effects of toxicants, including response vs. dose
- Use probit equations to determine response to dose.
- Understand exposure limits such as Threshold Limit Value (TLV) and Permissible Exposure Limit (PEL).

Reading

- Read an article on the toxicity of a given substance

18.1 Entry Routes of Toxicants

Route	Entry	Control/ Safeguards
Inhalation	Lungs	Ventilation, respirators, hoods
Ingestion	Mouth	Hygiene, gloves, Guidelines on eating, drinking, etc
Injection	Skin	Gloves, protective clothing
Absorption	Skin	Gloves, protective clothing

18.2 Toxin Blood Concentration

18.3 Responses to Toxicants

Irreversible Effects:

- Cancinogens (cancer) Like asbestos, tobacco, formaldehyde, and ionizing radiation
- Mutagens (genetic changes) Alkylating agents like diethyl sulfate and others
- Teratogens (birth defects) Like alcohol, lead, mercury, and thalidomide
- Reproductive toxins Like lead, mercury, and cadmium

Reversible Effects:

- Dermatotoxicants (skin)
- Neurotoxicants (nervous system)
- Hepatotoxicants (liver)
- Nephrotoxicants (kidneys)
- Pulmonotoxicants (lungs)
- Hemotoxicants (blood)

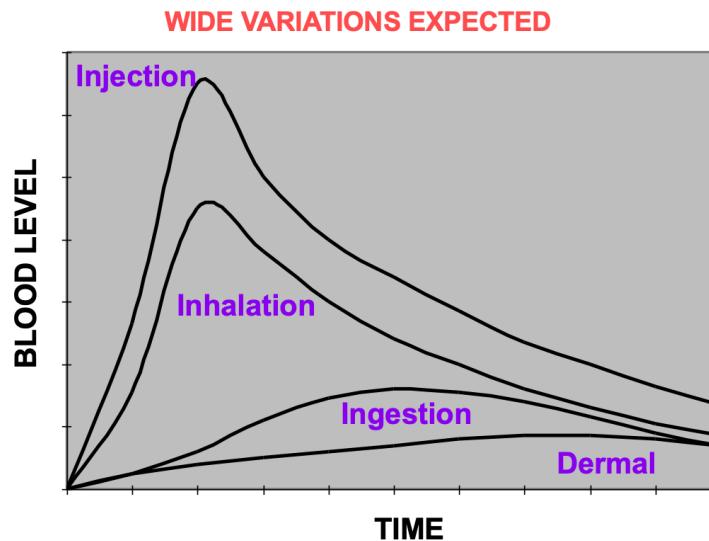


Figure 24: Toxin Blood Concentration Over Time

18.4 Toxin Storage and Elimination

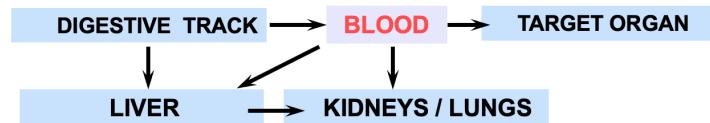


Figure 25: Toxin Storage and Elimination

Excretion: kidneys (urine), liver (bile), lungs (breath), skin (sweat)

Detoxification: liver (chemical changes through enzymes)

Storage: fat, bone, hair, nails, etc.

18.5 Dose-Response Relationships

Suppose we have the following data from a toxicology study with mice:

Dose (mg/kg)	Response (Death)
0.1	0
0.2	0
0.3	0
0.4	0
0.5	1 of 20
0.75	2 of 20
1.0	5 of 20
1.25	12 of 20
2	13 of 20
5	19 of 20

```

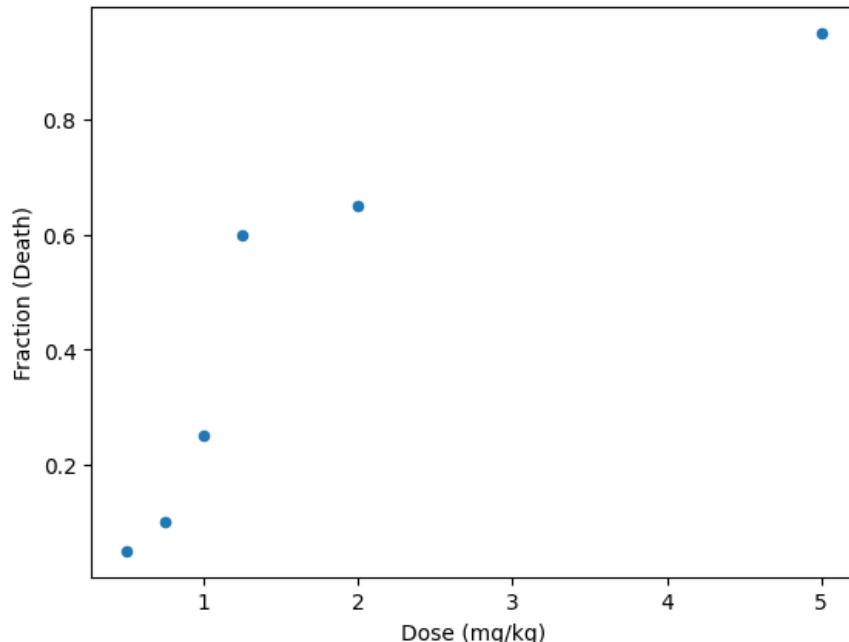
import numpy as np
import matplotlib.pyplot as plt
import pandas as pd

data = {'Dose (mg/kg)': [0.1, 0.2, 0.3, 0.4, 0.5, 0.75, 1.0, 1.25, 2, 5], 'Response (Death)': [0, 0, 0,
df = pd.DataFrame(data)
df['Fraction (Death)'] = df['Response (Death)'] / 20

df.plot(x='Dose (mg/kg)', y='Fraction (Death)', kind='scatter')

<Axes: xlabel='Dose (mg/kg)', ylabel='Fraction (Death)'>

```



Some questions we might ask:

- Were the mice that survived a lower dose then dosed with a higher dose?
- How does this toxicant affect humans? In the same way as mice?
- What is the LD50 (lethal dose for 50% of the population)?
- What would be a threshold dose?

If we fit a response curve to the data, we can answer some of those questions.

Lets fit a gaussian curve to the data and see what we get.

```

# fit a cumulative gaussian to the data
from scipy.optimize import curve_fit
from scipy.stats import norm

def cumulative_gaussian(x, mu, sigma):
    return norm.cdf(x, mu, sigma)

popt, pcov = curve_fit(cumulative_gaussian, df['Dose (mg/kg)'], df['Fraction (Death)'])

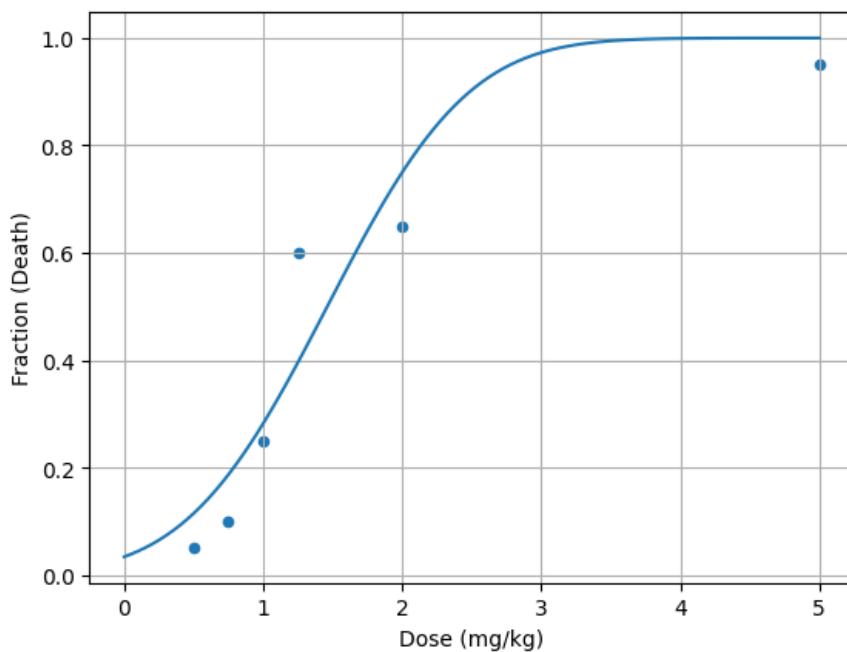
```

```

x = np.linspace(0, 5, 100)
y = cumulative_gaussian(x, *popt)

df.plot(x='Dose (mg/kg)', y='Fraction (Death)', kind='scatter')
plt.plot(x, y, label='fit'); plt.grid()
plt.show()

```



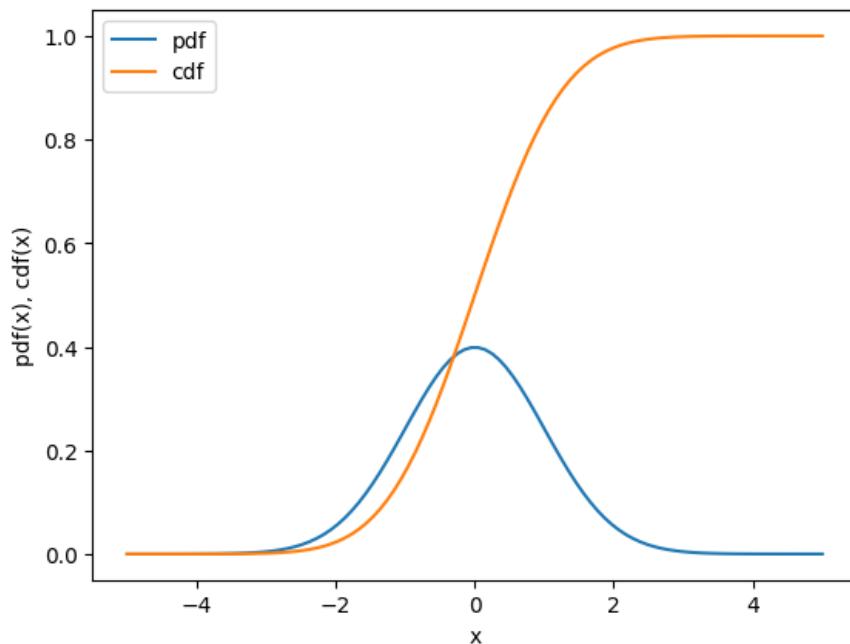
What's the cumulative distribution function for a gaussian curve?

It is the integral of the gaussian curve from negative infinity to x...

```

# plot of the gaussian curve
x = np.linspace(-5, 5, 100)
y = norm.pdf(x, 0, 1)
y2 = norm.cdf(x, 0, 1)
plt.plot(x, y, label='pdf');
plt.plot(x, y2, label='cdf');
plt.xlabel('x'); plt.ylabel('pdf(x), cdf(x)');
plt.legend();
plt.show()

```



From the above cumulative fit, we can calculate the LD50 and the threshold dose.

```
# Calculation of the LD50 and threshold dose

# LD50
mu, sigma = popt
ld50 = norm.ppf(0.5, mu, sigma) # ppf is the inverse of the cdf
#print the LD50 with 2 decimal places
print('LD50:', round(ld50, 2), 'mg/kg')

# threshold dose
threshold = norm.ppf(0.01, mu, sigma)
print(f'Threshold: {threshold:.2f} mg/kg')

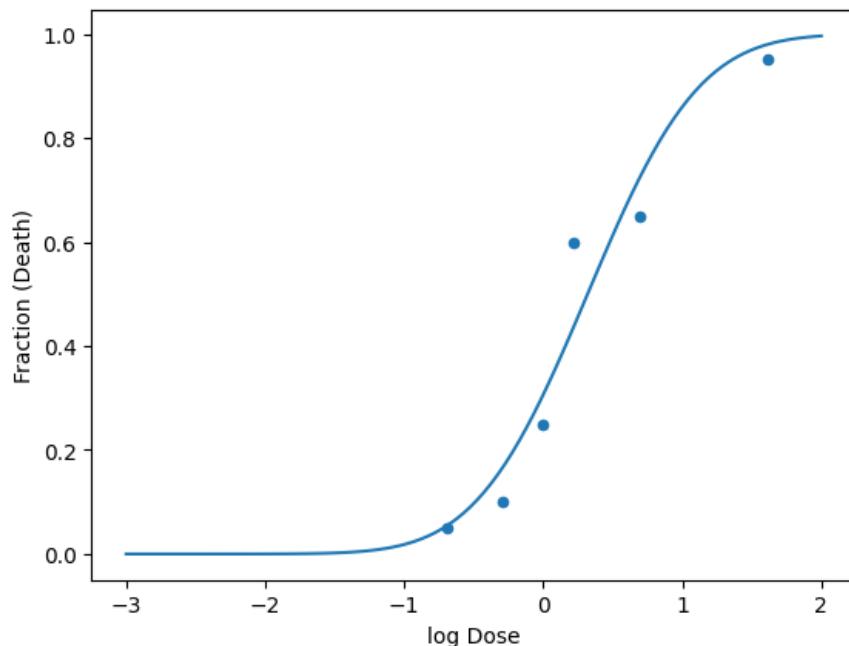
LD50: 1.45 mg/kg
Threshold: -0.18 mg/kg
```

Here we've given an estimate of the LD50 and the threshold dose (LD01). But wait, a negative value for the dose? That doesn't make sense.

In order to prevent that from happening, we can transform the dose or causitive variable (use the logarithmic function).

```
# log dose
df['log Dose'] = np.log(df['Dose (mg/kg)'])

# fit the cumulative gaussian to the log dose
pop, pcov = curve_fit(cumulative_gaussian, df['log Dose'], df['Fraction (Death)'])
x = np.linspace(-3, 2, 100)
y = cumulative_gaussian(x, *pop)
df.plot(x='log Dose', y='Fraction (Death)', kind='scatter')
plt.plot(x, y, label='fit');
plt.show()
```



Now lets try again on determining the LD50 and threshold dose.

```
# Calculation of the LD50 and threshold dose

# LD50
mu, sigma = popt
ld50 = np.exp(norm.ppf(0.5, mu, sigma)) # we need to transform back to the original scale with np.exp
#print the LD50 with 2 decimal places
print('LD50:', round(ld50, 2), 'mg/kg')

# threshold dose
threshold = np.exp(norm.ppf(0.01, mu, sigma)) # we need to transform back to the original scale with np
print(f'Threshold: {threshold:.2f} mg/kg')

LD50: 1.37 mg/kg
Threshold: 0.33 mg/kg
```

There is a slight difference in the LD50, which is expected as the weighting is different for the data in log space. In this case it is more conservative.

The threshold dose (1% chance of death) is also different (not negative) and thus realistic.

18.5.1 Probit Equation

It can be convenient to use the probit equation to determine the response to a dose. The probit equation is essentially the inverse of the cumulative distribution function of the normal distribution and can be used to linearize the dose-response relationship.

Transforming the fraction to a probit value...

```
# transform of the probability or fraction response to probit
def probit(p):
    return 5 + norm.ppf(p)

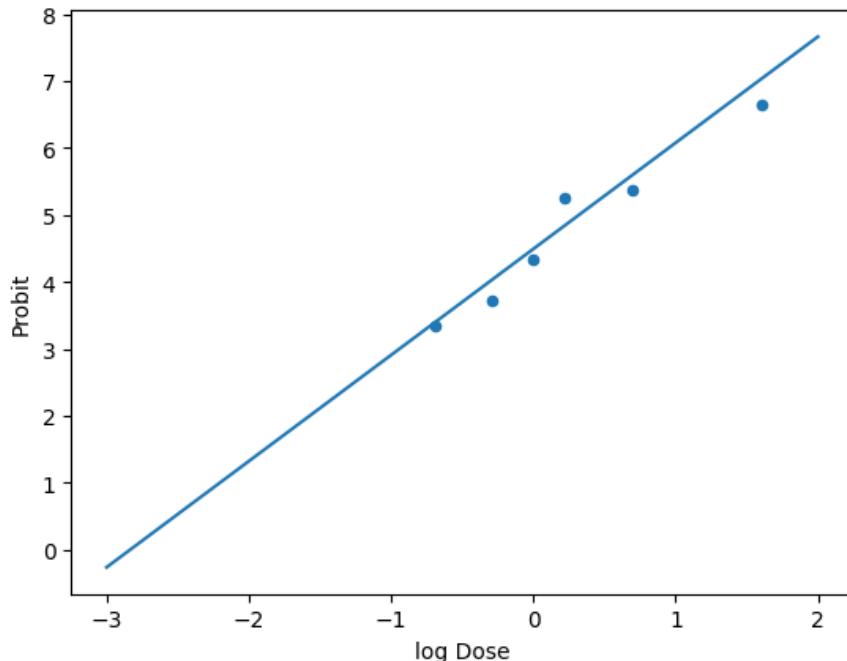
df['Probit'] = probit(df['Fraction (Death)'])
```

df

	Dose (mg/kg)	Response (Death)	Fraction (Death)	log Dose	Probit
0	0.10	0	0.00	-2.302585	-inf
1	0.20	0	0.00	-1.609438	-inf
2	0.30	0	0.00	-1.203973	-inf
3	0.40	0	0.00	-0.916291	-inf
4	0.50	1	0.05	-0.693147	3.355146
5	0.75	2	0.10	-0.287682	3.718448
6	1.00	5	0.25	0.000000	4.325510
7	1.25	12	0.60	0.223144	5.253347
8	2.00	13	0.65	0.693147	5.385320
9	5.00	19	0.95	1.609438	6.644854

```
# plot of the data with the probit scale
df.plot(x='log Dose', y='Probit', kind='scatter')
plt.plot(x, probit(y), label='fit')

[<matplotlib.lines.Line2D at 0x171041bb0>]
```



Instead of fitting a gaussian and then transforming the dose, we can fit the probit equation directly to the data. This will give us the two probit constants k_1 (intercept) and k_2 (slope) referenced in Table 2-5 in the textbook (Crowl and Louvar).

```
# fit a line (probit linear model) to the data
#first drop -inf values
df = df[df['Probit'] > 0]
```

```
k2,k1 = np.polyfit(df['log Dose'], df['Probit'], 1) # the first value is the slope and the second the intercept
print(f'k1: {k1:.2f}, k2: {k2:.2f}')
```

k1: 4.40, k2: 1.47

Once we have the probit constants, we can use them to determine the response to any dose, including the LD50 and threshold dose.

```
#using the probit constants to calculate the LD50 and threshold dose
ld50_log = (5 - k1) / k2
ld50 = np.exp(ld50_log)
print(f'LD50: {ld50:.2f} mg/kg')

# threshold dose
threshold_log = (probit(0.01) - k1) / k2
threshold = np.exp(threshold_log)
print(f'Threshold: {threshold:.2f} mg/kg')

LD50: 1.50 mg/kg
Threshold: 0.31 mg/kg
```

We can also transform from probit back to fraction response...

```
import math
def P(Y):
    if Y != 5:
        return 0.50*(1+(Y -5)/(abs(Y -5))*math.erf(abs(Y -5)/math.sqrt(2)))
    else:
        return 0.50
```

18.5.2 Probit Correlation Example

Suppose we use Table 2-5 in the textbook (Crowl and Louvar) to estimate the probability of death from exposure to a fireball (say the sun). The causitive variable is $t_{exposure} \cdot I^{4/3}/1E4$ where I is the radiation intensity. Say we stay out in the sun for 8 hours. The typical radiation intensity in full sun is 1000 W/m². What is the probability of death?

18.6 TLV and PEL

TLV (Threshold Limit Value) and PEL (Permissible Exposure Limit) are exposure limits for toxicants. They are typically given in units of concentration (e.g. ppm, mg/m³).

- TLV-TWA (Time Weighted Average) is the average concentration over an 8-hour workday that is believed to be safe for most workers.
- TLV-STEL (Short Term Exposure Limit) is the maximum concentration for a short period of time (15 minutes) that is expected to be safe.
- TLV-C (Ceiling) is the maximum concentration that should never be exceeded.

These TLV values are established by the American Conference of Governmental Industrial Hygienists (ACGIH).

OSHA (Occupational Safety and Health Administration) has established PEL values which are similar to TLV values.

IDLV (Immediately Dangerous to Life and Health) is the concentration that is immediately dangerous to life and health.

18.6.1 Example with Probit and TLV

Table 2-5 gives probit parameters for dying from ammonia. Calculate the LD50 from these parameters and compare it with the LD50 reported in the literature. Also, compare the TLV-TWA to determine a probability for death from the probit parameters.

19 Chemical Reactivity

Learning Outcomes

- Use the Gibbs free energy to make a stability estimate

Reading

- Foundations of Spiritual and Physical Safety: with Chemical Processes; Chapter 6, Sections 2

Download pdf of lecture freeform here: [physical/supportfiles/311Reactivity.pdf](#)

See also a pdf of mass and energy balances: [physical/supportfiles/MassAndEnergyBalances.pdf](#)

20 Static Control

Learning Outcomes

- Understand the concept of inerting
- Understand the concept of electrostatic charging, relation, and discharge
- Understand the concept of static control
- Understand basics of electrical classification and explosion proof equipment

Reading

- Foundations of Spiritual and Physical Safety: with Chemical Processes; Chapter 6, Sections 2.1

20.1 Inerting Approaches

Inerting is the process of replacing the atmosphere in a vessel with an inert gas (nitrogen, carbon dioxide, etc). This is done to prevent the formation of flammable/explosive mixtures. There are multiple approaches to purging and inerting:

- vacuum purge (removing the atmosphere from the vessel and replacing it with an inert gas in stages; stages used to prevent the container from collapsing)
- pressure purge (replacing the atmosphere in the vessel with an inert gas by pressurizing the vessel, also completed in stages)
- sweep purging (replacing the atmosphere in the vessel with an inert gas by flowing the inert gas through the vessel)
- siphon purging (replacing the atmosphere in the vessel with a liquid then filling with an inert gas)
- combination of the above

20.2 ESD and Static Control

Further info here:

Download pdf of lecture freeform here: [physical/supportfiles/ESD.pdf](#)

FLAMMABILITY PART 1

Clint Guymon

Brigham Young University

1st Jan, 2025

created in  Curvenote

Keywords Spiritual Safety, Process Safety, Chemical Engineering, Risk Assessment

Learning Outcomes

- Understand characteristics of fires and explosions
- Understand key parameters of flammability like LFL, UFL, etc.

Reading

- Foundations of Spiritual and Physical Safety: with Chemical Processes; Chapter 6, Sections 2.2

Flames are a common hazard in many industries. Flames are all around us and they serve purposes from conversion of chemical bond energy to heat, propulsion of rockets, to cooking in our homes. These scenarios are planned for and designed to safely occur. However, there are many scenarios where flames are not planned for and can cause catastrophic damage.

Fires cause billions of dollars in damage every year. In the United States alone, the National Fire Protection Association (NFPA) estimate that in 2022, local fire departments responded to an estimated 1.5 million fires. Those fires caused 3,790 civilian fire deaths and 13,250 reported civilian fire injuries. The property damage caused by these fires was estimated at \$18 billion. [See the NFPA Site Here for Further Information](#)

Learning Objectives:

- Describe the nature of fires and explosions.
- Define the fire triangle and explain how to use it to prevent flammable mixtures.
- Characterize the flammability of gases, liquids, and dusts.
- Estimate flammability parameters for mixtures.

1 Fires and Explosions

The below pie chart shows the fraction of fires per category for the approximately 4000 people that died in 2022. Notice that the majority of fires are residential fires.

Industrial loss of life and property is also due primarily to fires and explosions.



Figure 1: Chemical Processing Fire Example Image. Credit: <https://jenikirbyhistory.getarchive.net/media/fire-glowing-hot-372895>

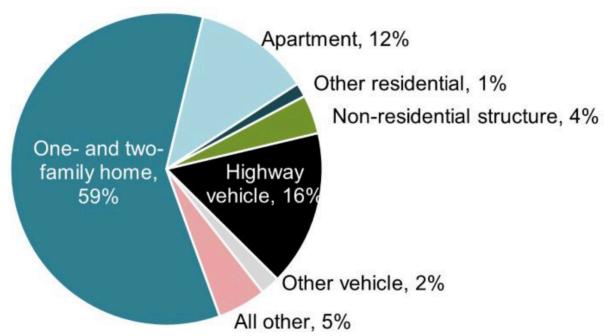


Figure 2: Fire Deaths by Category Pie Chart

1.1 What is a fire?

A rapid exothermic reaction. Or in other words, a fuel reacts with an oxidizer once ignited to produce a thermodynamically favored chemical change. Heat, light, and sound can be produced. The heat can be used to sustain the reaction, and the light and sound are often the first signs of a fire.

1.2 What is an explosion?

An explosion is a rapid release of energy in an uncontrolled manner. This can be due to a rapid exothermic reaction, or a rapid release of pressure. The energy release can be due to a chemical reaction, or a physical change in state.

1.3 Hazardous Effects of Fires and Explosions

- Thermal radiation
- Asphyxiation
- Toxic gases
- Blast waves
- Fragmentation

These effects can cause damage to property, injury, and loss of life.

2 How do fires start?

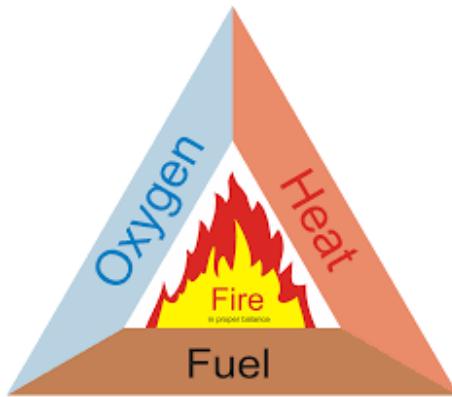


Figure 3: Fire Triangle. Credit to https://commons.wikimedia.org/wiki/File:Fire_triangle_2.svg

Fires and explosions require a fuel, an oxidizer, and an ignition source. This is known as the fire triangle.

Fuel

Fuels can be solid, liquid or gases:

- Solids: wood, wood byproducts, metal particles, combustible dusts, plastics, rubber, etc.
- Liquids: gasoline, diesel, kerosene, alcohols, etc.
- Gases: methane, propane, hydrogen, etc.

Oxidizer

Oxidizers are substances that provide oxygen to the reaction. Common oxidizers are:

- Solids: perchlorates, nitrates, etc.
- Liquids: hydrogen peroxide, nitric acid, sulfuric acid, etc.
- Gases: oxygen, chlorine, fluorine, etc.

Ignition Source

- Friction, Impact, Static Electricity, Electrical Sparks, Hot Surfaces, Open Flames, etc.

2.1 What actually burns?

In all but the most unique of circumstances, it is the vapor of a liquid or solid that burns. The vapor or gas mixes with the oxidizer and ignites. The heat from the ignition sustains the reaction.

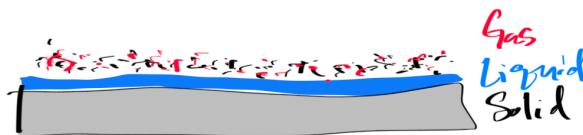


Figure 4: Surface Melt and Vaporization

3 How to Prevent Fires and Explosions

Ignition sources are plentiful and can be difficult to control. However, the fuel and oxidizer can be controlled. The most common way to prevent fires and explosions is to control the fuel and oxidizer. Often either the concentration of the fuel or the concentration of the oxidizer is controlled to prevent a fire or explosion.

3.1 How low or high do the concentrations need to be altered?

3.1.1 Lower Flammability Limit (LFL)

- **LFL:** **LFL** is the lowest concentration of fuel in air that will support a flame.
- **LOL:** **LOL** is the lowest concentration of a fuel in pure oxygen that will support a flame.
- **LOC:** Also can define **LOC** (Limiting Oxygen Concentration) as the lowest concentration of oxygen in air that could result in combustion for a given fuel. This can be defined for oxygen in air or for a different gas.
- Units are typically in volume percent (vol%) or equivalently mole percent (mol%).

3.1.2 Upper Flammability Limit (UFL)

- **UFL:** **UFL** is the highest concentration of fuel in air that will support a flame.
- **UOL:** **UOL** is the highest concentration of a fuel in pure oxygen that will support a flame.

- Units are typically in volume percent (vol%) or equivalently mole percent (mol%).

Typical Values for LFL and UFL

Substance	LFL (vol%)	UFL (vol%)
Methane	5	15
Propane	2.1	9.5
Hydrogen	4	75
Gasoline	1.4	7.6
Ethanol	3.3	19
Acetylene	2.5	83

Typical Values for LOC in Air

Substance	LOC (vol%)
Hydrogen	5
Methane	12
Ethane	11

3.2 Controlling the temperature

Flash point temperature is the lowest temperature at which a liquid gives off enough vapor to form an ignitable mixture with air near the surface of the liquid.

Typical Flash Points

Substance	Flash Point (°C)
Methane	-188
Propane	-104
Gasoline	-43
Methanol	11

Autoignition temperature is the lowest temperature at which a substance will spontaneously ignite without an external ignition source.

Typical Autoignition Temperatures

Substance	Autoignition Temperature (°C)
Methane	600
Toluene	536
Gasoline	280
Methanol	463

3.3 Graphical Image of Flammability Limits, Autoignition Temperatures, and Flash Points

4 Equipment used for experimental determination

4.1 Flash point

Closed cup apparatus

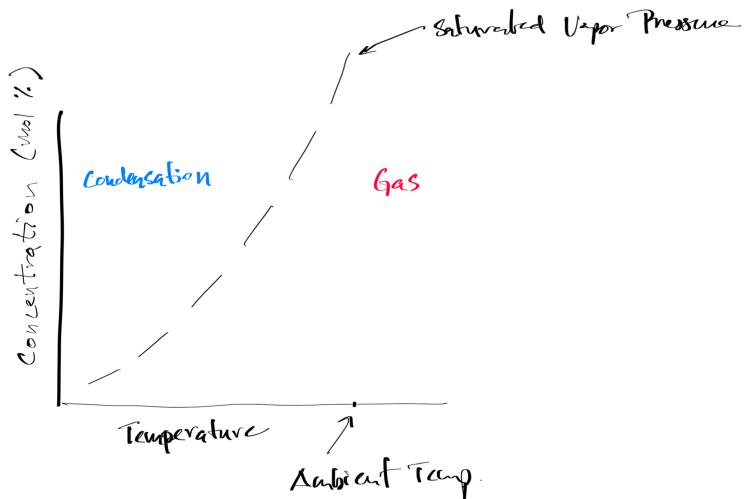


Figure 5: Graphical Image of Vapor Pressure

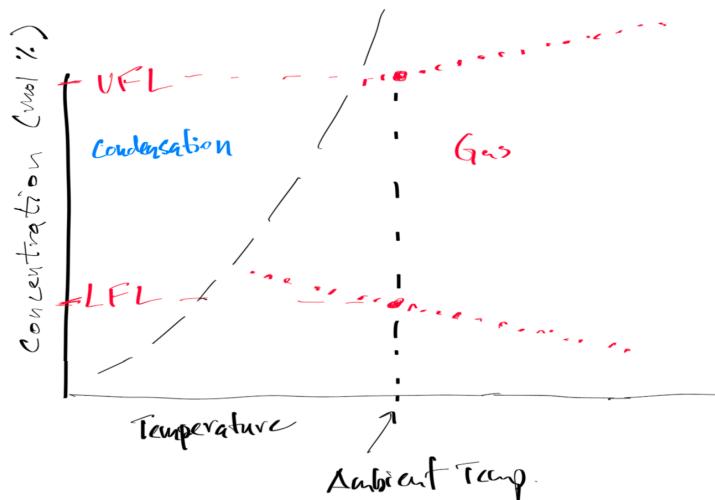


Figure 6: Graphical Image of LFL and UFL

4.2 Flammability limits

```

import numpy as np
import matplotlib.pyplot as plt
import pandas as pd

data = {'Fuel Conc.':[2.1,2.5,3.5,4,4.2,5.8,6.4,7,7.7], 'Max Pressure':[0,2.5,6,8,8.5,7.6,5,3,.03]}
df = pd.DataFrame(data)

df.plot(x='Fuel Conc.',y='Max Pressure',kind='scatter')
#fit a parabola to the data
p = np.polyfit(df['Fuel Conc.'],df['Max Pressure'],2)
#plot the parabola
x = np.linspace(2,8,100)
y = lambda x: p[0]*x**2 + p[1]*x + p[2]

```

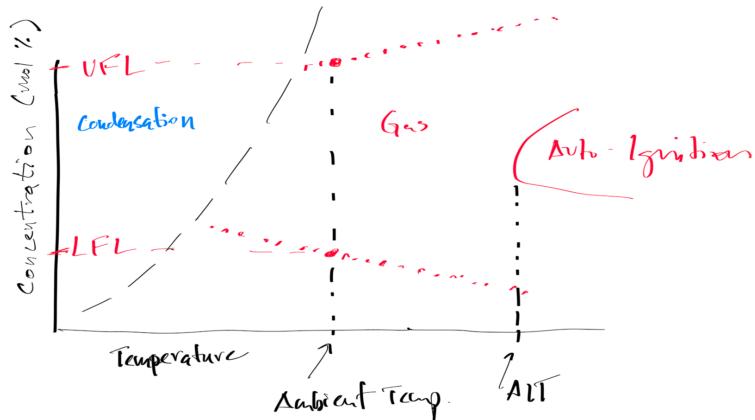


Figure 7: Graphical Image of Autoignition Temperatures

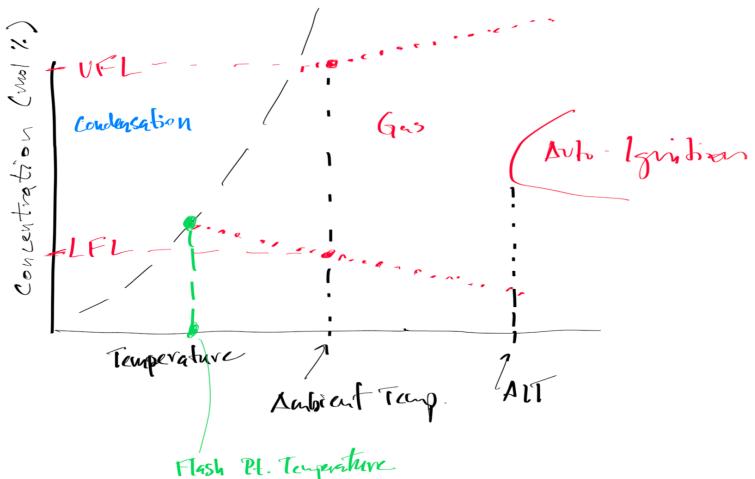


Figure 8: Graphical Image of Flash Point



Figure 9: Closed Cup Apparatus Image 1



Figure 10: Closed Cup Apparatus Image 2

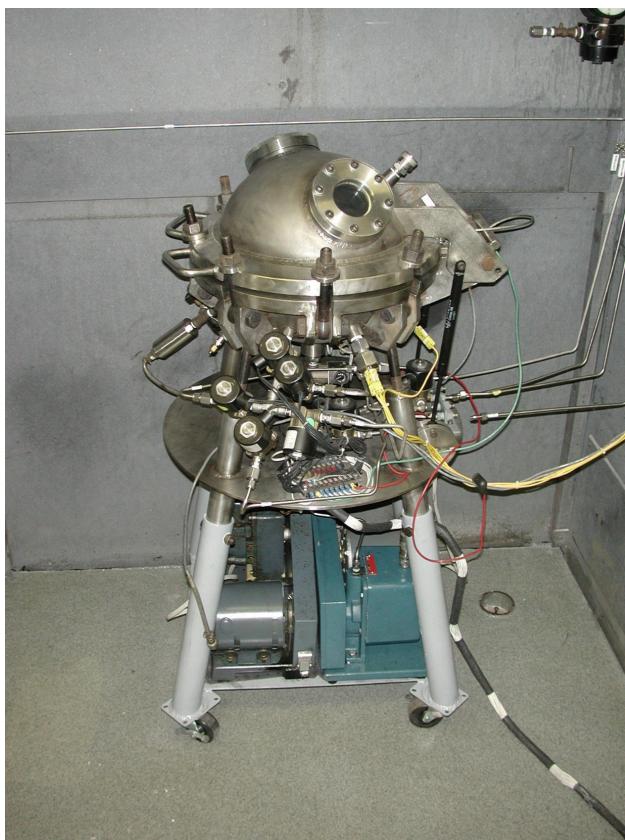
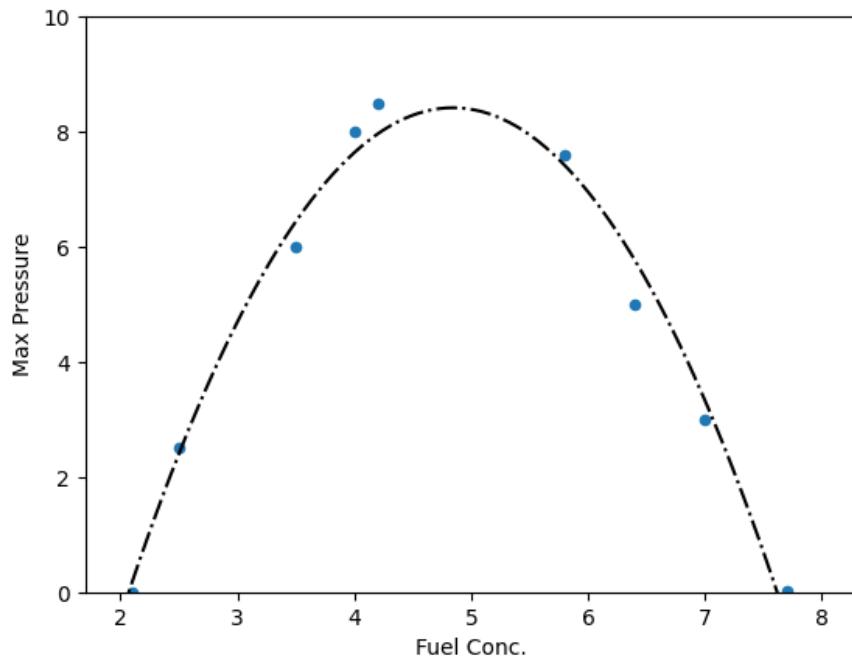


Figure 11: 20 Liter Sphere

```
plt.ylim(0,10)
plt.plot(x,y(x),'k -.')
plt.show()
```



5 Empirical Estimation of Flammabilities

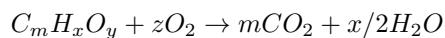
From Crowl and Louvar (4th edition of Chemical Process Safety, Chapter 6), the following empirical equations can be used to estimate the LFL and UFL for a gas or vapor:

Flash Point

$$T_f = a + \frac{b(c/T_b)^2 e^{-c/T_b}}{1 - e^{-c/T_b}} \quad (1)$$

where a,b, and c are constants, and T_b is the normal boiling point of the liquid and T_f is the flash point. See Crowl and Louvar for the constants.

Reaction Stoichiometry



How do you get the stoichiometric concentration for say propane in air?

Note



Note

There are 3.72 moles of nitrogen for every mole of oxygen in air. So the stoichiometric concentration of propane in air is:

$$\frac{1}{1 + 5 + 5 * 3.72} = 0.041 \quad (3)$$

LFL and UFL: Method 1

$$LFL = 0.55 \cdot C_{st} \quad UFL = 3.5 \cdot C_{st} \quad (4)$$

where C_{st} is the stoichiometric concentration (vol percent).

LFL and UFL: Method 2

$$LFL = \frac{0.55}{4.76m + 1.19x - 2.38y + 1} \quad (5)$$

$$UFL = \frac{3.5}{4.76m + 1.19x - 2.38y + 1} \quad (6)$$

LFL and UFL: Method 3

$$LFL = \frac{-3.42}{\Delta H_c} + 0.569\Delta H_c + 0.0538\Delta H_c^2 + 1.8 \quad (7)$$

$$UFL = 6.3\Delta H_c + 0.567\Delta H_c^2 + 23.5 \quad (8)$$

where ΔH_c is the heat of combustion in kJ/mol.

LFL and UFL: Mixtures

$$LFL = \frac{1}{\sum_i \frac{y_i}{LFL_i}} \quad (9)$$

where y_i is the mole fraction of the component and LFL_i is the LFL of the component. The UFL is calculated similarly.

UOL

$$UOL = \frac{UFL[100 + 1.87(100 - UFL_o)]}{UFL_o + UFL(1 + 1.87)} \quad (10)$$

where UFL_o is the oxygen concentration at the UFL. 1.87 is a fitting constant.

LOC

$$LOC = \left(\frac{LFL + 1.11UFL}{1 + 1.11} \right) \left(\frac{UFL_o}{UFL} \right) \quad (11)$$

where UFL_o is the oxygen concentration at the UFL. 1.11 is a fitting constant.

21 Flammability Part 2

Learning Outcomes

- Be able to reproduce a ternary flammability diagram

Reading

- Foundations of Spiritual and Physical Safety: with Chemical Processes; Chapter 6, Sections 2.2

Download lecture freeform here: <physical/supportfiles/311Flammability.pdf>

21.1 Python Flammability Diagram

Below code submitted by [Isaac Matthews](#), 2024.

Requirements for the equalateral flammability diagram below: `#pip install matplotlib, python-ternary`; the below code wont work if you install ternary,

```
import matplotlib.pyplot as plt
import ternary
from scipy.optimize import fsolve
ufl = 74
lfl = 4
stoic = 66.7 #stoichiometric ratio for hydrogen in oxygen
loc = 2

def flammabilityTriangle(name,lfl, ufl, stoic,loc,figsize = (10, 8)):
    # The stoic value is the stoichiometric ratio of fuel in pure oxygen
    lfl_o = (100 -lfl)*0.21; ufl_o = (100 -ufl)*0.21
    lfl_n = 100 - lfl - lfl_o; ufl_n = 100 - ufl - ufl_o
    slope = 1/(100/stoic - 1) # z/y or ratio of fuel to oxygen at stoichiometric mixture
    def eq(vars):
        x, y = vars #x is n2, y is o2
        denom = x+y*(1+slope)
        eq1 = loc/100 - y/(denom)
        eq2 = loc/100 + x/denom + y*slope/denom - 1
        return eq1, eq2
    mol_n2, mol_o2 = fsolve(eq, (0.5, 0.5)); mol_f = slope*mol_o2
    loc_f = mol_f/(mol_n2+mol_o2+mol_f)*100
    uol = ufl*(100+1.87*(100 -ufl_o))/(ufl_o+ufl*(1+1.87)) #upper flammability limit in pure oxygen
    lol = lfl
    data = [
        #nitrogen fuel oxygen
        [0, 0, 100],  # Pure Oxygen 0
        [79, 0, 21],  # Pure Air 1
        [0, 100, 0],  # Pure Fuel 2
        [100,0,0],    # pure n2 3
        [lfl_n, lfl, lfl_o],  #LFL 4
```

```

[ufl_n,ufl,ufl_o],      #UFL 5
[0,uol,100 -uol], #upper loc 6 (uol)
[0,stoic,100 -stoic], #left most stoic point 7
[100 -loc -loc_f, loc_f,loc],#intersection 8 (actual loc at stoichiometric point)
[0,lol,100 -lol], #lol 9
# Add more data points as needed
]
# Create a larger figure
whole = plt.figure(figsize=figsize)
box = whole.subplots()
# Create a ternary plot
fig, tax = ternary.figure(ax = box, scale=100)
#fix what terniary messes up
box.set_ylimits( -20,110)
box.set_xlim( -10,120)
box.set_aspect(1)
box.tick_params(axis='both', which='both', length=0,labelcolor = 'white') #if you can't beat them join them
tax.ticks(axis='lrb', linewidth=1, multiple=10, offset=0.02, clockwise=False)
# Plot data points
tax.scatter(data, marker='.', color='k', label='Data Points')

# Add a line between pure fuel and pure air
tax.line(data[2], data[1], color='green', linestyle=' -',label = "Air line")
#tax.line(data[9], data[8], color='red', alpha=0.6, linestyle=' - - ', label = "Flammability region")
tax.line(data[3], data[7], color='blue', alpha=0.9, linestyle=' - ', label = "Stoichiometric line")
#tax.line(data[6], data[8], color='red', alpha=0.6, linestyle=' - - ')

# - - - Corrected part for shading (hopefully for good this time!) - - -
# Define the vertices of the flammability region in ternary coordinates
flammability_vertices_ternary = [data[9], data[8], data[6]]

# Convert ternary coordinates to Cartesian (x, y) coordinates for matplotlib's fill
flammability_vertices_cartesian = ternary.helpers.project_sequence(flammability_vertices_ternary)

# Use the underlying matplotlib axes (box) to fill the region
box.fill(
    flamability_vertices_cartesian[0], # X coordinates
    flamability_vertices_cartesian[1], # Y coordinates
    color='red',
    alpha=0.1,
    label="Flammability Region (Shaded)"
)
# - - - End of corrected part - - -

# Customize the plot
#tax.set_title(f"Flammability Triangle for {name} in Air", fontsize=16)
tax.left_axis_label("Oxygen", fontsize=14, offset=0.1)
tax.right_axis_label(name, fontsize=14, offset=0.02)
tax.bottom_axis_label("Nitrogen", fontsize=14, offset= -.1)
tax.gridlines(color="lightgrey", multiple=10, linewidth=1, linestyle=' - -')

# Define labels for data points
labels = ["", "", "", "", "LFL", "UFL", "UOL", "", "", ""]

```

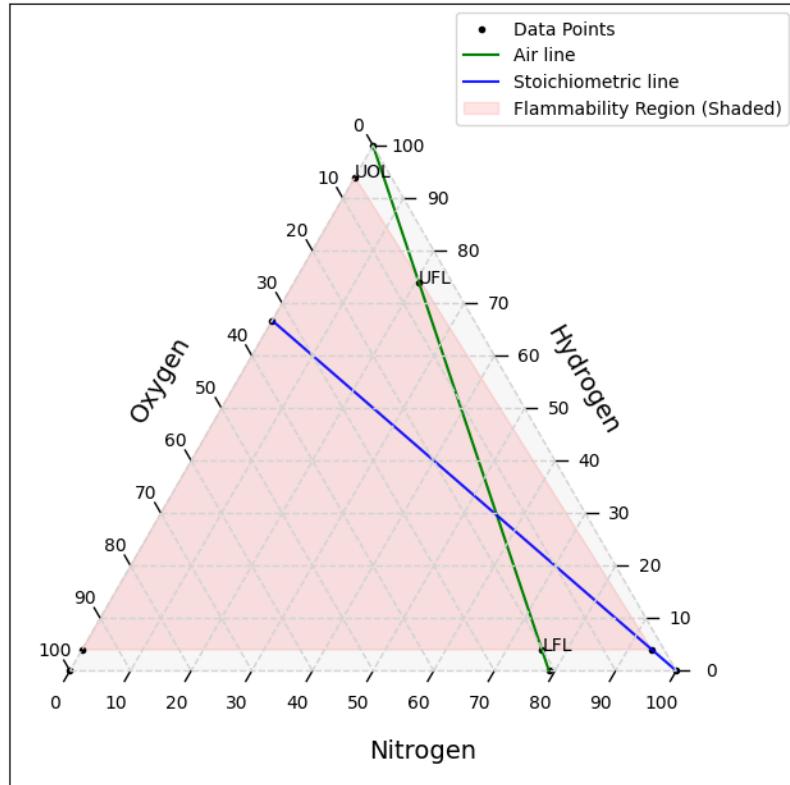
```
# Add labels for data points
for i, point in enumerate(data):
    tax.annotate(labels[i], position=point, fontsize=10)

# Add legend
tax.legend()

# Show the plot
plt.ticks = False
plt.show()

flammabilityTriangle("Hydrogen", lfl, ufl, stoic, loc)

/Users/clintguymon/opt/anaconda3/envs/jupyterbook/lib/python3.9/site-packages/ternary/plotting.py:148:
ax.scatter(xs, ys, vmin=vmin, vmax=vmax, **kwargs)
```



EXPLOSIONS

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1st Jan, 2025

created in  Curvenote

Keywords Spiritual Safety, Process Safety, Chemical Engineering, Risk Assessment

Learning Outcomes

- Understand the basics of explosions from:
 - Vapor Clouds
 - BLEVEs
 - TNT and high-explosives
 - Pressure vessels
- Be able to estimate over-pressures and associated damage
- Review GHS pictograms and NFPA 704 labels
- Review hazards analysis and flammability principles

Reading

- Foundations of Spiritual and Physical Safety: with Chemical Processes; Chapter 6, Sections 2.2

1 Vapor Cloud Explosions (VCE)

This a release of a flammable vapor cloud that then mixes with air and ignites.

1.1 In-class VCE demonstration

Isopropal alcohol has a LFL and UFL of 2% and 12% by volume.

We could calculate or estimate:

- energy from the event
- internal pressure and
- vent rate of the generated gases

Things to consider:

- ignition characteristics (laminar vs turbulent, top vs center ignition)
- flame speed
- hazards analysis

2 Boiling Liquid Expanding Vapor Explosions (BLEVE)

BLEVEs are a type of explosion that occurs when a vessel containing a liquid is heated to the point that the pressure exceeds the strength of the vessel. Once the vessel ruptures, the pressure falls rapidly and the hot liquid then quickly vaporizes and expands. It then can mix with air and ignite.

3 High-Explosive Blasts

Image of TNT showing a solid piece melting. TNT melts at a relatively low temperature (~80C). TNT is usually melt casted into bombs or other shapes.

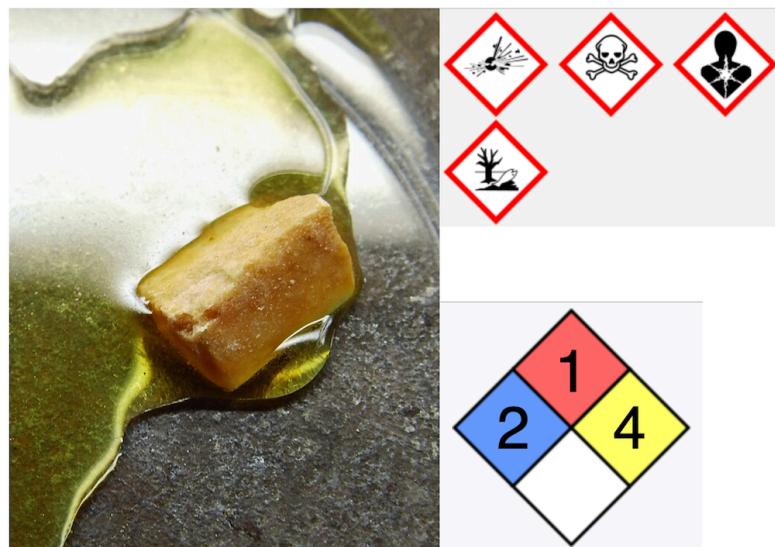


Figure 1: TNT Melt Casting, By Daniel Grohmann - Own work, CC BY-SA 3.0, <https://commons.wikimedia.org/w/index.php?curid=30126231>

3.1 Detonation

TNT detonates. That is, if boosted properly, the reaction front moves through the material at the detonation speed, approximately 7 km/s (much faster than the speed of sound in TNT).

3.2 Deflagration

TNT, if not properly boosted, may only burn or deflagrate. The deflagration or burning reaction lasts much longer and thus the energy released per time is much smaller.

3.3 TNT Equivalence and Blast Effects

TNT is a explosive that has been used for many years and is one of the most tested. TNT detonation blast pressures (both side-on and reflective), impulse (integral of the blast pressure with respect to time), and arrival

times have been experimentally measured for spherical and hemispherical (ground level) blasts of TNT at various distances and various TNT masses. The data for those tests are given in the TM5-1300 document or in other references like UFC 3-340-02. These data have been fit to a model that is used to assess the hazards from explosions (of TNT or otherwise). If the explosive is not TNT, testing or modeling is done to determine the equivalent TNT mass. The TNT model (with the scaled TNT mass) is then used to assess the hazards.

One very large hazard from TNT blasts is the shock wave (and blast wind) referred to as over-pressure. Typically, over-pressure is measured in psi (pounds per square inch) or kPa (kiloPascals). The over-pressure is the pressure above the ambient pressure. The over-pressure is a function of the distance from the explosion and the TNT mass.

Overpressure blast effects are typically categorized as follows:

- >0.4 psig: limited minor structural damage
- 0.4-1.0 psig: window breakage to partial demolition of houses
- 1-5 psig: significant damage to buildings to nearly complete destruction of houses
- >5 psig: severe damage

There is approximately 4184 J of energy per gram of TNT. You can use that as an estimate for TNT equivalence given an energy output from a blast.

3.4 TNT Overpressure Model

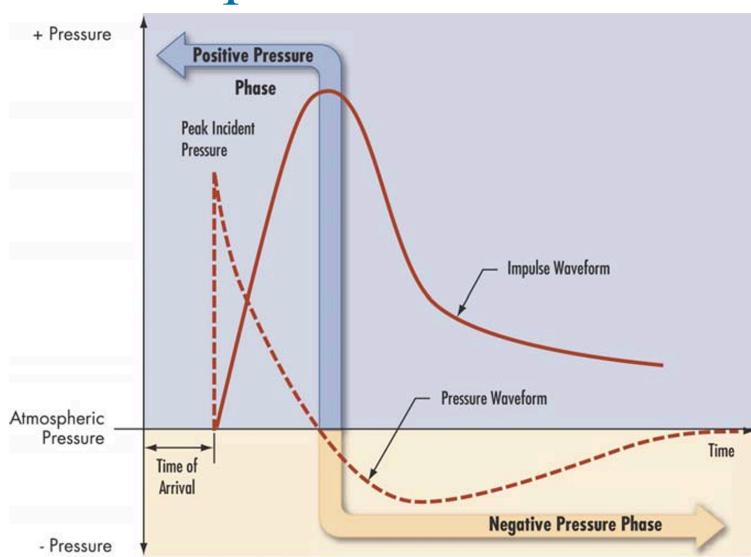


Figure 2: Image of the TNT blast pressure and overpressure as a function of time. Credit to https://www.fema.gov/pdf/plan/prevent/rms/155/e155_unit_vi.pdf

The peak side-on overpressure can be estimated for a given mass of TNT from the following equation (hemispherical blast or blast on the ground):

$$\frac{p_o}{p_a} = \frac{1616 \left[1 + \left(\frac{z_e}{4.5} \right)^2 \right]}{\sqrt{1 + \left(\frac{z_e}{0.048} \right)^2} \sqrt{1 + \left(\frac{z_e}{0.32} \right)^2} \sqrt{1 + \left(\frac{z_e}{1.35} \right)^2}} \quad (1)$$

where p_o is the overpressure in psig (gauge), p_a is the ambient pressure in psia, and z_e is the scaled distance ($\text{m}/\text{kg}^{1/3}$). z_e is the distance in meters divided by the TNT (or equivalent) mass to the $1/3$ power. Equation from G. F. Kinney and K. J. Graham. "Explosive Shocks in Air (Verlin, Germany: Springer-Verlag, 1985).

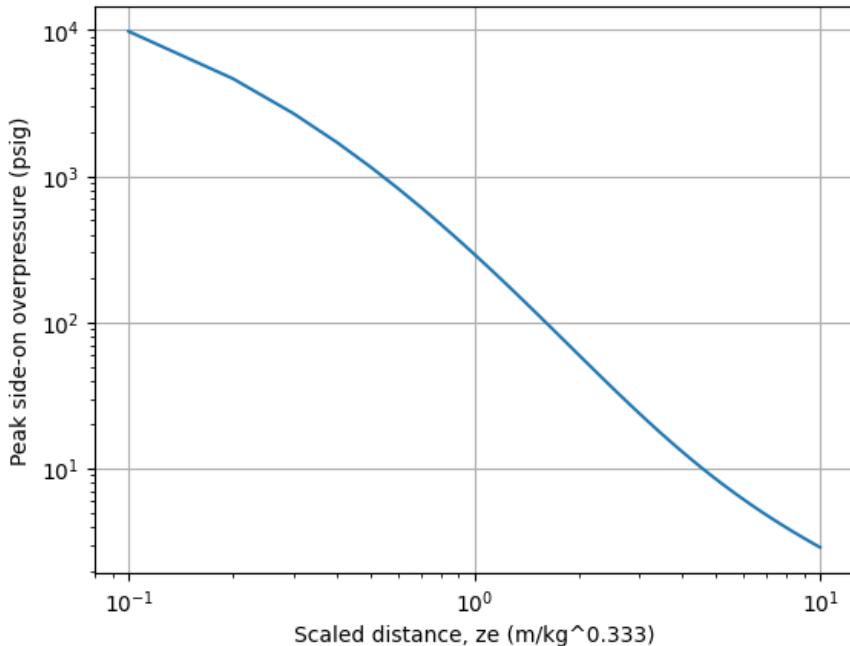
Note

More accurate alternatives to the above equation that are used throughout the defense community are described in UFC-340-02. The above equation is an estimate.

```
import numpy as np
import matplotlib.pyplot as plt

def overpressure(pa, ze):
    numerator = 1616*(1 + (ze/4.5)**2)
    denom1 = np.sqrt(1 + (ze/0.048)**2)
    denom2 = np.sqrt(1 + (ze/0.32)**2)
    denom3 = np.sqrt(1 + (ze/1.35)**2)
    return pa*(numerator/(denom1*denom2*denom3))

#plot the above relationship
ze = np.linspace(0.1, 10, 100)
pa = 14.7 #psi
po = overpressure(pa, ze)
plt.loglog(ze, po)
plt.xlabel('Scaled distance, ze ( $\text{m}/\text{kg}^{0.333}$ )')
plt.ylabel('Peak side-on overpressure (psig)')
plt.grid()
```


Note

Also given in the TM5-1300 document are the impulse as a function of the scaled distance. The impulse is the integral of the overpressure with respect to time. The damage from a blast depends both on the peak overpressure and the impulse. The impulse is a measure of the energy in the blast.

For example, using the above correlation, the peak overpressure at 100 m from a 1000 kg TNT blast is:

```
ze = 100/(1000**0.333)
po = overpressure(pa, ze)
print(f'At a distance of 100m, the peak side -on overpressure from a 1000 kg blast is {po:.2f} psig')

At a distance of 100m, the peak side -on overpressure from a 1000 kg blast is 2.89 psig
```

3.5 Munroe Effect and Explosive Devices

The [Munroe effect](#) is used in perforation guns for oil wells, armor piercing weapons, or other devices. The effect of the explosive can be significantly increased in a particular direction by shaping the explosive charge. The generated gases are focused in a particular direction and the pressure is thereby significantly increased.

3.5.1 Perforation Guns and Oil Recovery

Perforation guns are used in oil wells to create vias for oil to be recovered from otherwise impermeable layers. The gun has multiple perforation charges usually arranged in a spiral pattern. The charge creates a high pressure jet of solid copper or other malleable metal to punch a hole through the gun casing, through the bore lining and into the rock. The diameter of the holes vary but typically are about the diameter of your finger.



Figure 3: Shape charges in a perforating gun. Credit to <https://www.scotopetro.com/uploads/image/20180627/15/perforating-gun.jpg>

4 Pressurized Vessel Bursting

This is referred to in the book (Crowl and Louvar) as **Mechanical Explosions**.

```
P1 = 101325 # ambient pressure, Pa
P2 = np.linspace(101325, 1e7, 100) # pressure range, Pa
V = 1 # volume, m^3
gamma = 1.4 # ratio of specific heats
Ebrody = (P2 - P1)*V/(gamma - 1)/(1e6) # energy required to compress air, MJ
Eisoentropic = P2*V/(gamma - 1)*(1 - (P1/P2)**((gamma - 1)/gamma))/(1e6) # energy required to compress air
Eisothermal = P2*V*np.log(P2/P1)/(1e6) # energy required to compress air isothermally, MJ
Ecrowl = P2*V*(np.log(P2/P1) - (1 - P1/P2))/(1e6) # energy required to compress air using Crowl's method
n = P2*V/(8.314*298)

plt.plot(P2/1e5, Ebrody, label='Brody')
```



Figure 4: Images of shape charges with a copper lining. Credit to https://www.downhole-drillingtools.com/photo/pl21706160-steel_case_shaped_charges_for_oil_well_perforating_high_hardness_durable.jpg

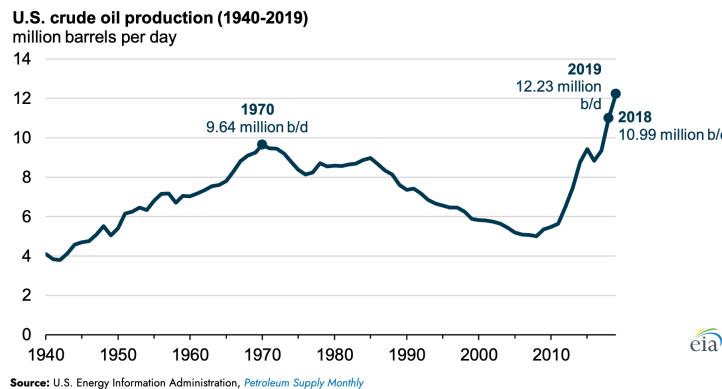
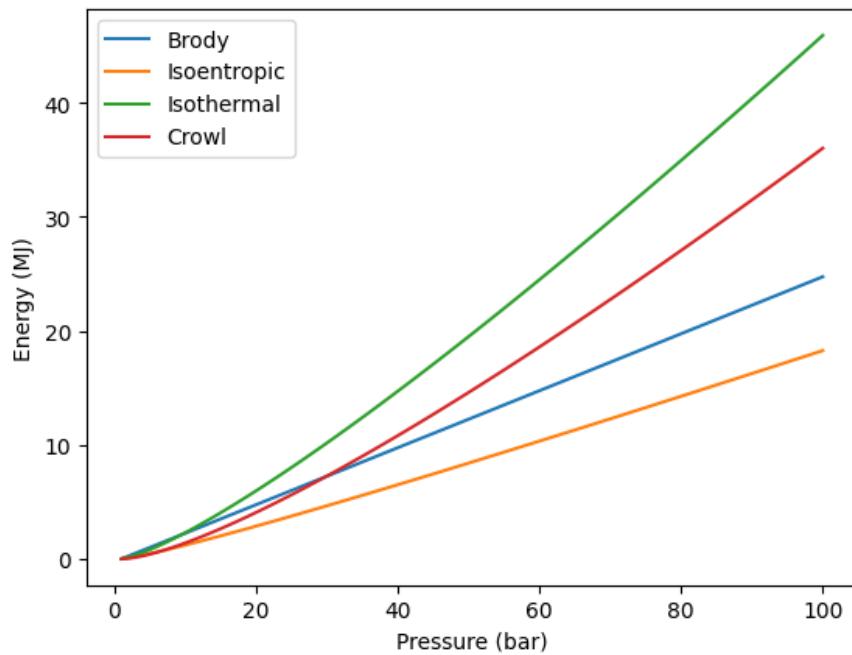


Figure 5: Crude Oil Production PLOT. Credit to <https://www.eia.gov/todayinenergy/detail.php?id=43015>

```

plt.plot(P2/1e5, Eisoentropic, label='Isoentropic')
plt.plot(P2/1e5, Eisothermal, label='Isothermal')
plt.plot(P2/1e5, Ecrown, label='Crown')
plt.xlabel('Pressure (bar)')
plt.ylabel('Energy (MJ)')
plt.legend(); plt.show()

```



*If you divide the energy by the number of moles in the volume (assuming room temperature) to get an energy per mole, you get the plot given in Figure 6-26 in the book.

The above plot can then be used to estimate a TNT equivalent mass for the given energy and then thereby estimate the overpressure at a given distance.

Note

The energy from fragments from a mechanical energy burst is approximately 5% of the product of the burst pressure of the structure (gauge) and the volume of the pressurized gas.

22 Mole Balances

Learning Outcomes

- Be able to setup and solve a mass balance using ordinary differential equations

Reading

- Foundations of Spiritual and Physical Safety: with Chemical Processes; Chapter 6 (Venting and Mass Balances)

Mass (mole) and energy balance problems are fundamental to chemical engineering. It takes practice to understand how to set up and solve these problems. These problems are part of multiple courses in chemical engineering, and they are also part of the Fundamentals of Engineering (FE) exam and proficiency exams given by chemical engineering departments. This course is the 2nd or 3rd time reviewing these principles. Example exam results demonstrating that more practice is needed are shown below.

Winter 2024

	Correct	Incorrect
Points	9	0
Percent of all students who selected option	29%	71%
Percent of high-scoring students (Q4) who selected option	86%	14%
Percent of low-scoring students (Q1) who selected option	0%	100%
Mean test score of students who selected option	96.01	81.13

Winter 2025

	Correct	Incorrect
Points	9	0
Percent of all students who selected option	38%	62%
Percent of high-scoring students (Q4) who selected option	94%	6%
Percent of low-scoring students (Q1) who selected option	11%	89%
Mean test score of students who selected option	79.55	71.66

Figure 26: Mass Balance Example Exam Results

22.1 Mass and Energy Balances

Helpful sheet: [General Mass and Balance Equations](#)

22.2 Why?: Concentration Estimates for Assessing Risk

Prior to implementing control techniques, it can be important to quantify the risk of exposure from a spill scenario of other toxic gas/ vapor release.

22.2.1 Total Mole (Mass) and Component Mole Balances

Given a control volume and:

- A release of toxic gas or vapor at a constant rate
- Addition of air at a constant rate
- Exit of the gasses based on the inlet conditions and assuming that the exit rate can be achieved without pressurization of the control volume
- Steady state conditions

Total molar balance:

$$\text{Rate of accumulation} = \text{Rate of inlet} - \text{Rate of exit} + \text{Generation rate} \quad (9)$$

$$\frac{dn_{tot}}{dt} = n_{in} - n_{out} + n_{gen} \quad (10)$$

Component balances:

$$\frac{dn_i}{dt} = n_{in,i} - n_{out,i} + n_{gen,i} \quad (11)$$

At steady state, the accumulation terms ($\frac{dn_{tot}}{dt}$ and $\frac{dn_i}{dt}$) are zero.

Other assumptions/ notation:

- concentration of interest, $C_i = n_i/V$,
- the exit rate of the total gases is Q_v^n , mol//time,
- the inlet rate of the composition of interest is Q^e , mol//time,
- $C_{ppm} = C_i RT/P \cdot 10^6$, where C_{ppm} is the concentration in parts per million (ppm), R is the ideal gas constant, T is the temperature, and P is the pressure.
- $n_{gen,i} = 0$, for the case of a spill or release of a toxic gas or vapor (new species are not generated).
- Perfect mixing of the gases in the control volume (no concentration gradients).

As such, the mole balance for the component of interest i is

$$0 = Q^e - C_i Q_v^n RT / P \quad (12)$$

$$C_i = \frac{Q^e}{Q_v^n RT / P} \quad (13)$$

If however, there are concentration gradients, the concentration could deviate significantly from the above estimate (larger or smaller).

22.2.2 Inlet composition from vaporization of a liquid

The inlet rate of the species of interest, Q^e , can be estimated from the vapor pressure of the liquid and the rate of vaporization and a mass transfer coefficient according to:

$$Q^e = k_m A(C_{sat} - C) \quad (14)$$

where k_m is the mass transfer coefficient, C_{sat} is the saturation concentration of the species close to the liquid surface, and C is the concentration of the species in the air, and A is the area of the spill.

k_m can be estimated from correlations or from experimental data or by comparison to another component with a known mass transfer coefficient (e.g. water, k_m^0):

$$k_m = k_m^0 \left(\frac{M}{M_0} \right)^{0.33} \quad (15)$$

where M is the molecular weight of the species of interest and M_0 is the molecular weight of water. k_m^0 is typically in the range of $0.1 - 10.0 \text{ cm/s}$ depending on the conditions.

C_{sat} can be estimated from the Antoine equation:

$$\log_{10} P_{sat} = A - \frac{B}{T + C} \quad (16)$$

where P_{sat} is the saturation pressure of the species of interest, and A , B , and C are constants that can be found in the literature. Where $C_{sat} = P_{sat}/RT$.

Incorporating those into the mole balance, we have:

$$0 = k_m A(C_{sat} - C_i) - C_i Q_v^n RT / P \quad (17)$$

$$C_i = \frac{k_m A}{Q_v^n RT / P + k_m A} C_{sat} \quad (18)$$

How would you solve the above if you would like the unsteady state concentration as a function of time? And there by obtain the Time Weighted Average (TWA) for a worker directly after a spill?

See [here](#) to view a video on a mole (mass) balance for a spill scenario. This video can be helpful for the homework. You can download the sheet used in the video here: [physical/supportfiles/Balance.pdf](#)

22.3 Additional Mass Balance Examples

Example

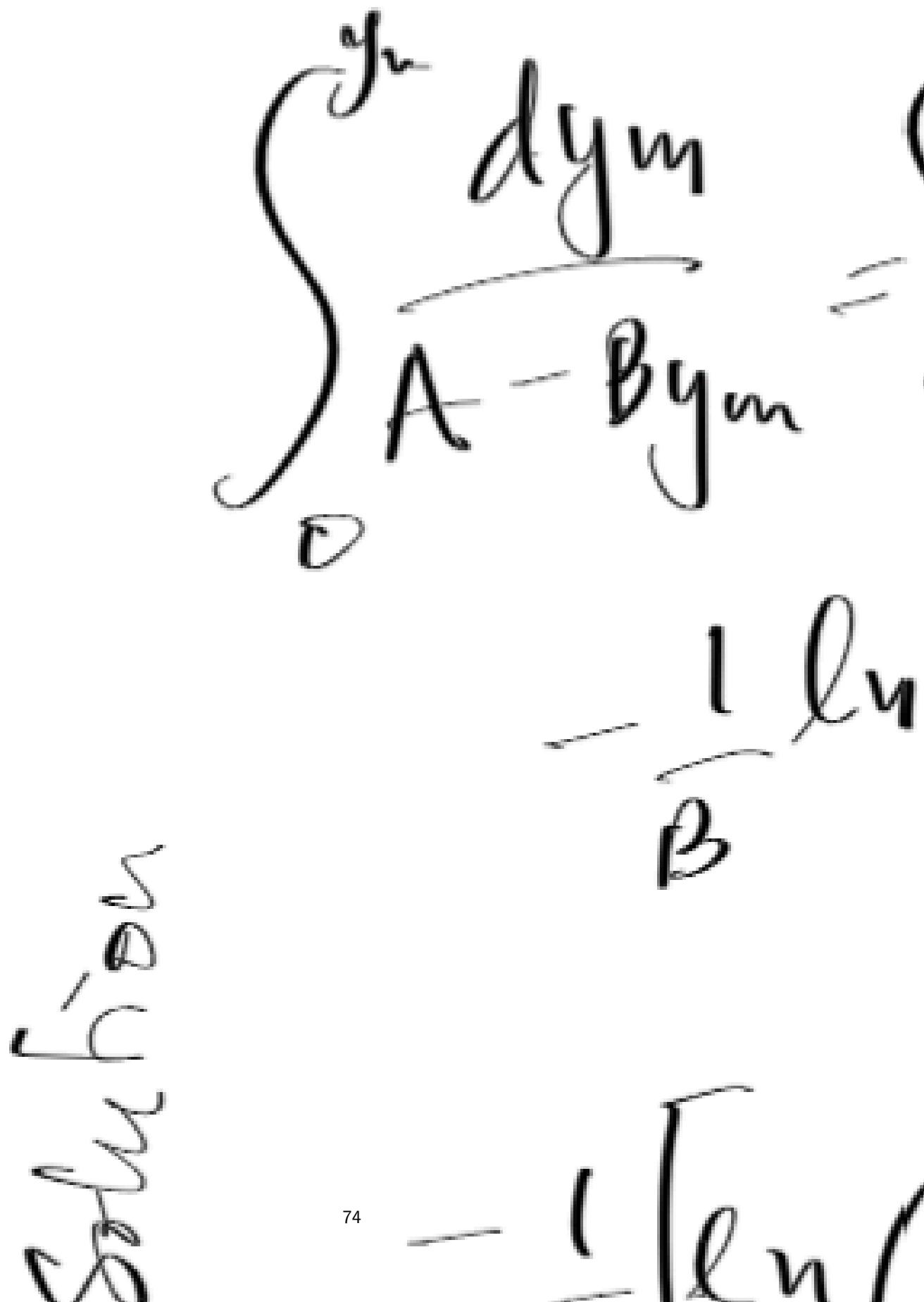
$$y_m = \frac{\text{moles of CH}_4}{\text{total moles}}$$

$$\frac{d n_{CH_4}}{dt} = d(n \cdot y)$$

* Assuming that
pressure

thus, $n \propto V$

$$\text{so } \frac{dn}{dt}$$



Examp



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22.4 Mass and Energy Balance Example

Example

In this example, we will consider a system where the mass and energy balance equations are constant over time. This means that the total mass and total energy in the system remain constant, even though individual components may change.

Energy balance

$$\frac{d\bar{U}}{dt} = \dot{n}_{air}^{\text{in}}$$

For gases: \bar{U}

(3)

$$\frac{\int nC_v dT}{dt}$$

```
#Mass and energy balance solution for Example 4
#      air flow into room at 20C, methane flow into room at 200C, air/methane mixture leaves the room
#      determine the fraction of methane and air temperature as a function of time

import numpy as np
import matplotlib.pyplot as plt
from scipy.integrate import odeint

# Parameters
Cv_m = 27 # J/mol -K specific heat of methane, (estimate) assumed constant but is a function of tempera
```

```

Cv_air = 29 # J/mol -K specific heat of air, (estimated) assumed constant but is a function of temperature
#stream flow rates
nin_air = 1 # mol/s air flow rate
nin_m = 1/7 # mol/s methane flow rate
#stream temperatures
Pairin = 101425 # Pa, pressure of air stream entering the room
Tairin = 20 + 273.15 # K, temperature of air entering the room
Tmin = 200 + 273.15 # K, temperature of methane entering the room
#room parameters
orifice_diameter = 0.2 # m (outlet diameter)
Cd = 0.6 # discharge coefficient
Pext = 101325 # Pa, external pressure
P_initial = Pext # Pa, constant pressure
T_initial = 20 + 273.15 # K, initial temperature of room
n_initial = 1000 # total moles in room, can be found from the volume and initial temperature and pressure
nm_initial = 0 # initial moles of methane in room

Rg = 8.314 # J/mol -K
T0 = 20 + 273.15 # K, reference temperature
Pref = 101325 # Pa, constant pressure

Vol = n_initial * Rg* T_initial/P_initial # m^3, volume of room
print(f'Volume of room = {Vol} m^3')
print(f'Air flow rate into room = {nin_air*Rg*Tairin/Pairin} m3/s')
print(f'Air flow rate into room = {nin_air} mol/s')

def derivatives(p,t):
    # changing parameters
    n, nm, T = p
    ym = nm/n
    Cv = ym * Cv_m + (1 -ym) * Cv_air # J/mol -K, specific heat of the mixture
    Mw = ym * 0.016 + (1 -ym) * 0.029 # kg/mol, molecular weight of the mixture
    P = n*Rg*T/Vol # Pa, pressure in the room
    rho = P*Mw/Rg/T # kg/m^3, density of the mixture

    # flow rate out, assume flow out is incompressible
    nout = Cd * np.pi/4 * orifice_diameter**2 * np.sqrt(2*(P -Pext)*rho)/Mw # mol/s

    # Mass balance
    # first total mass balance
    dndt = nin_air + nin_m - nout
    # then component balance
    dnmdt = nin_m - nout * ym

    # Energy balance
    dTdt = 1/(n*Cv)*(- Cv*(T -T0)*dndt + nin_air*(Cv_air+Rg)*(Tairin -T0) + nin_m*(Cv_m+Rg)*(Tmin -T0))

    return [dndt, dnmdt, dTdt]

# time points
t = np.linspace(0,1000,1000) # seconds

# solve ODE

```

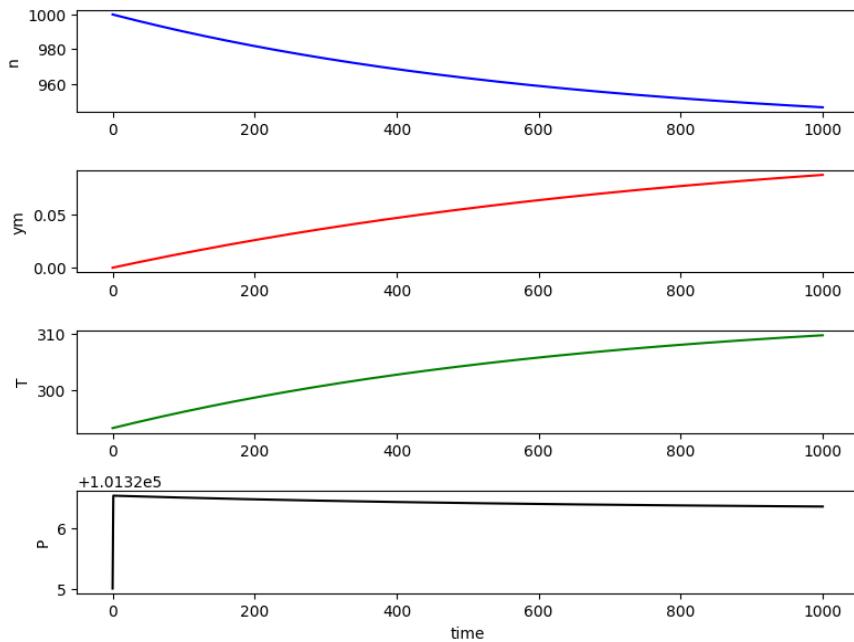
```

n0 = [n_initial, nm_initial, T_initial]
sol = odeint(derivatives, n0, t)

# plot results in a grid of subplots
fig, ax = plt.subplots(4, 1, figsize=(8, 6))
ax[0].plot(t, sol[:, 0], 'b', label='n')
ax[0].set_ylabel('n')
ax[1].plot(t, sol[:, 1]/sol[:,0], 'r', label='ym')
ax[1].set_ylabel('ym')
ax[2].plot(t, sol[:, 2], 'g', label='T')
ax[2].set_ylabel('T')
ax[3].plot(t, sol[:, 0]*Rg*sol[:,2]/Vol, 'k', label='P')
ax[3].set_ylabel('P')
ax[3].set_xlabel('time')
fig.tight_layout(pad = 1.0)
plt.show()

```

Volume of room = 24.053778435726617 m³
 Air flow rate into room = 0.024030062607838305 m³/s
 Air flow rate into room = 1 mol/s



23 Relief Action

Learning Outcomes

- Use orifice flow estimates in mass and energy balance calculations
- Estimate vent sizing for deflagrations
- Gain experience with mass and energy balance principles
- Review relief requirements for fire scenarios

Reading

- Mass and energy balances

Review of MAWP and max accumulation pressure or max overpressure (based on gauge pressure)

23.1 Venting for External Fires

As heat is input to the vessel, the liquid warms and expands and reaches the boiling point. The mass flow of vapor at that point is:

$$Q_m = Q / \Delta H_{vap} \quad (19)$$

where Q_m is the mass flow of vapor, Q is the heat input (estimated from Eq 10-34 and 10-35 in Crowl and Louvar), and ΔH_{vap} is the heat of vaporization. The vent area can then be sized based on the mass flow of vapor.

When the liquid is heated it expands according to the thermal expansion coefficient, β . The volume of the liquid is:

$$V = V_0(1 + \beta\Delta T) \quad (20)$$

where V_0 is the initial volume, β is the thermal expansion coefficient, and ΔT is the temperature change. This is found from the definition of the thermal expansion coefficient:

$$\beta = \frac{1}{V_0} \frac{dV}{dT} \quad (21)$$

23.2 Orifice Flow, Mass and Energy Balances with Reaction

23.2.1 First Example

Consider a 20L sphere where the methane is combusted with at least as much air as is stoichiometrically required. The combustion is complete and the products are:



Three moles of reactants produce 3 moles of products. At higher temperatures, the water vapor will be in the gas phase and there can be radicals. For the example here, we will assume that the water stays in the vapor phase and that the combustion is complete such that there is no overall change in the number of moles of gas.

What is the final pressure and temperature if there is no heat loss and the reaction rate is constant at 15 moles/sec/m³?

Note

Some simplifying assumptions:

- The burn rate is proportional to the total moles not just the moles of methane
- The burn rate transitions monotonically from it's highest value to zero instead of a step change

Here is a an image of the notebook thoughts on the scenario and the mass and energy balance:

The below hidden code cell contains:

- parameters for the 20L sphere and combustion reaction estimate (simplified)
- the sigmoid function for the burn rate (transition from full burn to zero at the end of the burn)
- the derivative function to be integrated
- the initial conditions
- the integration and solution

See this reference for more detailed information on combustion of methane in a 20L and larger spheres: [Mittal \(2017\)](#)

23.3 Second Example (Follow-on from First Example)

Consider the same conditions as the first example but what burst disk size would be required to prevent the pressure from exceeding 1 barg?

Note

Some simplifying assumptions:

- The above assumptions apply
- Assume that the area of the burst disk transitions from closed to open in a s-curve fashion once the burst pressure of the disk is reached with a parameter of t_{open} equal to the time that the burst disk is 67% open. This is also applied to the burn rate of the fuel.

You can download a pdf of the in-class notes here (including both the instructor and in-class version): [physical/supportfiles/EnergyMassVent.pdf](#)

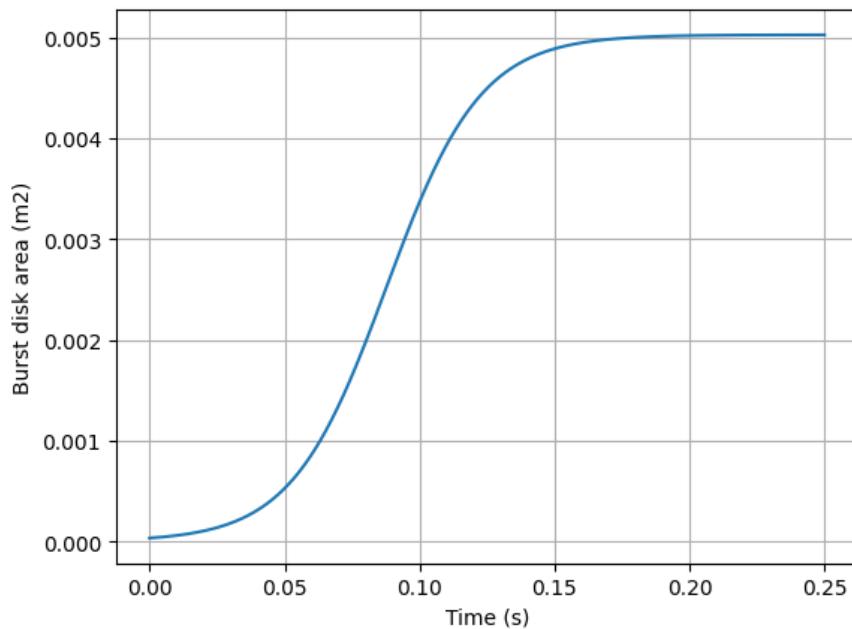
Additional parameters for the venting of the volume once the pressure reaches the burst pressure of the disk.

```
#Burst disk function
t_open = 0.1 #seconds, time to open burst disk to 67%
Pdisk = 2e5 #Pa, burst disk pressure, 1barg
Area_f = np.pi/4*(0.08)**2 #m^2, area of burst disk
barea = lambda t: Area_f*sigmoid(t,t_open) #sigmoid function to open burst disk
Cd = 0.95 #discharge coefficient
```

Warning

The below code will give non-realistic answers if the vent time is faster than the burn time. Vent time meaning the pressure is relieved prior to the burn completing.

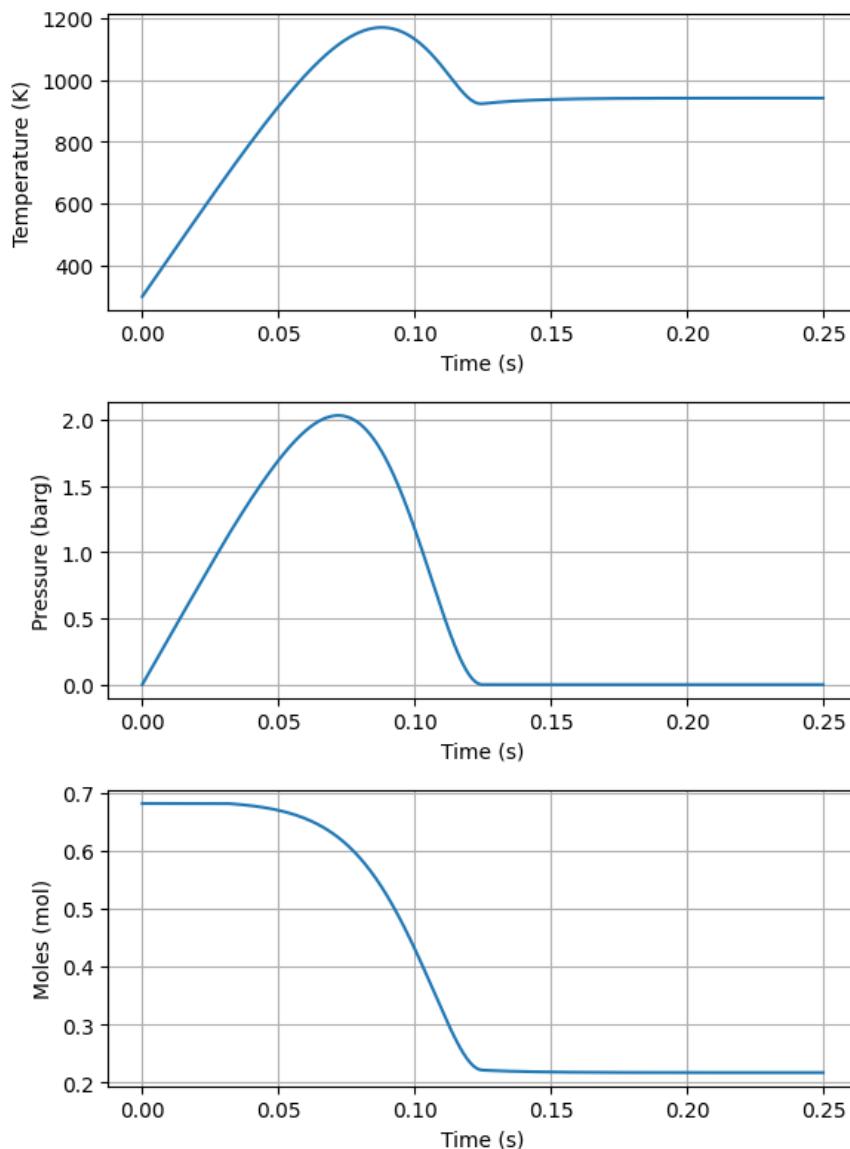
The area of the burst disk changes with time as it opens and moves out of the way. That transition is also estimated with a sigmoid function (it could also be done with using physics where $F = P/A = m*a$ and you can step through time as the burst disk moves). The area of the burst disk is shown in the below figure.



The below hidden code cell contains the moles of gas flowing out of the vent. The flow is based on the general equations discussed in the previous lecture. There's also an if statement such that if the pressure drops below the atmospheric value, there's flow of gas into the container from the atmosphere.

The below code cell shows the derivatives for moles and temperature for the venting. There's also if statements to account for the changing conditions when the burst disk ruptures and the relative sizes of the internal and external pressures.

The below code cell shows the integration and solution for the venting of the volume once the pressure reaches the burst pressure of the disk.



Notice how the pressure exceeds the burst pressure of the disk substantially as the energy from the burning is larger than that that can be vented. The accumulation and overpressure discussed in the previous lectures can be found knowing the MAWP of the vessel and the set pressure of the disk.

Note

The above example is an integrated solution to the approximate behavior of the burning and of the opening of the vent. Actual vent sizing for explosions can be more nuanced and is not covered in detail here. This is a simplified example to demonstrate some fundamental principles of kinetics, thermodynamics, and numerical methods with many simplifying assumptions.

24 Relief Sizing

Learning Outcomes

- Ability to estimate flow through an orifice for
 - incompressible liquid
 - compressible gas (choked and unchoked flow)
 - two-phase flow for a flashing fluid
- Perform preliminary sizing of a relief valve for a liquid, gas, and two-phase flow

Reading

- Mass and energy balances

24.1 Mechanical Energy Balance

Note

Constant Density, Frictionless, Constant Temperature Flow

$$\frac{\Delta P}{\rho g} + \frac{\Delta u^2}{2g} + \Delta z + \frac{F}{g} = \frac{-W_s}{\dot{m}g} \quad (23)$$

where ΔP is the change in pressure, Δu is the change in velocity, Δz is the change in elevation, ρ is density, F is the frictional losses, and W_s is the shaft work with respect to two points in the system.

If there is no friction and constant density and no shaft work and no change in elevation, the mechanical energy balance simplifies to:

Note

$$\frac{\Delta P}{\rho g} + \frac{\Delta u^2}{2g} = 0 \quad (24)$$

or assuming that the flow points are inside a tank where $P = P_{\text{o}}$ and $u = 0$ and outside the tank where $P = P_{\text{atm}}$ and $u = u$, then

$$\frac{P_o}{\rho} - \frac{P_{\text{atm}}}{\rho} = \frac{u^2}{2} \quad (25)$$

or

$$u = \sqrt{2 \left(\frac{P_o - P_{\text{atm}}}{\rho} \right)} \quad (26)$$

24.2 Incompressible Flow through an Orifice

Thus for incompressible flow, the velocity of the fluid can be determined from the pressure drop across an orifice. Although the flow is usually not frictionless, the velocity can be estimated from the pressure drop and the density of the fluid according to:

$$\dot{m} = AC_d \sqrt{2\rho\Delta P} \quad (27)$$

or

$$\dot{n} = \frac{AC_d}{M_w} \sqrt{2\rho\Delta P} \quad (28)$$

where \dot{m} is the mass flow rate, \dot{n} is the molar flow rate, M_w is the molecular weight, A is the area of the orifice, ρ is the density of the fluid, C_d is the discharge coefficient, and ΔP is the pressure drop across the orifice. For liquid flow, and estimate of the discharge coefficient is 0.65.

24.3 Gaseous flow through an Orifice: General Case

The flow of a gas through an orifice is also derived from an energy balance assuming adiabatic and frictionless flow. The flow is characterized by the pressure ratio, P_o/P_{atm} and associated Mach number, Ma . P_o is the absolute pressure of the volume. The Mach number can be found from:

$$Ma = \min \left(1, \sqrt{\frac{2}{\gamma - 1} \left(\left(\frac{P_o}{P_{atm}} \right)^{\frac{\gamma-1}{\gamma}} - 1 \right)} \right) \quad (29)$$

where γ is the ratio of specific heats (1.4 for air). The flow is choked when $Ma = 1$ and unchoked when $Ma < 1$.

The molar flow rate is given by:

$$\dot{n} = P_o A C_d \sqrt{\frac{\gamma}{RTM_w}} Ma \left[1 + \frac{(\gamma - 1)}{2} Ma^2 \right]^{\frac{\gamma+1}{2-2\gamma}} \quad (30)$$

where R is the gas constant and T is the temperature, P_o is the absolute pressure inside the vessel, C_d is the discharge coefficient (typically about 0.9). If you use all SI units (Pascal, meters, kilograms, mole: so pressure in pascal, area in meters, R in J/mol/K, and Mw in kg/mol), you'll get mole per second for \dot{n} . See Perry's Handbook for Chemical Engineers Equation 6-118 for more information.

24.4 Flashing Two Phase Flow Estimate

$$\dot{m} = f \frac{\Delta H_v A}{\nu_{fg}} \sqrt{\frac{1}{C_p T_s}} \quad (31)$$

where \dot{m} is the mass flow rate, f is a factor depending on the scenario (less than 1), ΔH_v is the heat of vaporization, A is the area of the orifice, ν is the specific volume change of the liquid as it flashes ($\nu_g - \nu_l$), C_p is the heat capacity of the fluid, and T_s is the saturation temperature of the fluid at the set pressure. See Chapter 4 of Crowl and Louvar for more information.

24.5 Relief Valve Sizing

The above equations can be rearranged to solve for the area of the orifice, A , for a given flow rate and other conditions. Note that the discharge coefficient, C_d , is a function of the geometry of the orifice and the flow conditions. The discharge coefficient is typically determined experimentally with viscosity, downstream piping,

backpressure, and other factors influencing the value. Estimates for some of those parameters can be found in Chapter 10 of Crowl and Louvar. For a preliminary estimate, a value of 0.65 is often used for liquid flow and 0.9 for gas flow.

Relief Valve Sizing in some instances does required verification with actual flow per the AMSE Boiler and Pressure Vessel Code.

Note

See in-class examples

Download a pdf of the example using freeform here: <physical/supportfiles/GasFlowExample311.pdf>

24.5.1 In Class Example: Venting CO₂ from 2L Bottle

A two liter bottle is half filled with water. There is a relief valve on the top designed to relieve at 60 psig with a flow of 61 scfm. What is the flow rate of CO₂ through the relieve per the above equations?

```
import numpy as np

#first find the Mach number
gamma = 1.3 #specific heat capacity ratio for CO2, estimate
P1 = 60 + 12.5 #initial pressure, estimate, psia
Patm = 12.5 # atmospheric pressure, psia
Ma = min(1, np.sqrt(2/(gamma -1)*((P1/Patm)**((gamma -1)/gamma) -1))) #Mach number

Ma
1

#now calculate the molar flow rate
R = 8.314 # gas constant, J/(mol*K)
Temp = 295 # temperature, K
Area = np.pi/4*(1/4*0.0254)**2 # area of the pipe, m^2
Cd = 0.9 # discharge coefficient
Mw = 0.04401 # molar mass of CO2, kg/mol
# molar flow rate, mol/s
ndot = P1*6894.76*Area*Cd*np.sqrt(gamma/(R*Temp*Mw))*Ma*(1+(gamma -1)/2*Ma**2)**((gamma+1)/(2 -2*gamma))
print(f'The molar flow rate is {ndot:0.2f} mol/s')

The molar flow rate is 0.92 mol/s

#now convert that molar flow rate into scfm, PV = nRT
Tstandard = 298.15 # standard temperature, K
Pstandard = 101325 # standard pressure, Pa
scmps = ndot*R*Tstandard/Pstandard #units of m^3/s
scfm = scmps*60*(3.281**3)
print(f'The flow rate in scfm is {scfm:0.1f}')

The flow rate in scfm is 47.4
```

Why is this number different than the reported flow rate of CO₂ through the relief valve? Could the diameter of the relief be slightly larger?

How would you get the generation rate of CO₂ from the sublimation of dry ice?

$$Q = hA(T_{water} - T_{ice})mdot = Q/\Delta H_{vap} \quad (32)$$

Does area (A) change? How would you get the heat transfer coefficient (h)?

25 Mass and Energy Balances

Learning Outcomes

- Be able to understand a mass and energy balance

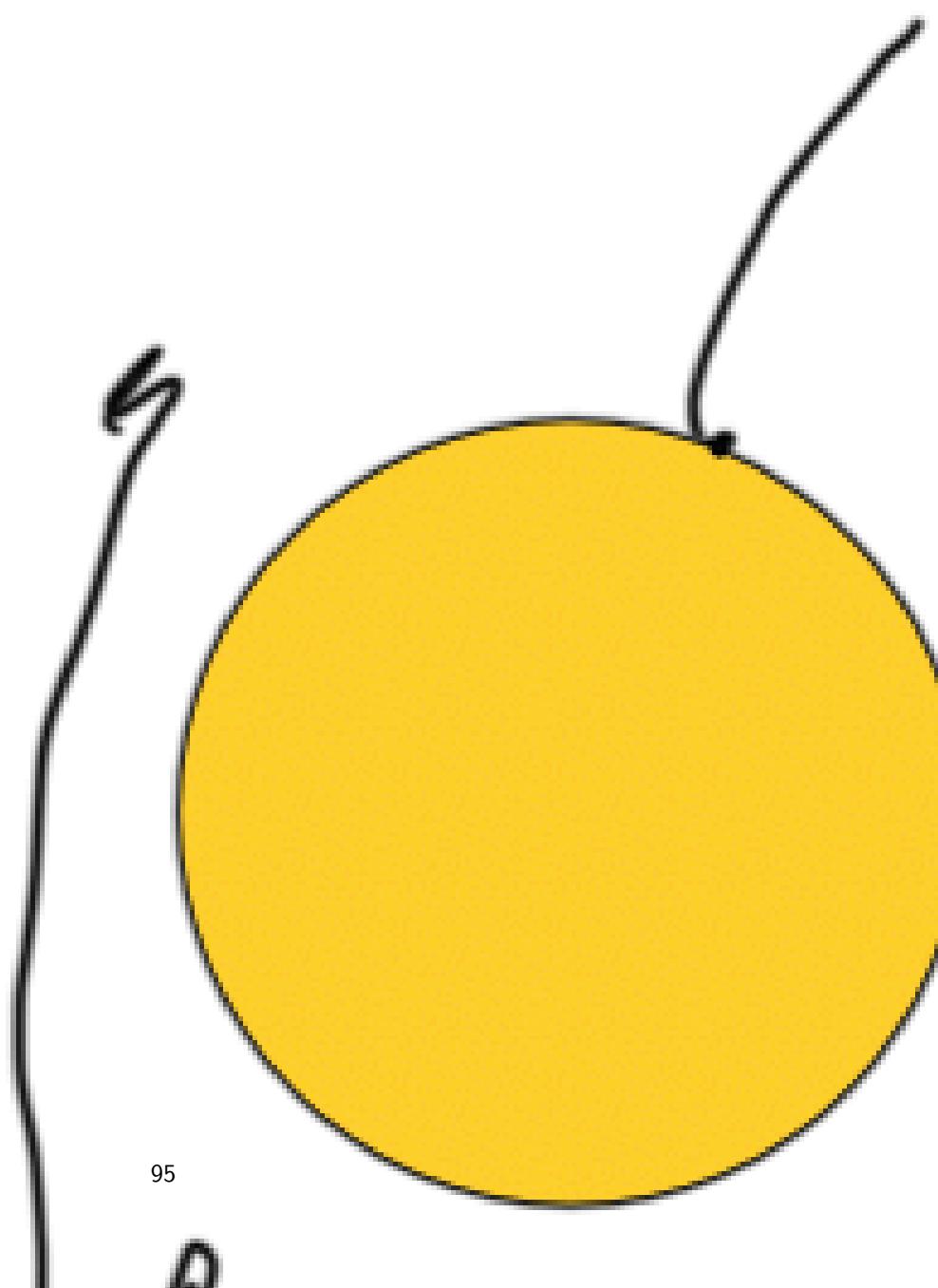
Reading

- Mass and energy balances

In previous discussions on environmental remediation, we have discussed ways in which material can be transferred from one location to another or that it can be broken down and then transferred. The rate of that transfer depends on the concentration immediately next to the surface and out in the middle of the fluid. Principles of vapor-liquid equilibrium (concentration next to the surface) and mass transfer are reviewed here.

25.1 Heat and Mass Transfer Preview

25.1.1 Heat Transfer: Convection



Solving the

$$m C_p \frac{dT}{dt}$$

$$dT$$

$$\frac{T_f - T_i}{T_f}$$

The

and

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25.1.2 Mass Transfer: Convection

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Her

25.2 Vapor Liquid Equilibrium Preview

25.2.1 Raoult's Law

25.2.2 Henry's Law

26 Reliefs

Learning Outcomes

- Understand the importance of **pressure protection**
- Identify and understand the different **types of pressure protection devices**
- Understand **where and why** pressure protection devices are used

Reading

- Foundations of Spiritual and Physical Safety: with Chemical Processes; Chapter 7, Sections 2-3

26.1 Pressure Protection

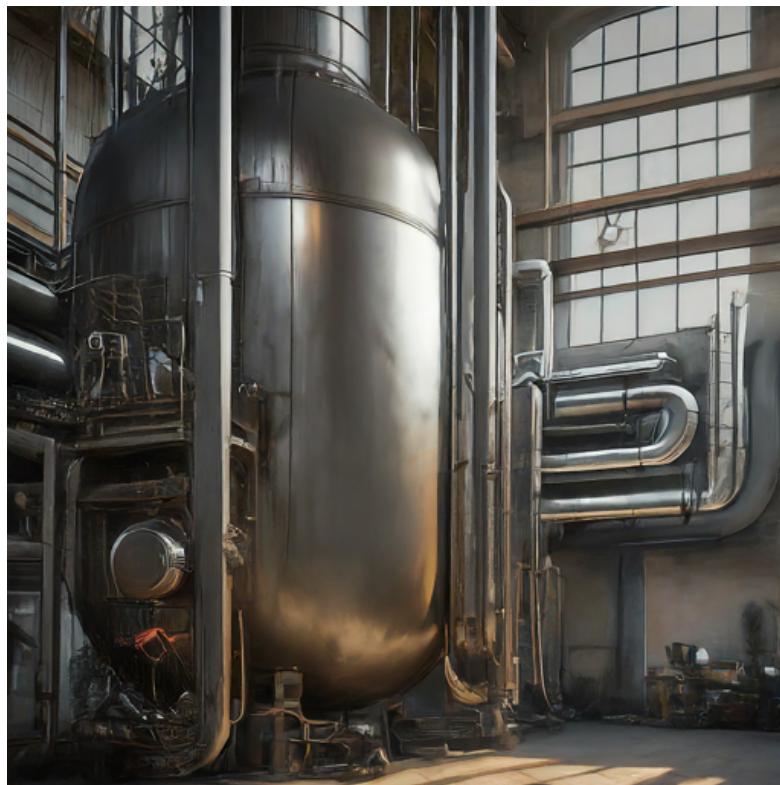


Figure 27: AI Generated Image of a Reactor

What would be the consequences if the reactor in the image above were to over-pressurize?

- The reactor could **explode**, causing damage to the plant and surrounding area
- The reactor could **release hazardous chemicals into the environment**

- The reactor could **release hazardous chemicals into the plant**, causing harm to personnel

Explosion approximate consequences:

```
#Potential energy from exploding reactor
ReactorVolume = 50 #m^3 (13,200 gallons)
VoidFraction = 0.67 #67% void fraction
Contents = 'Acetone'
BurstPressure = 10 #bar
ContentMass = ReactorVolume * (1 - VoidFraction) * 785 #kg/m^3, Acetone density estimate
CombustionHeat = 30.819e6 #J/kg: 1790 kJ/mol, molecular weight 58.08 g/mol

#Energy from bursting reactor scales with burst pressure and void volume:
BurstEnergy = BurstPressure * ReactorVolume * 1e5/(1.4 -1)*(1 -1/BurstPressure)**((1.4 -1)/1.4) #Joules
print('BurstEnergy, MJ: ', BurstEnergy/1e6)
CombustionEnergy = ContentMass * CombustionHeat #Joules
print(f'CombustionEnergy, MJ: {CombustionEnergy/1e6:.2f}')
#energy to power 1 homes for a year
EnergyPerYear = 100e6 #J
print(f'Energy could power {(CombustionEnergy+BurstEnergy)/EnergyPerYear:.2f} homes for a year')

BurstEnergy, MJ: 121.29319730813798
CombustionEnergy, MJ: 399183.10
Energy could power 3993.04 homes for a year
```

What steps could be taken to prevent the reactor from over-pressurizing?

Note

- Effective control of the rate of the reaction(s)
- Specific strategies to control side reactions
- Effective reactor cooling
- **Pressure Relief Devices** can be used to prevent an over-pressurization scenario
- RAGAGEP (Recognized and Generally Accepted Good Engineering Practices) should be followed

Code requirements (RAGAGEP) for pressure relief devices are found in Boiler and Pressure Vessel Code (ASME), Section VIII, Division 1, API 520, and others.

Many vessels are required to have pressure relief protection including

- Pressure vessels
- Blocked-in sections of liquid-filled piping
- Heat exchangers
- Storage tanks

What are some ways that elevated pressures could occur?

Note

- Overheating
- Runaway reaction
- Blocked outlet
- Fire exposure
- External pressure
- Thermal expansion
- Overfilling
- Equipment failure
- Control system failure
- Operator error
- Instrumentation failure

26.2 Types of Pressure Protection Devices

26.2.1 Spring Operated Relief Valves

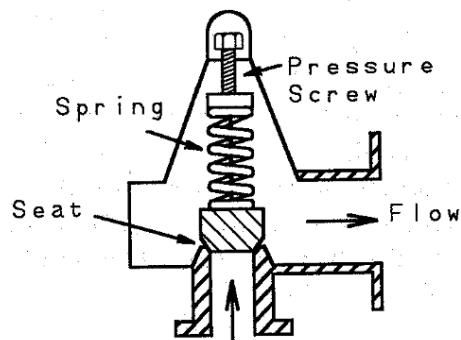


Figure 28: Drawing of the internal components of a spring operated relief valve.

Some components of spring operated relief valves include:

- Spring - the spring is compressed by the process pressure
- Valve plug - the plug is lifted off the seat when the spring force is overcome by the process pressure
- Nozzle - the nozzle directs the flow of the relieving fluid
- Seat - the plug seals against the seat to prevent flow

Comments on spring operated relief valves:

- very common



Figure 29: Image of a spring operated relief valve installed.

- versatile: can be used for gas or liquid
- reliable
- susceptible to chatter
- relieving pressure affected by temperature, back pressure, and accumulation
- flow decreases with increasing back pressure

26.2.2 Balanced Bellows Relief Valves

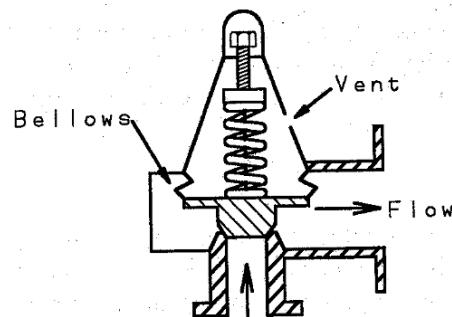


Figure 30: Drawing of the internal components of a balanced bellows relief valve.

Some components of balanced bellows relief valves include:

- Bellows - the bellows is a flexible diaphragm that is used to sense the process pressure
- Valve plug - the plug is lifted off the seat when the bellows force is overcome by the process pressure
- Nozzle - the nozzle directs the flow of the relieving fluid
- Seat - the plug seals against the seat to prevent flow

Comments on balanced bellows relief valves:



Figure 31: Image of a balanced bellows relief valve installed.

- similar to spring operated relief valves
- relieving pressure is not affected by back pressure
- flow decreases with increasing back pressure
- spring is protected from the process fluid
- flow through the valve can be impacted by back pressure

26.2.3 Pilot Operated Relief Valves

Some comments on pilot operated relief valves:

- relieving pressure not affected by back pressure
- can operate very close to set pressure
- potential for back flow
- o-ring seals limit some applications

26.2.4 Buckling Pin Relief Valves

Comments on buckling pin relief valves:

- similar to a rupture disk
- o-ring seals used and can limit some applications
- less susceptible to corrosion (vs rupture disk)
- can be operated closer to the set pressure (vs rupture disk)
- can operate at very low set pressures

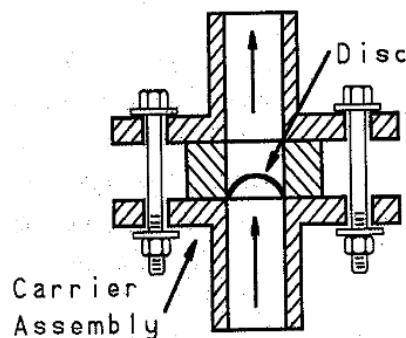


Figure 32: Drawing of the internal components of a rupture disk device.



Figure 33: Image of a rupture disk.

26.2.5 Rupture Disks

Relief valves are often used in conjunction with rupture disks. Rupture disks are used to protect the relief valve from the process fluid. Rupture disks are often used in applications where the process fluid is corrosive, toxic, or would otherwise damage the relief valve.

Rupture disks are often made of a thin metal that is designed to rupture at a specific pressure. The rupture disk is installed in a holder that is designed to contain the disk fragments when the disk ruptures. Some other characteristics of rupture disks include:

- often used in conjunction with relief valves
- often used in applications where the process fluid is corrosive, toxic, or would otherwise damage the relief valve or small leaks over time would present risks to people and the environment
- one-time use (does not close after relieving)
- pieces of disk can be a hazard in the process
- rapid response
- there are multiple types:
 - reverse buckling
 - tension loaded
 - scored
 - pre-fragmented

- composite
- solid
- knife blade
- slotted

26.3 Some Definitions

Term	Definition
Set Pressure	The pressure at which the relief device is set to open
Relief Pressure	The pressure at which the relief device actually opens
MAWP	Maximum Allowable Working Pressure, maximum gauge pressure permissible at the top of the vessel at the designated temperature
MAWT	Maximum Allowable Working Temperature, the maximum temperature at which the vessel is permitted to operate
MDMT	Minimum Design Metal Temperature, the lowest temperature at which the vessel is permitted to operate
Operating Pressure	The pressure at which the vessel is intended to operate; no more than 90% of the MAWP
Accumulation	The pressure increase over the MAWP that occurs when the relief device is operating; expressed as a percentage of the MAWP
Overpressure	The pressure increase over the set pressure that occurs when the relief device is operating; expressed as a percentage of the set pressure
Back Pressure	The pressure at the outlet of the relief device; composed of two components: pressure from downstream and pressure required for frictional losses
Blowdown	The difference between the set pressure and the relief reseating pressure
Maximum allowable accumulation pressure	Sum of the accumulation and the MAWP
Relieving pressure	The pressure at which the relief device is fully open and relieving: set pressure plus overpressure

Code comments:

- The maximum normal operating pressure can never exceed the MAWP, even momentarily. However, the actual pressure during the relieving process may exceed the MAWP.
- Pressure tests (to verify strength) are often performed at 1.5 times the MAWP. Tests use water typically (gas tests would yield a much more violent failure if the vessel were to fail during the test).
- For a single relief, the maximum set pressure is the MAWP.
- During the relieving process, the overpressure cannot exceed the MAWP by more than the following percentages:
 - 110% for vessels equipped with a single pressure relief device.
 - 116% for vessels equipped with supplemental pressure relief devices.
 - 121% for fire exposures.
- For supplemental relief devices, the max. set pressure is 105% of the MAWP.

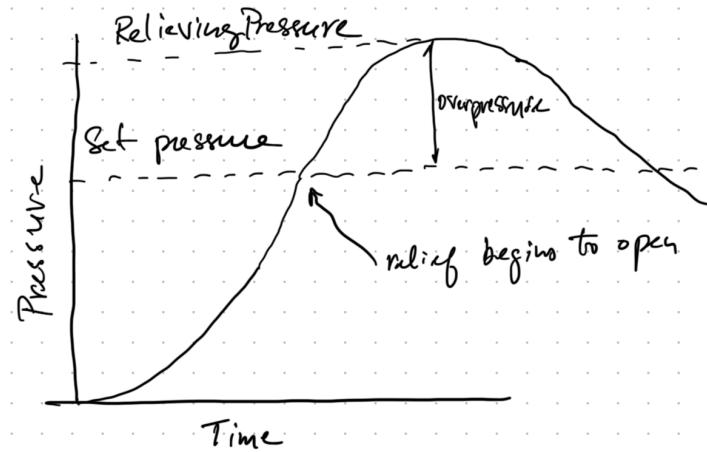


Figure 34: Plot of set pressure, relieving pressure, accumulation, and overpressure for a pressure relief device.

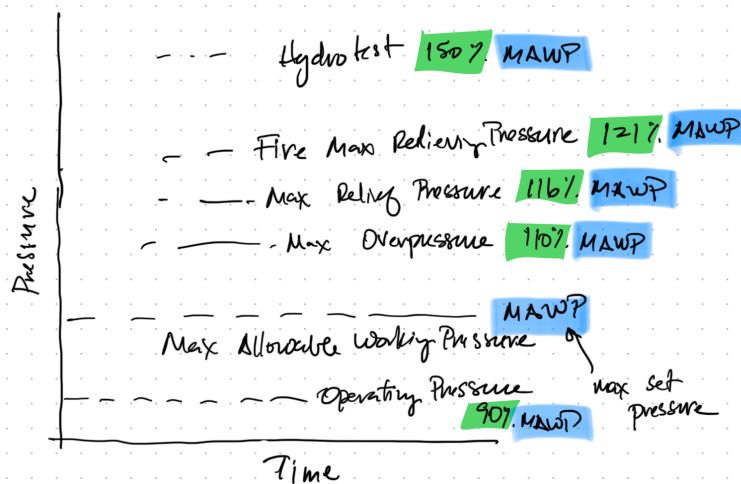


Figure 35: Plot of the various pressures associated with a pressure relief device.

26.4 Where and Why Pressure Protection Devices are Used

26.4.1 Vessels

All vessels, including reactors, storage tanks, heat exchangers, towers and drums.

26.4.2 Positive Displacement Pumps, Compressors, and Turbines

These devices can be blocked in by a closed valve, causing the pressure to rise. These processing pieces may have an internal relief valve.

26.4.3 Piping

Piping is not normally required or recommended to have pressure relief protection as piping can typically withstand pressures higher than the vessels they supply. However, there are some exceptions:

- blocked-in sections of liquid-filled piping that may be heated or otherwise pressurized
- heat traced piping

- long lines (thermal expansion)
- loading or transfer lines beyond the property line
- lines with history of overpressure
- lines that may be exposed to high pressures
- per the hazards analysis

26.4.4 Examples of Where Pressure Protection Devices are Used

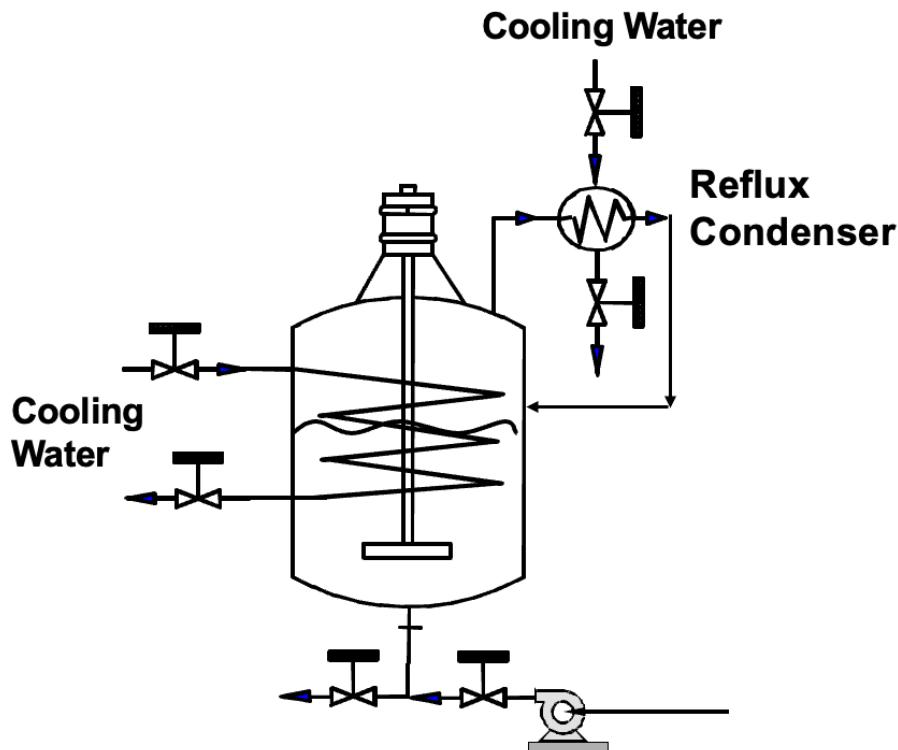


Figure 36: Example drawing of a reactor with cooling and reflux.

Note

- Blocked in heating coils.
- Blocked in cooling water line on reflux condenser.
- Relief on reactor – variety of scenarios.
- Relief on pump – need to check with manufacturer of pump.
- Side reaction? Incompatibility?
- Fire?

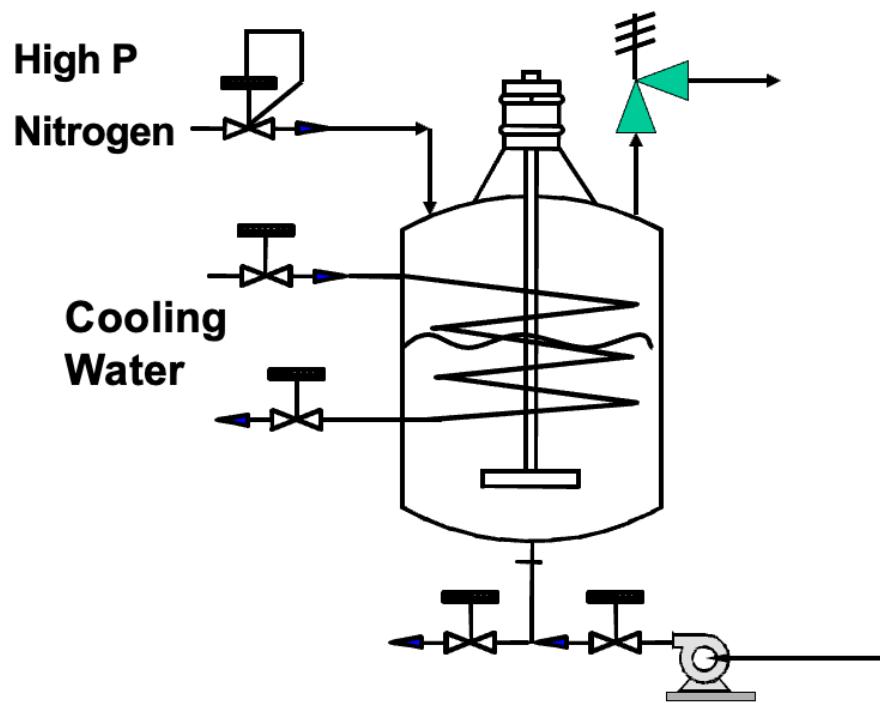


Figure 37: Image of a reactor with pressure relief device present on the reactor.

Note

- Failure of high pressure nitrogen regulator
- Hole in cooling water coil.
- Pump continues to run after filling.
- Fire exposure
- Runaway reaction
- Blocked outlet

26.5 Relief Effluent Handling

Oft times, the relief effluent cannot simply be released to the atmosphere. The effluent may be toxic, flammable, or otherwise hazardous. The effluent may also be at a high temperature or pressure. Some options for handling the effluent include:

- Flare
- Vent to a scrubber
- Vent to a thermal oxidizer

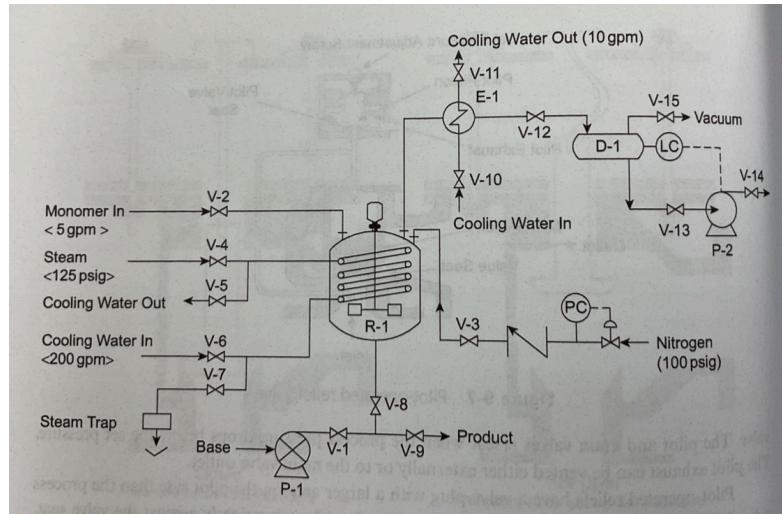


Figure 38: Process flow diagram of a polymerization process. *Source: Crowl and Louvar, Chemical Process Safety, 4th Edition, Figure 9-8.

- Vent to a condenser
- Vent to a knock-out drum

27 Engineering Controls

Learning Outcomes

- Control Techniques

Reading

- Foundations of Spiritual and Physical Safety: with Chemical Processes; Chapter 7, Sections 4-8

Inerting (Vacuum/Pressure purging); Piping/Bonding/Grounding; Work Permits; Hot Work.

27.1 Control Techniques

There are multiple control techniques that can be used to reduce the exposure to workers from a toxic gas or vapor. These include:

Inherent Safety: Designing the process to eliminate or reduce the use of toxic gases or vapors.

- **Substitution:** Replace the toxic gas or vapor with a less toxic or non-toxic alternative.
- **Minimization:** Reduce the amount of toxic gas or vapor that is used in the workplace.
- **Isolation:** Use of barriers or other methods to separate the toxic gas or vapor from workers.

Engineering Controls: Use of ventilation, enclosures, or other engineering controls to reduce the concentration of the toxic gas or vapor in the workplace.

Administrative Controls: Use of work practices, policies, and procedures to reduce the exposure of workers to toxic gases or vapors.

Personal Protective Equipment (PPE): Use of PPE such as respirators (full or half face) or supplied air respirators to reduce the exposure of workers to toxic gases or vapors.

27.1.1 Engineering Controls

Ventilation: Ventilation occurs with HVAC systems where air is circulated and filtered. However, most of the air is recirculated and only a small fraction is replaced with fresh air. The recirculation of air can lead to a build up of toxic gases and/or distribute them to other areas of the workplace.

Ventilation where outside air is brought in can help reduce the concentration of toxic gases or vapors but it has significant energy costs.

Typical ventilation occurs with negative rather than positive pressure systems. Know the difference between positive and negative pressure systems and why one might be used over the other.

Local Ventilation: Hoods

Hoods are effective at containing and expelling toxic gases or vapors. However, they can be expensive to install and maintain. They also require a significant amount of energy to operate.

28 RAGAGEP and PSM

Learning Outcomes

- Be able to recognize RAGAGEP with details
- Be able to name multiple parts of PSM and why they are important

Reading

- Foundations of Spiritual and Physical Safety: with Chemical Processes; Chapter 8

Process safety management also covers important topics besides Process Safety Information and Process Hazard Analysis.

28.1 RAGAGEP

Following significant industrial accidents, government regulations were put in place to create a safer work environment. OSHA or the Occupational Safety and Health Administration was established in the early 70's. They and others collected and set Recognized and Generally Accepted Good Engineering Practices (RAGAEP). Some of the substantial practices have been codified into law. These practices are the minimum standards that must be followed to ensure a safe work environment. Some of which are given below:

Regulations:

- OSHA 29 CFR 1910.119 Process Safety Management (PSM)
- EPA 40 CFR 68 Risk Management Programs (RMP)
- DHS 6 CFR 27 Chemical Facility Anti-Terrorism Standards (CFATS)
- PHMSA/ DOT Shipment of Hazardous Chemicals 49 CFR Parts 100-185

Codes

- NFPA 70: National Electrical Code
- ASME Boiler and Pressure Vessel Code

Standards

- NFPA 45, 68, 69
- Many others

28.2 OSHA 29 CFR PSM Elements

Required for those meeting the Threshold Quantities

- Employee Participation

- **Process Safety Information**
- **Process Hazards Analysis**
- Operating Procedures
- Training
- Contractors
- Pre-Startup Safety Review
- Mechanical Integrity
- Hot Work Permits
- Management of Change
- Incident Investigation
- Emergency Planning and Response
- Audits
- Trade Secrets

28.3 14 Points of PSM: OSHA 1910.119

1. Employee Participation
 - Employees participate with process hazards analysis (PHAs) for example
2. Process Safety Information
 - Understanding the hazards of the process
 - process chemistry
 - phase diagram
 - inventory or processing amounts
 - safe upper and lower limits for temperature, pressure, etc.
 - consequences of deviation, etc.
3. Process Hazards Analysis
 - **FMEA** Failure Modes and Effects Analysis
 - **HAZOP** Hazards and Operability Study
 - **FTA** Fault Tree Analysis
 - Others: LOPA, What-If, Checklist, etc.
 - Hazards addressed
 - Previous incidents and near misses evaluated and included
 - Engineering and administrative controls (safeguards)
 - Consequences of failure
 - Facility siting (location of the facility relative to other facilities and the public)
 - Qualitative and quantitative evaluations
 - Team effort
 - System to address findings and recommendations
 - Revalidation (every 5 years)
 - Documentation
4. Operating Procedures

- startup, shutdown, normal operations, emergency operations, etc.
- operating limits
- safety and health considerations
- safety systems
- Accessible and reviewed regularly
- Lock and Tag Out procedures
- Confined Space Entry procedures

5. Training

- Initial and refresher training
- Documentation

6. Contractors

- Prequalification (safety record, training, etc.)
- Informed on PHA and operating procedures by the owner
- Injury and illness records
- Documentation

7. Pre-Startup Safety Review

- Required with new processes or significant modification
- RAGAGEP (Recognized and Generally Accepted Good Engineering Practices)
- Procedures required to be in place (operating, maintenance, emergency, etc)
- PHA completed
- Training completed
- Documentation

8. Mechanical Integrity

- covers pressure vessels, tanks, prvs, piping, emergency systems, controls, pumps, etc.
- written procedures required
- training for maintenance personnel
- Regular inspection with testing
- Documentation

9. Hot Work Permits

- Required for welding, cutting, brazing, etc. on covered processes
- Fire prevention and protection measures
- Inspection of area
- Fire watch
- Documentation

10. Management of Change

- Required for changes in process chemicals, technology, equipment, procedures, etc.
- Procedures to manage changes and their consequences
- Training required on consequences of changes
- Documentation

11. Incident Investigation

- Required for incidents that resulted in, or could have resulted in, a catastrophic release
- Team effort started within 48 hours

- Report generated
- System required to address findings
- Report reviewed with employees
- Report retained for 5 years

12. Emergency Planning and Response

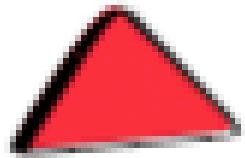
- Emergency action plan documented and implemented including evacuation, alarms, training, drills, etc.

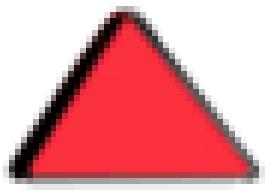
13. Compliance Audits

- Required every 3 years
- Team effort
- Report generated
- System required to address findings
- 2 most recent reports retained

14. Trade Secrets

- PSI (Process Safety Information) must be available to employees and contractors
- Confidential information can be protected
- Employees have access to PSI, the PHA, and other PSM documentation





Process hazard

- will

- can

- do

- Hazard
- Incident
- Emergency
- Consequence
- Facility

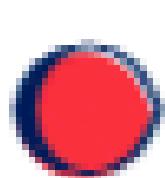
• Operating
• with Hev

- S

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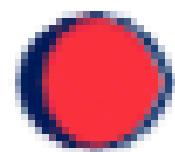
- S

- C



Principles

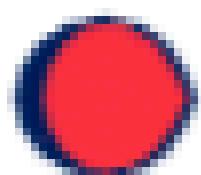
- Personal
- Professional
- Safe Work
- Protection
- Training



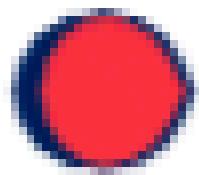
Manager
•



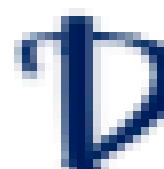
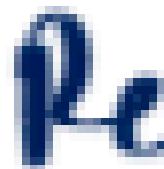
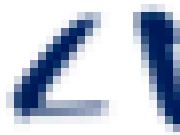
Incident



Emergency



Complaint



28.4 Example Cases

28.4.1 Pressure drop

Pressure drop in a hydrogenation reactor from clogged support plate after change in charcoal blend.

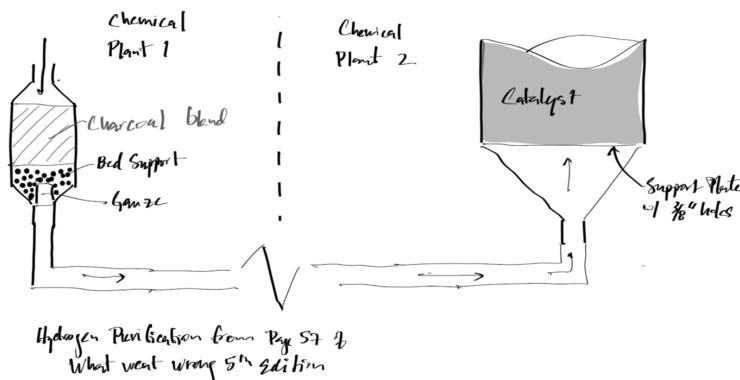


Figure 39: Image of the process where a hydrogenation reactor from a clogged support plate resulted after change in the charcoal blend.

28.4.2 Process change

Nitration occurs with OH groups replaced by NO₂ groups. A nitration reaction was carried out at low temperature and then heated to 90°C for 30min and then cooled. Instead of active cooling, the reactor was left to cool down on its own and it exploded throwing pieces 75m away (see reference 7 in Section 2.6 in What Went Wrong, 5th Edition). (Autoignition can be at lower temperature with longer exposure times.)

28.4.3 Gasoline flammability

A man who wanted some gasoline for cleaning decided to siphon it out of the tank of a company vehicle. He inserted a length of rubber tubing into the gasoline tank. Then, to fill the tubing and start the siphon, he held the hose against the suction nozzle of an industrial vacuum cleaner. The gasoline caught fire and two vehicles were destroyed and eleven damaged. (Quoted from What Went Wrong, 5th Edition, Section 3.3.3(a))

28.4.4 Ethylene Oxide

The above system with the ethylene oxide pump was setup such that the Pump1 could only operate (engineering controls) when:

- the circulation pump (pump2) was running
- the temperature was above 115°C, as otherwise the ethylene oxide would not react
- the temperature was below 125°C, otherwise the reaction was too fast

Accident scenario:

The operator thought he had the valve at the bottom of the reactor open but didn't and running the pump with a dead suction led to the temperature rising, satisfying the conditions for the ethylene oxide to be introduced (pump was running and temperature was between 115 and 125°C). He saw the pressure rise (no reaction occurring as ethylene oxide is a gas) so he allowed more heat to the heat exchanger. He then realized that the valve was closed and opened it. An explosion resulted as the reaction occurred very quickly and released a lot of heat.

This scenario taken from What Went Wrong, 5th Edition, Section 3.2.8.

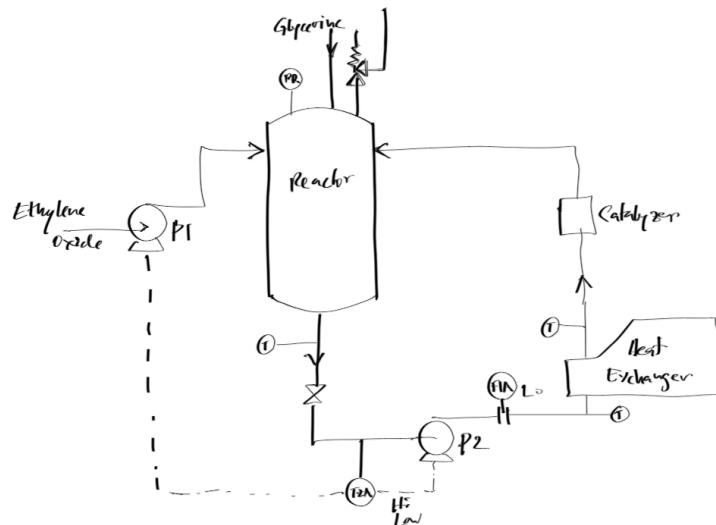


Figure 40: Process flow drawing of an ethylene oxide reactor system.

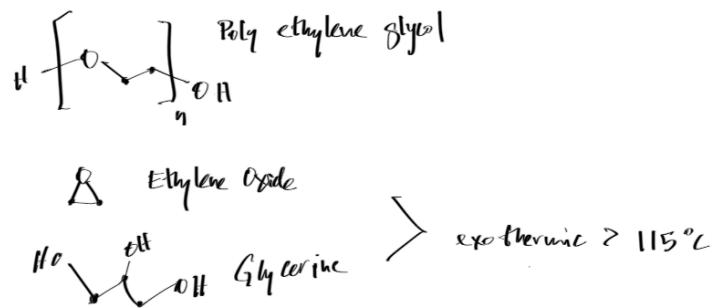


Figure 41: Image of polyethylene glycol, ethylene oxide and glycerine molecules.

28.4.5 Hot Work

Many accidents have occurred from maintenance or other activities with welding, cutting, etc that have ignited flammable materials.

29 RAGAST

Learning Outcomes

- Be able to discuss important points of RAGAST

Reading

- Foundations of Spiritual and Physical Safety: with Chemical Processes; Chapter 9

Accepted Scriptural Texts

30 Hazardous Communication

Learning Outcomes

- Understand the purpose and components of the Hazardous Communication Standard
- Become more familiar with the 9 Hazard Classes of the GHS
- Understand the 16 Components of a Safety Data Sheet (SDS)
- Understand the elements of GHS Labeling
- Be familiar with the GHS Pictograms
- Understand the NFPA 704 Diamond

Reading

- Foundations of Spiritual and Physical Safety: with Chemical Processes; Chapter 10

Hazardous Communication is required by OSHA to ensure that the hazards of all chemicals produced or imported are evaluated, and that information concerning their hazards is transmitted to employers and employees. This information is transmitted through the use of Safety Data Sheets (SDS) and labels. The regulation requiring this is [29 CFR 1910.1200](#).

Global Harmonized System of Classification and Labelling of Chemicals (GHS) is a system for standardizing and harmonizing the classification and labelling of chemicals. It satisfies the requirement of many countries to have a single system of classification and labelling of chemicals.

30.1 Opening Activity

- How would you think it best to communicate hazards to a toddler or 3-5 year old on the hazards in a typical household
 - Guns?, Chemicals?, Hot Surfaces?, Electricity?, Sharp Objects?
- How would you want to be communicated to about hazards in your workplace?
 - Chemicals, Machinery, Electrical Hazards, Fire Hazards, etc.?

30.2 Nine (9) Hazard Classes of Materials and Articles

1. Explosives
2. Gases
3. Flammable Liquids
4. Flammable Solids
5. Oxidizing Substances
6. Toxic and Infectious Substances
7. Radioactive Material

8. Corrosives
9. Miscellaneous Dangerous Goods



Figure 42: Image of the different hazard class labels of materials and articles.

30.2.1 Explosives

- HD1.1: Mass explosion hazard
- HD1.2: Projection hazard
- HD1.3: Fire hazard
- HD1.4: No significant hazard
- HD1.5: Very insensitive substances
- HD1.6: Extremely insensitive substances

See Video examples from Safety Management Services, Inc.

30.2.2 Gases

- HD2.1: Flammable gases
- HD2.2: Non-flammable, non-toxic gases
- HD2.3: Toxic gases

30.2.3 Flammable Liquids

- Flammable liquids: flash point <60°C
- Combustible liquids: flash point >60°C and <93°C

30.2.4 Flammable Solids

- HD4.1: Flammable solids
- HD4.2: Spontaneously combustible
 - Pyrophoric: ignite spontaneously in air
 - Self-heating: heat up in air
- HD4.3: Dangerous when wet

30.2.5 Oxidizing Substances

- HD5.1: Oxidizing substances
- HD5.2: Organic peroxides

30.2.6 Toxic and Infectious Substances

- HD6.1: Poisonous substances
- HD6.2: Infectious substances

30.2.7 Radioactive Material

- HD7: Radioactive material

30.2.8 Corrosives

- HD8: Corrosives

30.2.9 Miscellaneous Dangerous Goods

- HD9: Miscellaneous dangerous goods

30.2.10 Hazardous Materials Table

The hazardous materials table is a list of hazardous materials and their proper shipping names, hazard classes, identification numbers, packing groups, and special provisions. The table is in 49 CFR 172.101: [49 CFR 172.101](#)

[49 CFR 172.101](#) has many of the details on shipping and handling of hazardous materials. You are not required to know this for any exam but it may prove valuable to you to know where to find this information.

30.3 SDS Components

1. Identification
2. Hazard(s) identification
3. Composition/information on ingredients
4. First-aid measures
5. Fire-fighting measures
6. Accidental release measures
7. Handling and storage
8. Exposure controls/personal protection
9. Physical and chemical properties

10. Stability and reactivity
11. Toxicological information
12. Ecological information
13. Disposal considerations
14. Transport information
15. Regulatory information
16. Other information

See also: <https://www.osha.gov/laws-regulations/standardnumber/1910/1910.1200AppD>

30.3.1 SDS Examples

- [Gasoline](#)
- [Water](#)
- [PETN](#)

30.4 GHS Pictograms

Health Hazard



- Carcinogen
- Mutagenicity
- Reproductive Toxicity

Gas Cylinder



- Gases Under Pressure

Flame Over C



- Oxidizers

Source: <https://www.osha.gov/sites/default/files/publications/OSHA3491QuickCardPictogram.pdf>

30.5 GHS Labeling

GHS Labeling requirements include:

- Product Identifier
- Signal Word
 - Danger (more severe)
 - Warning
- Hazard Statement
- Pictograms
- Precautionary Statement
- Supplier Information
- [Gasoline](#)
- [Ethanol](#)

Classwork Assignment: What would a GHS label for PETN look like? What should the SDS Contain?

30.6 NFPA 704 Diamond

NFPA diamonds are required by OSHA to be placed on containers of hazardous materials. The diamond is divided into four sections, each with a color and number. The colors and numbers are as follows:

- Red: Flammability
- Blue: Health
- Yellow: Reactivity
- White: Special Hazards

NFPA 704 Diamonds are not required by OSHA; however, local municipalities or fire departments may require them.

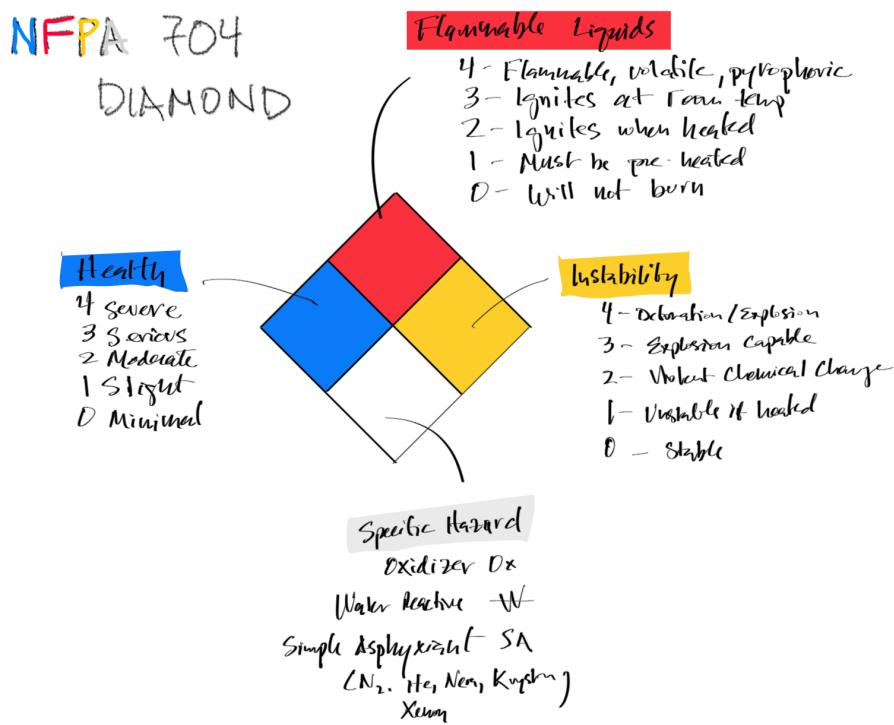


Figure 43: Drawing of the NFPA 704 Diamond with the colors and numbers for flammability, health, reactivity, and special hazards.

31 AI Tools in Safety

Learning Outcomes

- Understand the basics of AI Tools
- Be able to effectively use AI Tools in safety analysis

Reading

- Foundations of Spiritual and Physical Safety: with Chemical Processes; Chapter 11

32 Energy Overview

Learning Outcomes

- Review Energy Units and "Horse Sense"
- Understand the different energy types
- Understand quantities and fractions of energy used in US
- Understand the growing energy demands by 1/2 the world's population in BRICS countries
- Understand some of the challenges and opportunities in the energy sector

Reading

- Energy overview reference

32.1 Units Review

- BTUs: British Thermal Units
 - Energy required to raise 1 pound of water by 1 degree Fahrenheit
- Calories
 - Energy required to raise 1 gram of water by 1 degree Celsius
- Joules
 - 1 calorie = 4.184 Joules
- Watts
 - Power or rate of energy use in Joules per second
 - A human can generate about 300 Watts of power on an exercise bike for a sustained time period
- Kilowatt-hours
 - Energy used by a 1 kW device in 1 hour
- Quad: 1 quadrillion BTUs
 - This is the amount of energy in 170 million barrels of oil

32.1.1 Example Unit Problems

How many BTU's to heat 1 L of water from 60°F to 212°F?

How many BTUS's to vaporize that same 1L of water at 212°F?

32.2 Energy Types

- Fossil
 - Coal
 - Oil
 - Natural Gas
 - Tar Sands
- Nuclear
- Solar
 - Photovoltaic
 - Concentrated Solar Power
- Renewable
 - Wind
 - Hydro
 - Geothermal
 - Biomass
 - Ocean

32.3 US Energy by Source with Losses

Figure 44: Estimate US Energy Consumption. Source: https://flowcharts.llnl.gov/sites/flowcharts/files/2022-04/Energy_2021_United-States_0.png

How many cubic miles of oil are used in the US in a year?

Note

About 1 cubic mile

There are significant losses in use of the energy. For example, a coal plant is only about 33% efficient in converting the energy in coal to electricity. A gasoline engine is only about 20% efficient in converting the energy in gasoline to motion. The rest is lost as heat.

32.3.1 Energy loss example

The energy density of gasoline is about 45 MJ/kg. If a car gets 30 miles per gallon (at 60 miles per hour), how many MJ of energy are used to go 30 miles? What is the efficiency of the car?

How will you set this up?

Note

Assumptions:

- Force from drag is $F_d = 1/2\rho v^2 C_d A$, where ρ is air density, v is velocity, C_d is drag coefficient, and A is frontal area. The drag coefficient for a car is about 0.3, the frontal area is about 2 m², and the air density is about 1.2 kg/m³.
- The resistance from rolling friction, $F_r = C_r mg$, where C_r is the coefficient of rolling friction, m is mass, and g is acceleration due to gravity. The coefficient of rolling friction is about 0.01 for cars and the mass of the car is about 1500 kg.

- The energy of a moving car is $E = 1/2mv^2$.
- The energy of a force acting over a distance is $\int Fdx$.

32.4 BRICS

The BRICS countries (Brazil, Russia, India, China, South Africa) are expected to use more energy as development continues.

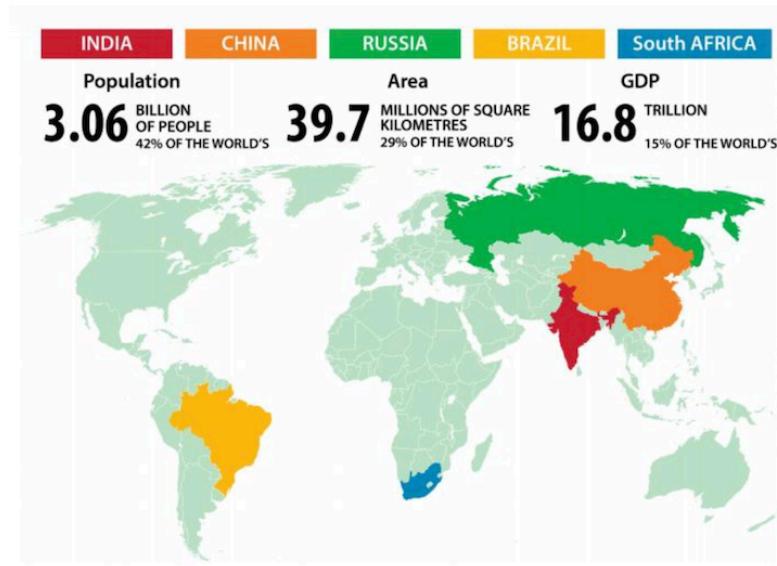


Figure 45: Population and GDP of the BRICS countries. Source: <https://unacademy.com/content/upsc/study-material/international-relations/importance-of-brics-for-india/>

32.5 Increasing Energy Use

32.6 Energy per Person

32.7 Inflation Reduction Act (2022)

The Inflation Reduction Act (IRA) is a United States federal law enacted on August 16, 2022. It is the most significant piece of climate legislation in U.S. history. The IRA provides \$369 billion in climate change programs over 10 years. It also includes provisions to lower healthcare costs, reduce the federal deficit, and invest in domestic energy production.

32.7.1 Key provisions of the IRA include:

- **Tax credits for renewable energy:** The IRA extends and expands tax credits for solar, wind, and other renewable energy sources. This includes a 30% investment tax credit (ITC) for solar projects and a production tax credit (PTC) for wind projects.
- **Electric vehicle incentives:** The IRA provides tax credits for electric vehicles (EVs) and plug-in hybrid electric vehicles (PHEVs).
- **Energy efficiency programs:** The IRA includes funding for energy efficiency programs, such as rebates for energy-efficient appliances and home retrofits.

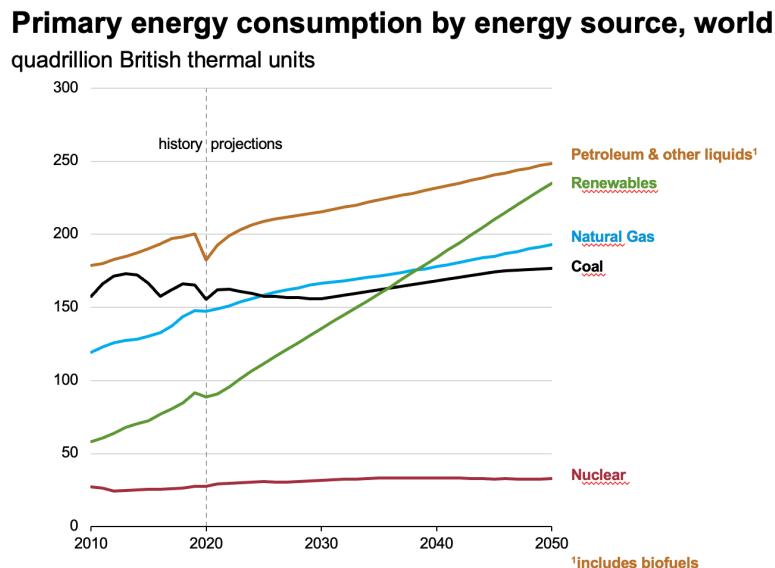


Figure 46: Primary energy consumption by energy source. Credit [EIA.org](https://www.eia.gov/), International Energy Outlook 2021

Figure 47: Energy use per person, source: <https://ourworldindata.org/energy-access#>.

- **Carbon capture and storage:** The IRA provides tax credits for carbon capture and storage (CCS) projects, which can help reduce greenhouse gas emissions from fossil fuel power plants.

32.8 IRA Expected Environmental Benefits

- **Reduction in greenhouse gas emissions:** The IRA is expected to reduce U.S. greenhouse gas emissions by about 40% by 2030 compared to 2005 levels.
- **Increased renewable energy generation:** The IRA is expected to increase the share of renewable energy in the U.S. electricity mix to about 70% by 2030.
- **Job creation:** The IRA is expected to create millions of jobs in the renewable energy sector, including jobs in manufacturing, installation, and maintenance of renewable energy systems.

32.9 Energy Future

The US Energy Information Administration (EIA) is a government organization that provides data and analysis on energy production, consumption, and trends. The EIA provides projections of energy consumption and production through 2050 and can be found on their website: <https://www.eia.gov/outlooks/aoe/>

Figure 48: Energy related CO2 emissions, source: <https://www.eia.gov/outlooks/aoe/>

Some Comments:

- Total CO2 emissions are expected to decline despite the increase in energy use and population
- Coal is declining due to its challenges:
 - Mercury, SOx, NOx, CO2, and particulates

- Natural Gas is increasing due to its lower emissions, abundance, and economics
- Petroleum will face a slow decline but there is not yet a feasible replacement as a transportation fuel and as a raw material for chemical production
- Transition to renewables will not/cannot happen on order of 10 years (maybe even 30) without societal upheaval
- Nuclear is a viable option but has its own challenges
- Energy storage is likely to grow in importance
- Ultimately, we'll need to use many forms of energy

D&C 104: 17 Says: "For the earth is full, and there is enough and to spare; yea, I prepared all things, and have given unto the children of men to be agents unto themselves."

And the next verse says: "Therefore, if any man shall take of the abundance which I have made, and impart not his portion, according to the law of my gospel, unto the poor and needy, he shall, with the wicked, lift up his eyes in hell, being in torment."

32.10 Energy Ethics

Per the AICHE Code of Ethics (<https://www.aiche.org/about/code-ethics>), and the National Society of Professional Engineers (<https://www.nspe.org/resources/ethics/code-ethics>) engineers should "hold paramount the safety, health, and welfare of the public."

How does that ethics code apply to helping developing nations get access to energy?

FOSSIL FUELS AND NUCLEAR

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1st Jan, 2025

created in  Curvenote

Keywords Spiritual Safety, Process Safety, Chemical Engineering, Risk Assessment

Learning Outcomes

- Characterize the four major fossil fuel types (Coal, Petroleum, Natural Gas, Tar Sands) based on their formation, extraction, and application.
- Analyze the economic mechanisms, such as Energy Return on Investment (EROI), that favor fossil fuel utilization.
- Explain the operational principles of nuclear energy and contrast its reliability and risk profile with fossil fuel systems.

Reading

- Fossil fuels review article
- Nuclear energy review article

1 Coal

Coal has been used for many years to provide power to millions of homes and businesses. Coal is the most abundant fossil fuel in the United States. Fossil fuels are formed from the remains of ancient plants and animals, buried and altered over millions of years. The three main types of fossil fuels are coal, oil, and natural gas.

The United States has more coal than the rest of the world has oil. There is still enough coal underground in this country to provide energy for the next 250 years or more per the U.S. Department of Energy. There is enough coal in the world to last us more than 1,000 years.

1.1 Coal Types

Peat

Bituminous Coal

Chemical Structure, CHNSO_{Hg}



Figure 1: Image of peat from [https://commons.wikimedia.org/wiki/File:Peat_\(49302157252\).jpg](https://commons.wikimedia.org/wiki/File:Peat_(49302157252).jpg).



Figure 2: Image of coal from [https://commons.wikimedia.org/wiki/File:Bituminous_coal_\(Ferron_Sandstone_Member,_Mancos_](https://commons.wikimedia.org/wiki/File:Bituminous_coal_(Ferron_Sandstone_Member,_Mancos_)

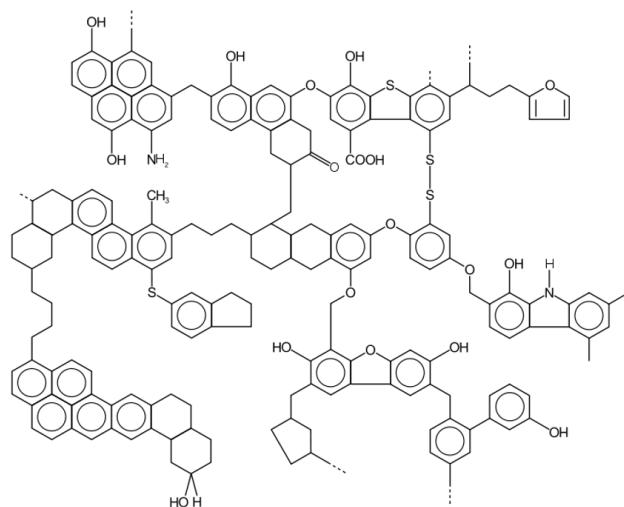


Figure 3: Chemical structure of coal showing the main chemical structures present.

- Sulfur
- Nitrogen
- Mercury
- CO₂ (Coal emits 60% more CO₂ than natural gas per kWh (0.37 kg/kWh compared to 0.23 kg/kWh))
- Ash

1.2 Coal History

- 300 BC - Greek scientist Theophrastus reportedly said: "Among the materials that are dug because they are useful, those known as coals are made of earth, and, once set on fire, they burn like charcoal."
- Newcomen Engine (1712)
- 1769 James Watt invents the steam engine, which ran on coal.
- 1882 Thomas Edison opens the first commercial power plant in New York City, which was powered by coal.

1.3 Coal Use

- Principally used for electricity generation
- >8 billion tons per year are used ([source](#)).
- China uses 4 billion tons per year ([source](#))
- Taking into account the thermodynamic efficiency of electricity generation, coal produces approximately 2 kWh per kg.
- Current US coal-fired power plant capacity is <200,000 MW
- >2400 coal-fired power plants in the world

1.4 Coal Technology Frontiers

- Combined Cycle Gas Turbine (CCGT) and Integrated Gasification Combined Cycle (IGCC)
- Clean coal/Carbon capture and sequestration (CCS)
- Gasification and liquefaction for fuels and chemicals

1.5 Power Plant

2 Petroleum

Petroleum, a naturally occurring mixture of hydrocarbons, is a primary energy source due to its high energy density. Through refining, it provides fuels for transportation (gasoline, diesel, jet fuel) and serves as a feedstock for lubricants, plastics, and various petrochemicals. Chemical engineers seek to optimize its extraction and refining processes while mitigating its environmental impact.

Petroleum production around the world ranges from:

- 23 million barrels per day in the Middle East
- 16 million barrels per day in the Americas
- 20 million barrels per day in Russia and Africa

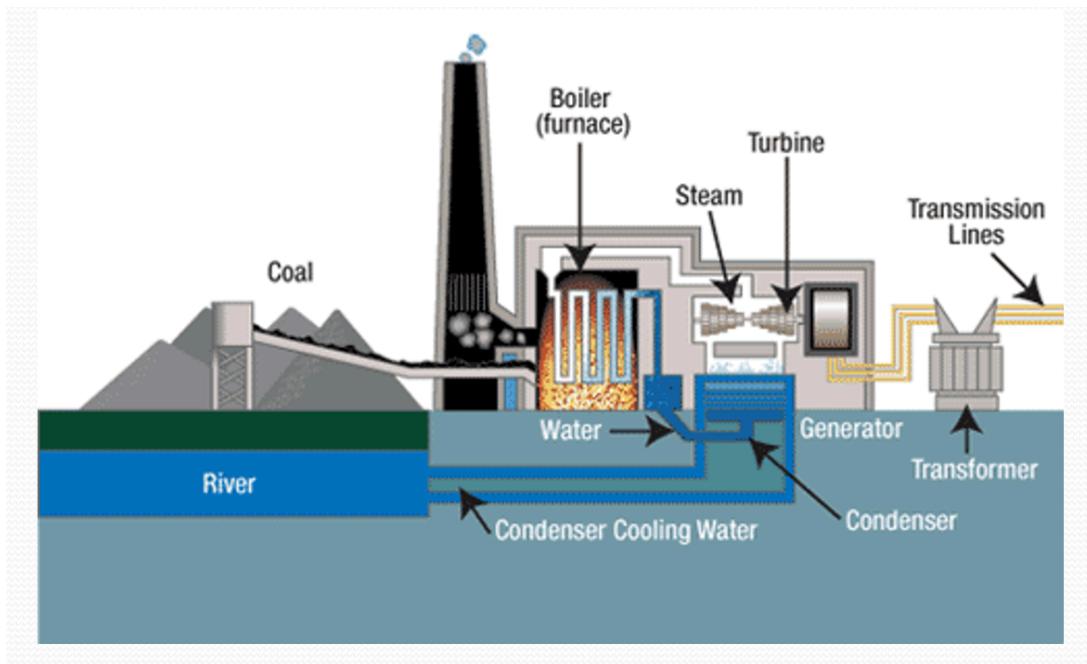


Figure 4: Image of a power plant as a general process flow diagram.

2.1 Petroleum Revenue

350 billion dollars in revenue in US alone in 2022 (<https://www.statista.com/statistics/294614/revenue-of-the-gas-and-oil-industry-in-the-us/>)

2.2 Petroleum Reserves

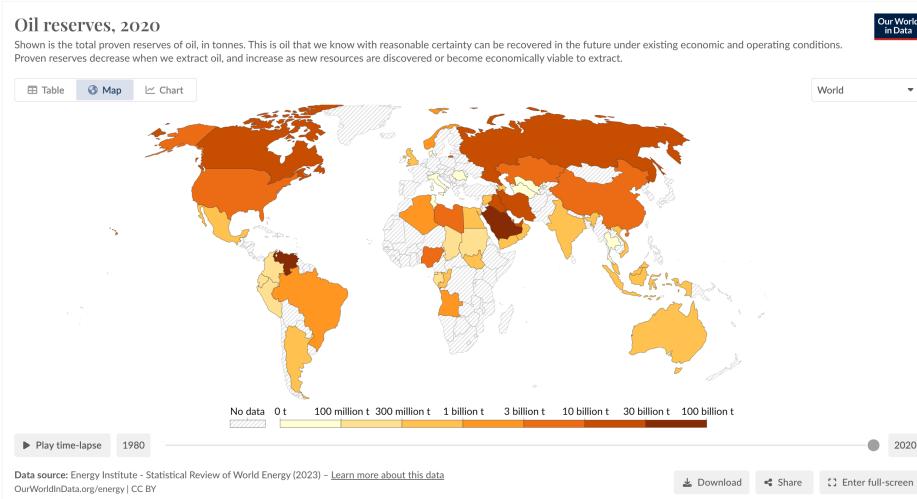


Figure 5: Oil reserves map as of 2020. See: <https://ourworldindata.org/grapher/oil-proved-reserves?time=2020>

2.3 Upstream Operations

- Exploration
 - Seismic surveys

- Borehole Logging
- Drilling
- Production

2.4 Downstream Operations

- Refining
- Transportation
- Distribution

Products from refining:

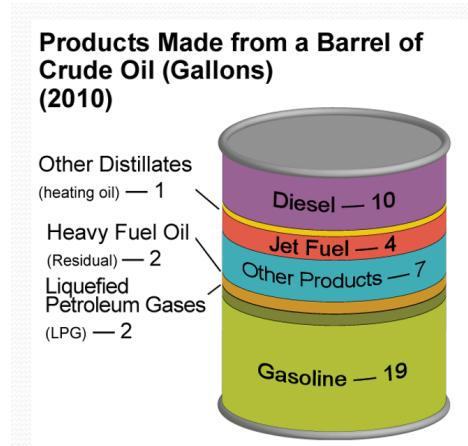


Figure 6: Image of products from petroleum refining.

3 Natural Gas

- Principally methane, but contains varying amounts of other compounds, including heavier hydrocarbons (ethane, propane, butane, pentane) and other gases (carbon dioxide, hydrogen sulfide).
- Natural gas can be “associated” with oil deposits or isolated, “non-associated” resources. It can also be associated with coal beds.
- Until recently, associated natural gas was burned off because it was not economical to transport it to where it was usable.
- Used for electricity generation; home heating, cooking, and clothes drying; transportation; and fertilizer manufacture
- Peaking power plants are commonly natural gas plants
- Can be used to make liquid fuels using Fischer-Tropsch process
- LNG transportation is huge and growing business

3.1 Natural Gas Reserves

- 7,000 trillion cubic feet (tcf) of proven reserves
- Current world production is near 120 tcf per year

4 Tar Sands

- Canada and Venezuela have the largest reserves
- Must be heated to flow
- Polycyclic Aromatic Hydrocarbons (PAHs or Asphalt)
- Estimated to be twice the reserves of conventional oil

5 Fossil Fuel Concerns

Fossil fuel use is very widespread and is a key piece of our energy infrastructure. However, there are concerns about the environmental impact of fossil fuel use. These include:

- Air pollution
- Water pollution
- Greenhouse gas emissions
- Land use
- Resource depletion (limited supply)

6 Cooking with Solid Fuels

- Used for cooking in many parts of the world (1/3 of the world's population or 2.5 billion people)
- Include wood, charcoal, coal, dung, and crop residues
- Often burned in open fires or simple stoves
- Often burned in poorly ventilated spaces, leading to indoor air pollution
- Often burned in rural areas in developing countries, where access to cleaner fuels is limited

7 Nuclear Energy

Nuclear energy has many benefits over conventional fossil fuels. However, it is also currently limited due to the very remote risks that could have far-reaching consequences. The Nuclear Regulatory Commission (NRC) is the U.S. government agency responsible for regulating nuclear power plants. It can take decades to build a nuclear power plant due to the regulatory process.

7.1 Fission of Large Atoms

Fission occurs when a neutron strikes the nucleus of a uranium-235 atom, causing it to split into two smaller nuclei and release energy in the form of heat and gamma radiation. This releases additional neutrons, which can then strike other uranium-235 nuclei, causing a chain reaction. The heat is used to produce steam, which spins a turbine to produce electricity.

7.2 Massive Energy Density

1 kg of uranium-235 can produce the same amount of energy as 2.7 million kg of coal. Or 3 million kg of oil. Or 17,000,000 m³ of natural gas.

7.3 Nuclear Energy is Clean

Nuclear energy is clean in that it does not produce greenhouse gases or other emissions. The waste produced is small in volume and can be stored safely.

7.4 Nuclear Energy is Safe and Reliable

Lowest risk of death of industrial power processes.

Nuclear power plants operate at full power 90% of the time. This is much higher than other types of power plants.

7.5 Comments (Dr. Matt Memmott)

- There is enthusiasm for nuclear power in the US energy plan, BUT...
- Large reactor solutions are not likely in developed countries (different story for China, UAE, South Korea, etc)
- Industry can't justify development based on cost vs. return
- Market's no longer favor large baseload nuclear
- Any nuclear future must include
 - Smaller installations
 - Non-electricity products (in addition to electricity)
 - Inherent safety
 - Load-follow capabilities

33 Climate and Energy

Learning Outcomes

- Be able to identify key climate indicators and the complex interplay between those key parameters

Reading

- Foundations of Spiritual and Physical Safety: with Chemical Processes; Chapter 11

The Earth gets energy from the sun and core of the earth is still quite hot. The energy from the sun is the main driver of the climate on Earth. The energy from the sun is not evenly distributed over the Earth's surface. The equator gets more energy than the poles. The energy from the sun is absorbed by the Earth and then re-emitted as infrared radiation. The Earth's atmosphere absorbs some of this infrared radiation and re-emits it back to the Earth's surface. This is the greenhouse effect. Without this greenhouse effect, we would be living in a much colder world.

Relatively recently, the concentration of atmospheric carbon dioxide has been increasing, although the concentration of CO₂ has been estimated to be higher in the past. It is believed that the recent increase in CO₂ is due primarily to burning of fossil fuels.

Note

Reading: <https://earthobservatory.nasa.gov/features/EnergyBalance/page2.php>.

33.1 Heat from the Core of the Earth

The core temperature of the Earth is estimate to be 6,000 C under very high pressures, composed primarily of iron ([Anzellini et al. \(2013\)](#)). The heat flux to the surface from the core is on average 0.1 W/m².

33.2 Heat from the Sun

The heat flux from the sun is approximately 1360 W/m² (oscillating every 24 hours depending a little on the time of year and latitude). The Earth's surface temperature is about 15 C. The Earth's surface temperature is determined by the balance between the energy from the sun and the energy from the core.

The energy incident on the atmosphere from the sun, is absorbed and re-emitted by the Earth's surface, primarily as infrared radiation. That incident radiation has a wide range of wavelengths. Water, a very powerful greenhouse gas varies from 1-4% of the atmosphere (depending on many factors). The concentration of CO₂ is about 0.04% or 400 ppm of the atmosphere.

33.3 Mass Balance

The mass of the atmosphere is estimated to be 5.15e18 kg. The amount of fossil fuels burned by the world is approximately 136 terawatt-hours. If the average energy density of fossil fuels is 40 MJ/kg, then the mass of fossil fuels burned is 3.4e12 kg.

```
atmosphere = 5.15e18 #kg
molesinatmosphere = atmosphere/0.029 #moles
energyff = 136e6 #megawatts, energy from fossil fuels burned
```

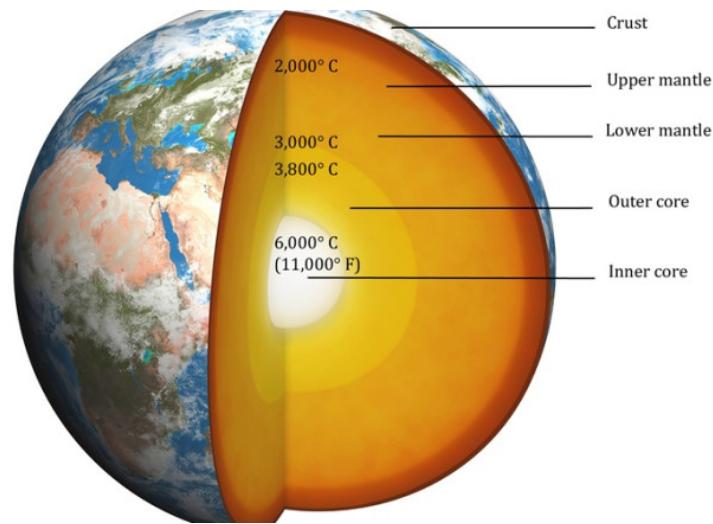


Figure 49: Image of the Earth showing the core and mantle from <https://www.discovermagazine.com/planet-earth/taking-the-temperature-of-earths-core>.

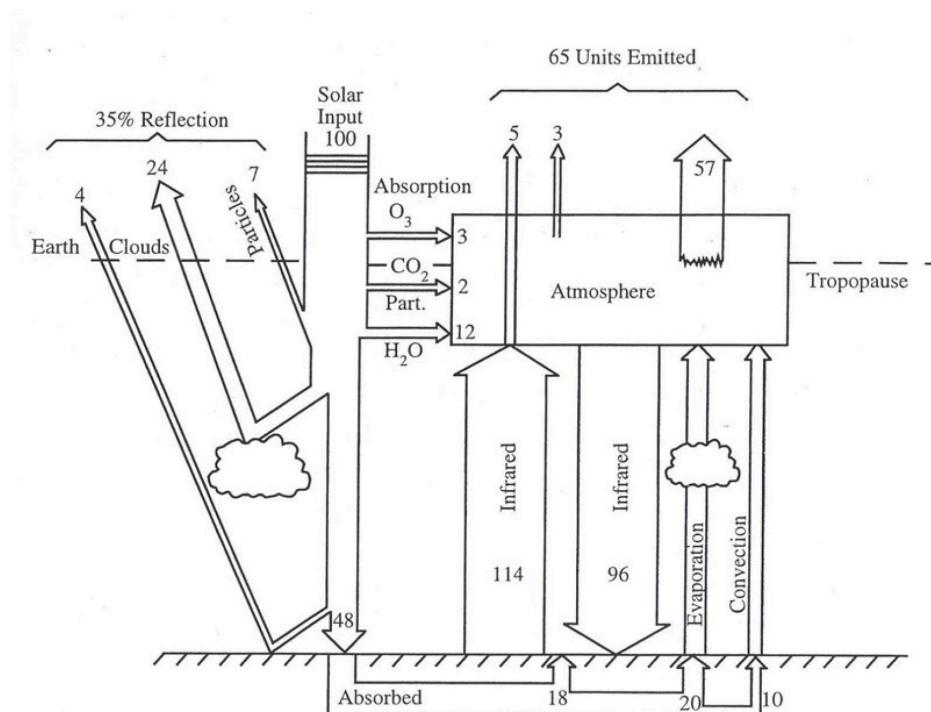


Figure 50: Image of the Earth's heat balance. Similar images and information in <https://earthobservatory.nasa.gov/features/EnergyBalance/page2.php>.

```
ffburned = energyff/40 #kg of fossil fuels burned
co2emitted = 35*1e9*1000 #billion tons of CO2 emitted to kg
molesCo2emittedperyear = co2emitted/0.044 #moles of CO2 emitted per year
```

$$\frac{dn_{CO_2}}{dt} = n_{CO_2}^{in} - n_{CO_2}^{out} \quad (33)$$

```
dnco2dt = molesCo2emittedperyear/molesinatmosphere*1e6 #ppm of CO2 emitted per year
print(f'The estimated rate of change of CO2 in the atmosphere is {dnco2dt:.2f} ppm/year')
```

The estimated rate of change of CO₂ in the atmosphere is 4.48 ppm/year

Currently the rate of increase of ppm of CO₂ is about 2 ppm/year. Thus, the approximately other half of the CO₂ is absorbed by the oceans and elsewhere.

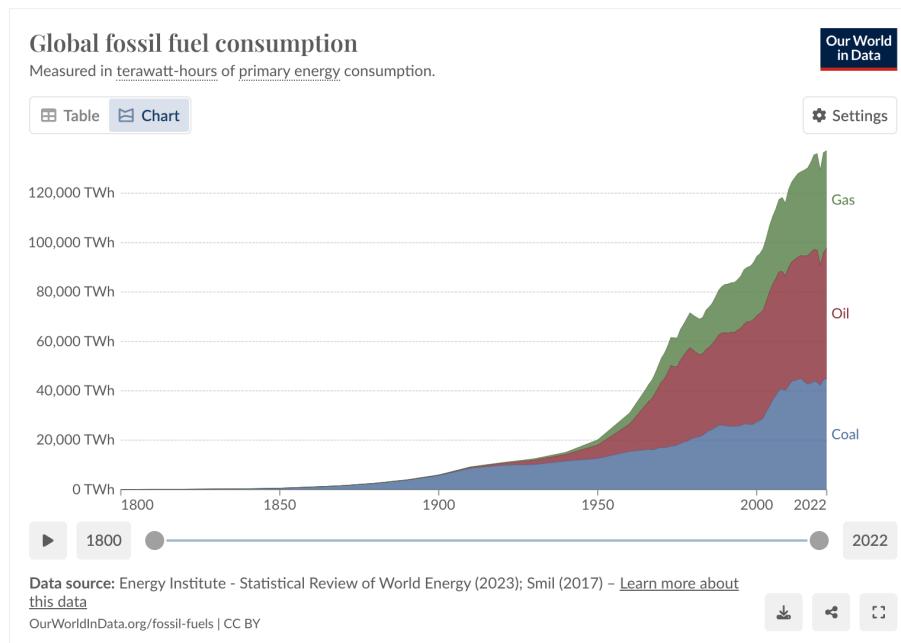


Figure 51: Global fossil fuel consumption as a function of time from <https://ourworldindata.org/grapher/global-fossil-fuel-consumption>.

33.3.1 Carbon Cycle

Carbon dioxide is produced by the oxidation of carbon. Many sources of oxidation occur naturally including:

- respiration of animals
- decomposition of organic matter (aerobic bacteria)
- volcanic activity
- forest fires
- oceanic release of CO₂
- weathering of rocks (carbonate rocks)

Carbon dioxide is removed from the atmosphere by:

- photosynthesis
- oceanic uptake of CO₂
- deposition of carbon in sediments

33.3.2 Oxygen Cycle

Oxygen is produced when water is split by photosynthesis or through other reduction mechanisms. Oxygen is consumed by respiration of animals and decomposition of organic matter. The oxygen cycle is closely linked to the carbon cycle.

33.3.3 Water Cycle

Water is evaporated from the surface of the Earth and then condenses in the atmosphere. The water cycle is driven by the energy from the sun. The water cycle is closely linked to the amount of energy incident on the Earth's surface and the amount absorbed and reflected by the atmosphere.

33.3.4 Industrial Revolution and Energy Needs

The industrial revolution began in the 18th century in England. The industrial revolution was driven by the need for energy to power machines. The primary source of energy was coal. As more people have come to earth, the energy needed to support each other has increased together with our quality of life. More energy use correlates with a higher quality of life.

33.4 Energy Balance

With the same energy input and output, the Earth's temperature is stable. It is estimated, that the increase in green house gases, primarily CO₂ (and water) is causing the Earth's temperature to increase. The Earth's temperature is increasing at a rate of about 0.2 C per decade. The Earth's surface atmospheric temperature has increased by about 1 C since the industrial revolution (in the last 150 years). The Earth's temperature has been higher in the past, but the rate of change now is much faster.

$$\frac{dnU}{dt} = n_{in}(H_{in} + 1/2Mv_{in}^2 + Mgz_{in}) - n_{out}(H_{out} + 1/2Mv_{out}^2 + Mgz_{out}) + Q + W_s \quad (34)$$

What does a simple mass balance of the atmosphere yield in terms of a temperature change if there is an increase in the Earth's surface radiation of 1 W/m²?

33.5 Correlation

Increasing concentration of CO₂ appears to be correlated (with causation) with the burning of fossil fuels for our energy needs.

There is correlation with that increasing concentration of CO₂ and the Earth's temperature. It's also correlated with the rise in sea levels, melting of glaciers, and other changes in the Earth's climate.

What should be done?

34 Environmental Legislation

Learning Outcomes

- Identify key pieces of legislation to help with safety and the environment

Reading

- Environmental Legislation Review

Severe smog in cities like New York and LA as well as the Cuyahoga river in Ohio catching fire in 1969 as well as scientific evidence of the hazards of air pollution such as Rachel Carson's *Silent Spring* (1962) motivated the US government to pass a series of environmental laws in the 1970s. These laws have been instrumental in cleaning up the environment and improving public health.

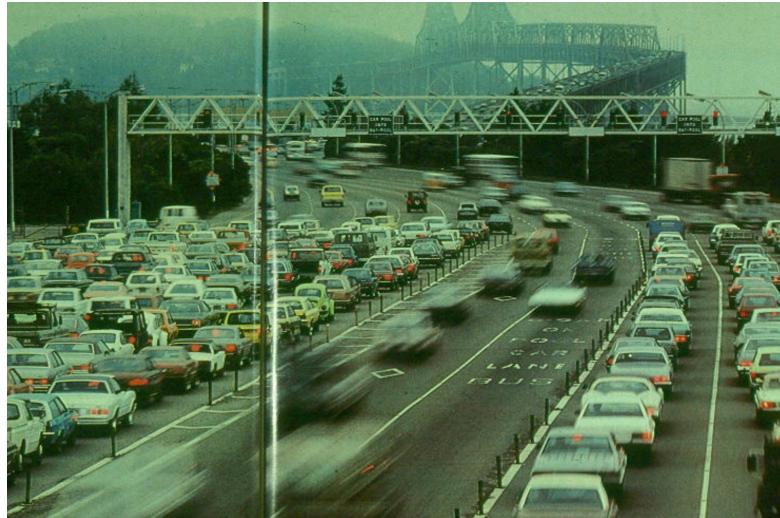


Figure 52: Image of smog in Los Angeles in the 1970s.

34.1 NEPA (National Environmental Policy Act, 1970)

It established the **EPA (Environmental Protection Agency)** and required environmental impact statements (EIS) for any project that received federal funding.

Without government oversight and regulation, it is unlikely that market forces would be sufficient to protect the environment. Why? Some examples:

- Catalytic converters
- Smokestack scrubbers
- Lead-free gasoline
- PCBs (polychlorinated biphenyls)
- DDT (dichlorodiphenyltrichloroethane)

34.2 Toxic Substances Control Act (TSCA, 1976)

- Assesses risks before introduction into the environment
- Ensures production and use do not present unreasonable risks to human health or the environment
- Premanufacture notification required for new chemicals
 - Name and structure
 - Use
 - Amount
 - Byproducts
 - Health and environmental effects
- EPA has authority to ban or restrict production

34.3 Federal Insecticide, Fungicide, and Rodenticide Act (FIFRA, 1947)

- Requires registration of all pesticides
- EPA has authority to ban or restrict production
- Requires labeling of all pesticides
 - Active ingredients
 - Instructions for use
 - Limitations
- Will not cause unreasonable adverse effects on the environment

34.4 Clean Air Act, 1970

The Clean Air Act is a comprehensive federal law that

- regulates air emissions from stationary and mobile sources (vehicles had to have catalytic converters)
- authorizes the Environmental Protection Agency (EPA) to establish National Ambient Air Quality Standards (NAAQS) to protect public health and the environment
- sets emission standards for hazardous air pollutants and
- establishes a cap-and-trade program for sulfur dioxide and nitrogen oxides.

Figure 53: EPA released plot of air quality trends from 1990 to 2022 showing significant reductions in key air pollutants.

<https://www.epa.gov/air-trends/air-quality-national-summary>

34.4.1 Catalytic Converters

Hot gases from the engine are passed over a catalyst (platinum and rhodium) that causes the gases to react with each other and convert them to less harmful gases. CO and other unburned hydrocarbons are converted to CO₂ and H₂O. NO_x is converted to N₂ and O₂.

What about SO₂ and particulates? (DERA, diesel emissions reduction act)

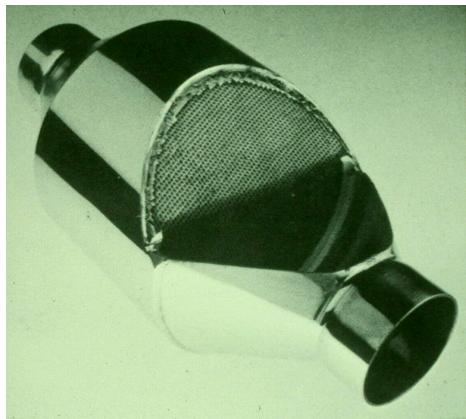


Figure 54: Image of a catalytic converter.

34.5 Clean Water Act, 1972

The Clean Water Act is a federal law that

- regulates the discharge of pollutants into the nation's waters
- sets water quality standards for surface waters
- authorizes the EPA to establish effluent limitations for industrial discharges
- regulate stormwater runoff from industrial facilities
- provides funding for wastewater treatment facilities
- establishes a permit program for discharges into navigable waters.

34.6 Resource Conservation and Recovery Act (RCRA), 1976

RCRA is a federal law that

- regulates the management of hazardous waste
- requires the EPA to establish standards for the treatment, storage, and disposal of hazardous waste
- outlines waste characterization: ignitability, corrosivity, reactivity, and toxicity
- requires cradle-to-grave tracking of hazardous waste
- states that treatment, storage, and disposal facilities must have permits and documentation

34.6.1 Comprehensive Environmental Response, Compensation, and Liability Act (CERCLA), 1980 and Superfund Amendments and Reauthorization Act (SARA), 1986

- Identify and clean up hazardous waste sites
- Establishes a trust fund to pay for cleanups
- Requires responsible parties to pay for cleanups
- Sets priorities for cleanup (National Priorities List)

See <https://www.epa.gov/superfund>

34.7 Pollution Prevention Act, 1990

- Reduce or eliminate pollution at the source
- Encourage source reduction over waste management
- Promote the use of non-toxic or less toxic substances, materials, and processes
- Encourage the use of innovative technologies

34.8 Energy Independence and Security Act (EISA), 2007

To move the United States toward greater energy independence and security, to increase the production of clean renewable fuels, to protect consumers, to increase the efficiency of products, buildings, and vehicles, to promote research on and deploy greenhouse gas capture and storage options, and to improve the energy performance of the Federal Government.

Provisions:

- Increase fleet gas mileage to 35 mpg by 2020
- Hybrid vehicle incentives
- Biofuels increase
- Greater efficiency required for light bulbs (25% by 2012; 200% by 2020)
- Initiatives for energy efficiency in buildings and industry
- Support for R&D in solar, geothermal, carbon sequestration, etc.

34.9 Inflation Reduction Act (IRA), 2022

The Inflation Reduction Act includes many provisions to help with increasing the energy efficiency of buildings and other infrastructure “to avoid, reduce, utilize, or sequester greenhouse gas emissions.”

<https://kw-engineering.com/>

34.10 Short US Legislative Summary

Early Foundations

- The Homestead Act (1862): While primarily focused on Western expansion, this act encouraged the settlement and development of lands, sometimes leading to unsustainable resource use.
- Establishment of Yellowstone National Park (1872): The first national park in the world, setting a precedent for land preservation and marking a shift towards conservation.
- Forest Reserve Act (1891): Gave the President power to set aside public lands as forest reserves, paving the way for the National Forest System.
- Antiquities Act (1906): Empowered the President to designate National Monuments, protecting sites of historical, cultural, or scientific significance.

Pollution-Focused Legislation

- Rivers and Harbors Appropriation Act (1899): Prohibited dumping refuse into navigable waters, an initial step towards water pollution control.

- The Clean Air Acts (1963, major amendments in 1970, 1977, 1990): A series of laws establishing national air quality standards, regulating emissions from various sources (factories, cars, etc.), and setting a framework for cooperation between federal and state governments regarding air quality.
- The Clean Water Act (1972): The cornerstone of water pollution control efforts, aimed at making surface waters fishable and swimmable by regulating pollutant discharges and setting water quality standards.
- Safe Drinking Water Act (1974): Established national drinking water standards and regulations, with a focus on protecting public health from contaminants.
- Toxic Substances Control Act (1976): Regulates the manufacture, import, processing, distribution, and disposal of chemicals, with the goal of protecting human health and the environment.
- Oil Pollution Act (1990): Created in response to the Exxon Valdez oil spill, this law aims to prevent and respond to oil spills, holding responsible parties accountable for cleanup and damages.

Protecting Species & Habitats

- Lacey Act (1900): One of the first wildlife protection laws, combating illegal trade in wildlife and plants.
- Endangered Species Act (1973): Powerful conservation tool for identifying at-risk species and creating plans to prevent extinction and promote recovery.
- National Wildlife Refuge System Improvement Act (1997): Provides guidelines and comprehensive management framework for the US National Wildlife Refuge System.

Hazardous Substances and Waste

- Resource Conservation and Recovery Act (RCRA) (1976): Regulates the handling of hazardous waste, with a “cradle-to-grave” scope to promote responsible disposal and reduce environmental risk.
- Comprehensive Environmental Response, Compensation, and Liability Act (CERCLA) (1980): Also known as “Superfund,” established a program to fund the cleanup of contaminated hazardous waste sites, holding polluters accountable.
- Pollution Prevention Act (1990): Emphasizes source reduction and pollution prevention, aiming to reduce or eliminate waste at the source.

Broadening Environmental Policy

- National Environmental Policy Act (NEPA) (1970): Requires federal agencies to evaluate the environmental impacts of proposed projects with potential for significant effects, promoting informed decision-making.
- Establishment of the Environmental Protection Agency (EPA) (1970): Consolidation of federal environmental programs into a single agency, granting the EPA broad authority to implement and enforce environmental laws.

34.11 Unintended Consequences

For the most part, government regulation has been successful in helping to clean and protect the environment. However, some government policies on either a local or national level can have unintended consequences. For example, recently some cities or states have banned single-use plastic bags. Instead, customers were given the option to reuse or purchase larger more massive plastic bags. This has led to an increase in the amount of plastic waste and some health risks with reusing bags.

<https://www.foxnews.com/opinion/why-plastic-bag-bans-failing>

35 Pollution Prevention

Learning Outcomes

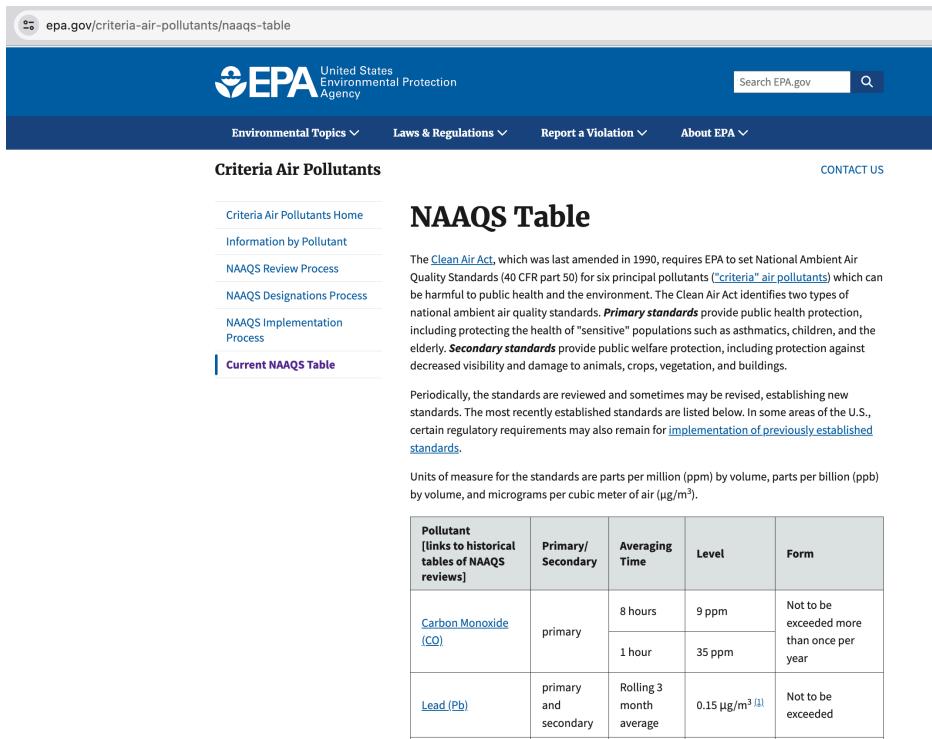
- Be able to download and analyze air quality data
- Be able to discuss key legislation pieces on air quality

Reading

- Pollution Prevention Review

35.1 Air Quality

35.1.1 National Ambient Air Quality Standards (NAAQS)



The screenshot shows the EPA website's header with the URL 'epa.gov/criteria-air-pollutants/naaqs-table'. Below the header, there's a navigation bar with links to 'Environmental Topics', 'Laws & Regulations', 'Report a Violation', and 'About EPA'. On the right side of the header is a search bar. The main content area has a title 'Criteria Air Pollutants' and a sub-section titled 'NAAQS Table'. A descriptive paragraph explains the Clean Air Act and the purpose of NAAQS. Below this is a table with two rows of data.

Pollutant [links to historical tables of NAAQS reviews]	Primary/ Secondary	Averaging Time	Level	Form
Carbon Monoxide (CO)	primary	8 hours 1 hour	9 ppm 35 ppm	Not to be exceeded more than once per year
Lead (Pb)	primary and secondary	Rolling 3 month average	0.15 µg/m ³ [1]	Not to be exceeded

Figure 55: Image of the National Ambient Air Quality Standards (NAAQS) from the EPA website at <https://www.epa.gov/criteria-air-pollutants/naaqs-table>

35.1.2 Air Quality Map

35.1.3 Air Data

Link: <https://epa.maps.arcgis.com/apps/webappviewer/index.html?id=5f239fd3e72f424f98ef3d5def547eb5&extent=-146.2334,13.1913,-46.3896,56.5319>

[epa.gov/outdoor-air-quality-data/interactive-map-air-quality-monitors](https://www.epa.gov/outdoor-air-quality-data/interactive-map-air-quality-monitors)

An official website of the United States government [Here's how you know](#) ▾

 United States Environmental Protection Agency

Environmental Topics ▾ Laws & Regulations ▾ Report a Violation ▾ About EPA ▾

Outdoor Air Quality Data

Air Data Home

Frequent Questions about AirData

Learn about Air Data

Interactive Map

Pre-generated Data Files

Download Daily Data

Download Raw Data (API)

Air Quality Index Report

Air Quality Statistics Report

Monitor Values Report

Monitor Values Report - Hazardous Air Pollutants

Air Quality Index Daily Values Report

CONTACT US

Interactive Map of Air Quality Monitors

The AirData Air Quality Monitors app is a mapping application available on the web and on mobile devices that displays monitor locations and monitor-specific information. It also allows the querying and downloading of data daily and annual summary data.

Map layers include:

- Monitors for all criteria pollutants (CO, Pb, NO₂, Ozone, PM₁₀, PM_{2.5}, and SO₂)
- PM_{2.5} Chemical Speciation Network monitors
- IMPROVE (Interagency Monitoring of Protected Visual Environments) monitors
- NATTS (National Air Toxics Trends Stations)



Figure 56: Image of the EPA's website where you can find maps of air quality monitors. Link: <https://www.epa.gov/outdoor-air-quality-data/interactive-map-air-quality-monitors>

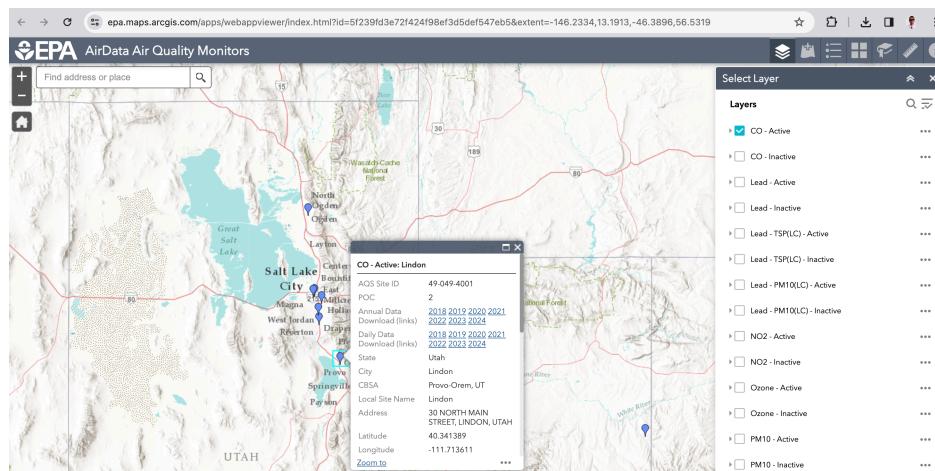


Figure 57: Image of the EPA's Air Data website where you can download air quality data for different locations with Utah shown.

Click the layers and choose CO and navigate to your location.

HW:

- If I worked outside and otherwise spent the whole day exposed to the air in the city of Provo, what would have been my TWA exposure to CO on 1/1/2020?
- How does that value compare to the NAAQS for CO? How does it compare to the PEL for CO?
- Plot the CO levels near Provo for the months of January-May 2020. Add the PEL and NAAQS levels for CO to the plot.

35.1.4 National Emission Standards for Hazardous Air Pollutants (NESHAP)

188 NESHAP standards have been established for 174 source categories. These standards limit the amount of hazardous air pollutants that may be emitted from a source. Chemicals such as benzene, mercury compounds, selenium compounds, asbestos, vinyl chloride, and many others are regulated by NESHAP standards.

35.2 Pollution Prevention Act (PPA), 1990

Focuses on pollution prevention (P2) as the nation's primary pollution strategy. Hierarchy:

- Source reduction
- In process recycling
- On-site recycling
- Off-site recycling
- Treatment
- Disposal
- Release

Requires P2 efforts for TRI (Toxic Release Inventory) permits. TRI permits are required for facilities that manufacture, process, or use more than a threshold amount of a listed toxic chemical. The PPA also requires the EPA to establish a P2 information clearinghouse.

- In-process recycling is the reuse of materials within a process.
- On-site recycling is the reuse of materials within a facility.
- Off-site recycling is the reuse of materials outside a facility.
- Treatment is the use of physical, chemical, or biological processes to reduce the toxicity or volume of waste.
- Disposal is the final disposition of waste.
- Release is the discharge of waste into the environment.

35.3 Source Reduction

Source reduction is the reduction or elimination of waste at the source. The intent is to reduce:

- energy use
- raw material use
- waste minimization
- environmental releases
- used solvents
- waste water
- air emissions

Reducing the amount of waste generated in a significant increase in the efficiency of the process. For example, if a process generates 1000 pounds of waste and 100 pounds of product, the process efficiency is 10% ($100/1100$). If the process is modified to generate 10 pounds of waste and 100 pounds of product, the process efficiency is 91% ($100/110$).

Case Scenario - production of nitric acid:

- The production of nitric acid generates a large amount of NOx emissions.
- The process can be modified to reduce the amount of NOx emissions.

Some additional specific examples of source reduction include:

- LED lighting
- Higher efficiency furnaces
- Higher efficiency air conditioners

HW: Research a source reduction scenario and provide a brief summary.

35.3.1 Waste Minimization

- Substitution of less hazardous materials
- Process modification
- Inventory control
- Equipment optimization
 - Fugitive emissions (Gold capture air particulate in gold processing)

35.4 Sustainability

Sustainability means meeting the needs of today without compromising the ability of future generations to meet their needs

35.5 Life-Cycle Analysis

1. Scope
 - Establish system boundaries
 - Determine functional unit (including life expectancy)
2. Inventory
 - Inputs: raw materials, energy
 - Outputs: products, byproducts, wastes, emissions
3. Impact assessment
 - Environmental impacts of all steps in life cycle
4. Improvement analysis
 - Generate alternatives
 - Consider each step
5. Cradle-to-grave analysis
 - Consider all steps in life cycle
 - Consider end use
 - Consider disposal

35.6 Superfund Amendments and Reauthorization Act (SARA)

A superfund site is any land in the United States that has been contaminated by hazardous waste and identified by the EPA as a candidate for cleanup because it poses a risk to human health and/or the environment. The Superfund program was established by the Comprehensive Environmental Response, Compensation, and Liability Act (CERCLA) in 1980. The Superfund Amendments and Reauthorization Act (SARA) was passed in 1986 to amend CERCLA. SARA expanded the Superfund program and added new provisions to the law. SARA also established the Emergency Planning and Community Right-to-Know Act (EPCRA).

Some prominent superfund sites include:

- Love Canal, New York
- Times Beach, Missouri
- Rocky Flats, Colorado

35.6.1 Love Canal

The Love Canal site is located in Niagara Falls, New York. The site was originally a canal that was dug in the late 19th century to provide hydroelectric power to the city. The canal was abandoned and used as a chemical waste dump in the 1940s and 1950s. In the 1970s, residents of the Love Canal neighborhood began to report health problems, including birth defects, miscarriages, and cancer. Investigations revealed that the site was contaminated with over 20,000 tons of hazardous waste, including dioxin, benzene, and other chemicals. The Love Canal site was declared a federal emergency in 1978, and the residents were evacuated. The site was later cleaned up and capped, and is now a public park.

HW: Research a superfund site and provide a brief summary.



Figure 58: Image of the restored Love Canal site, now a public park.

35.7 Bioaccumulation

Bioaccumulation is the accumulation of substances, such as pesticides, or other chemicals in an organism. Bioaccumulation occurs when an organism absorbs a substance at a rate faster than that at which the substance is lost. This can occur through inhalation, ingestion, or direct contact. The substance can accumulate in the organism's tissues, and can be passed on to the next trophic level in a food chain. Bioaccumulation can have harmful effects on organisms, and can lead to biomagnification, which is the increase in concentration of a substance as it moves up the food chain.

35.8 Solubility

Solubility is the ability of a substance to dissolve in a solvent. The solubility of a substance is dependent on the temperature and pressure of the solvent. The solubility of a substance can be expressed as the amount of solute that can be dissolved in a given amount of solvent. The solubility of a substance can be determined experimentally, and can be used to predict the behavior of the substance in a given solvent.

What happens if the solubility of a substance is exceeded? The substance will precipitate out of solution into a 3rd phase. This can be a solid, liquid, or gas depending on the substance and the solvent.

35.8.1 Henry's Law

Henry's Law states that the concentration of a gas in a liquid is directly proportional to the partial pressure of the gas above the liquid. The solubility of a gaseous species is dependent on the temperature and pressure of the system. Henry's Law can be used to predict the concentration of a species in a liquid:

$$y_i P = H_i x_i \quad (35)$$

where: y_i is the mole fraction of species i in the gas phase, P is the pressure of the gas above the liquid, H_i is the Henry's Law constant for the species i , and x_i is the mole fraction of the species in the liquid.

Henry's law is very similar to **Raoult's Law**, which states that the partial pressure of a species in the vapor phase is directly proportional to the product of the mole fraction of the species in the solution and the pure component saturated vapor pressure of that species. Both 'laws' are limit cases where Henry's Law is for dilute solutions and Raoult's Law is for ideal solutions.

36 Remediation

Learning Outcomes

- Be able to identify remediation processes with details
- Be able to discuss remediation principles relative to a person's spiritual life

Reading

- <https://www.churchofjesuschrist.org/study/general-conference/2006/10/the-atonement-can-clean-reclaim-and-sanctify-our-lives?lang=eng>
- Remediation principles review

36.1 Spiritual Healt

The Atonement of Jesus Christ Can Clean, Reclaim, and Sanctify Our Lives

<https://www.churchofjesuschrist.org/study/general-conference/2006/10/the-atonement-can-clean-reclaim-and-sanctify-our-lives?lang=eng>

36.2 Fate and Transport

36.2.1 Thought Experiment - Tree Leaves

What happens to tree leaves?

Do they not just keep building up in layers?

Wouldn't the tree's just eventually be buried in leaves?

36.2.2 Thought Experiment - Tire Tread

Wear does all the tire tread go from use of millions of tires?

Why doesn't it build up on the highway's or surroundings?

How are those pieces transported?

36.2.3 Hydrologic Cycle

Water moves through the air, on the ground, and in the ground. It rains, water flows downhill on the surface, and water infiltrates into and out of the ground (aquifers).

Water is a universal solvent, and it can dissolve many substances. Water can also carry substances in solution, suspension, or as a colloid. Some of those substances are toxic.

We depend on water for drinking, agriculture, and industry.

Image source: <https://www.sciencefacts.net/water-cycle.html>

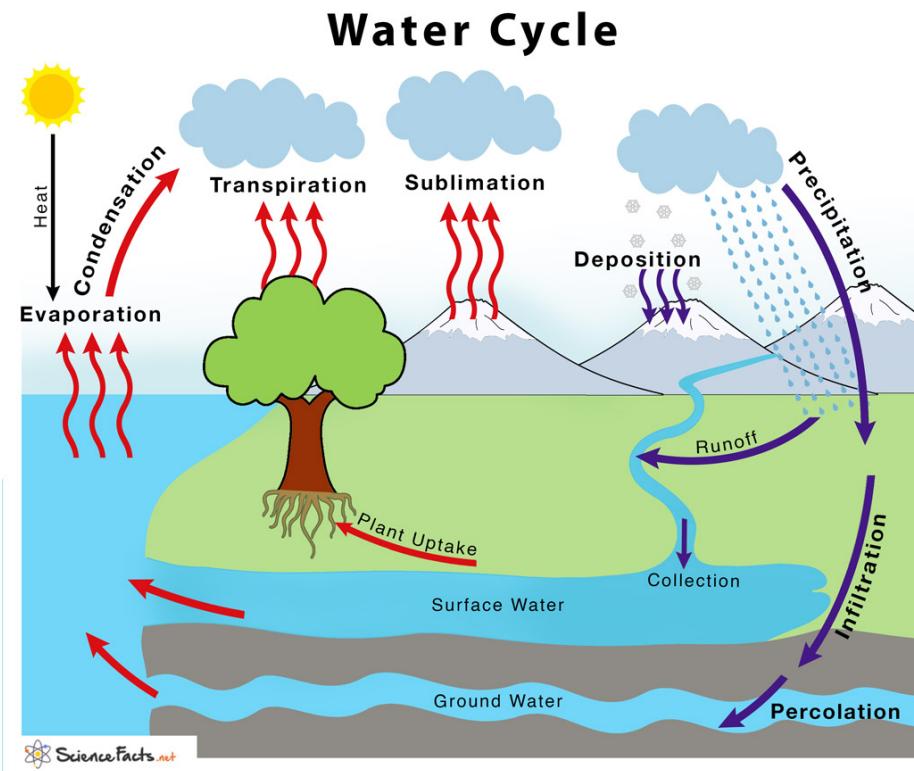


Figure 59: Image of the water cycle. See also the USGS website at <https://water.usgs.gov/edu/watercycle.html>.

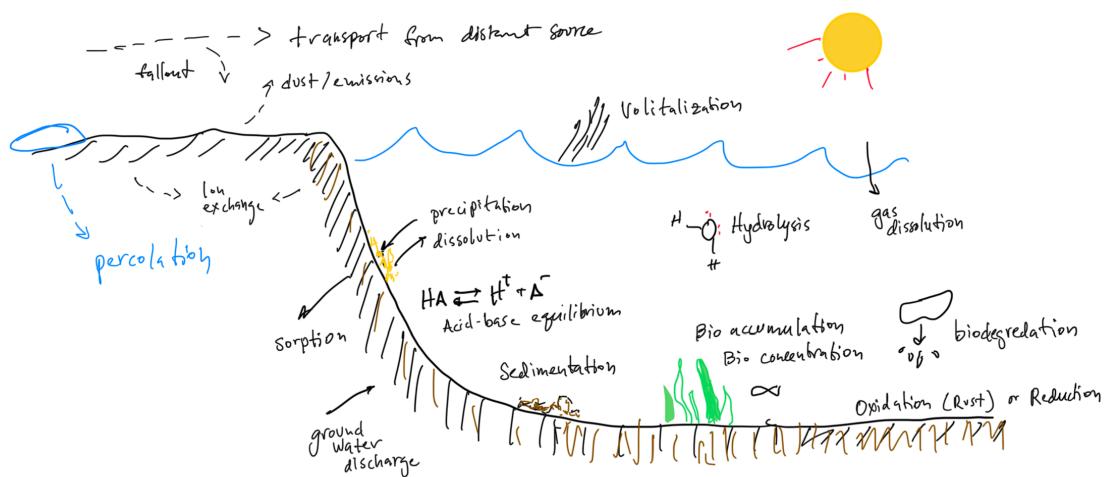


Figure 60: Image of fate processes.

36.2.4 Fate Processes

36.3 Environmental Remediation

Remediation: the action of reversing or stopping environmental damage.

36.3.1 Soil Washing

The soil is excavated and washed with water or other solvents to remove contaminants. The water is then treated to remove the contaminants.

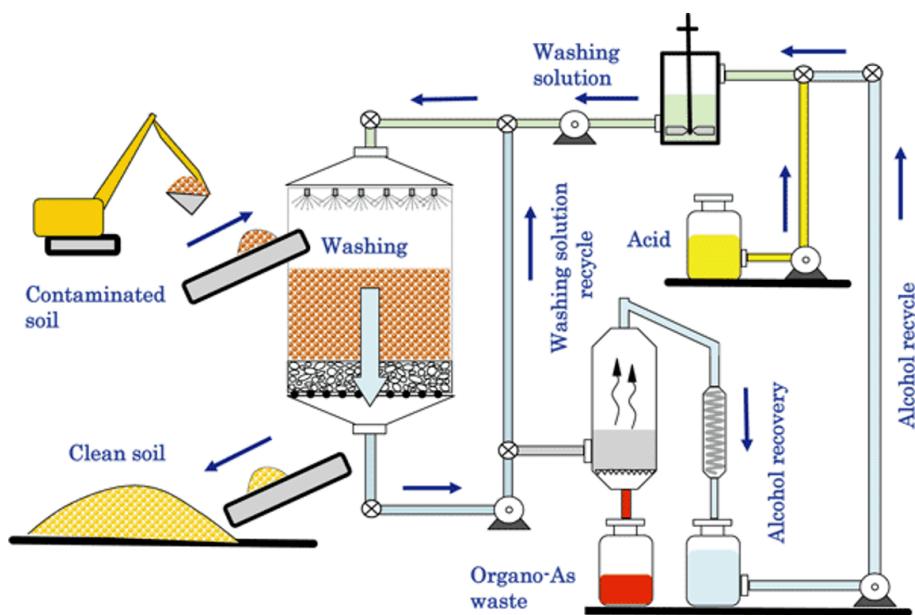


Figure 61: Remediation process with washing and scrubbing of gases.

36.3.2 Demonstration

500mL syring and a makeshift sand charcoal filter showing how large particles are screened but smaller molecules like dyes are not or that those smaller molecules can be washed or eluted out of the makeshift filter.

36.3.3 Soil Roasting/ Incineration

Soil roasting is a thermal treatment process that uses heat to remove contaminants from soil.

36.3.4 Vitrification or Encapsulation

Vitrification is the process of converting a material into a glass-like substance

36.3.5 Video on Vitrification at PNNL

https://www.youtube.com/watch?v=l-3we_QTK24

36.3.6 Landfilling

Contaminated soil is excavated and placed in a landfill.

Double lining with FML (Flexible Membrane Liners) and a dense clay layer is common practice to prevent leachate from contaminating groundwater.

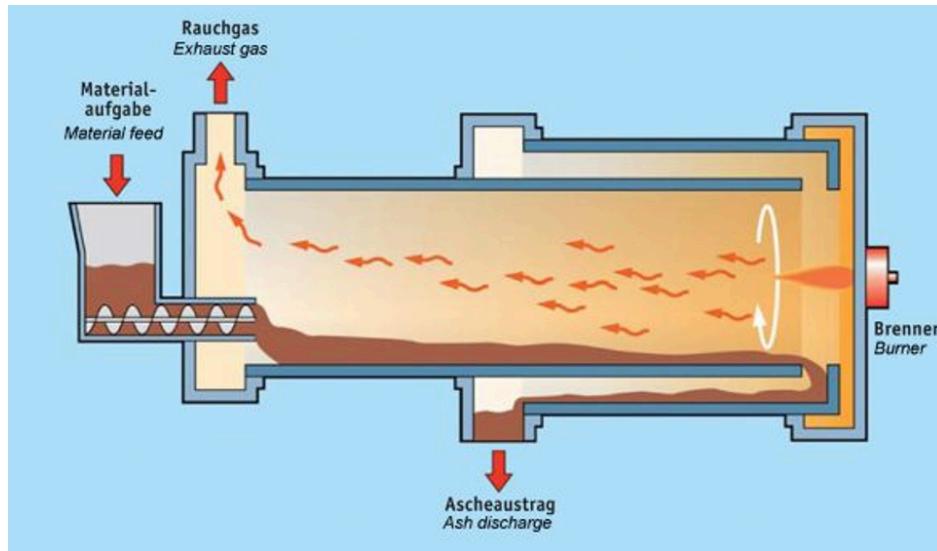


Figure 62: Image of a soil roasting process.

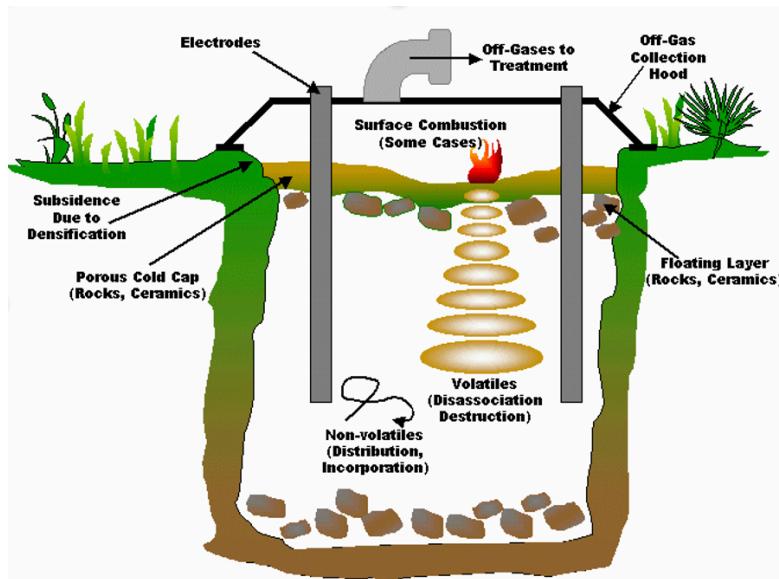


Figure 63: Image of a vitrification process.

Figure 64: Image with layer details and barriers at a landfill.

36.3.7 Pump and Treat

Groundwater is pumped to the surface and treated to remove the contaminants.

36.3.8 Volatilization

Volatilization is the process of converting a solid or liquid into a gas.

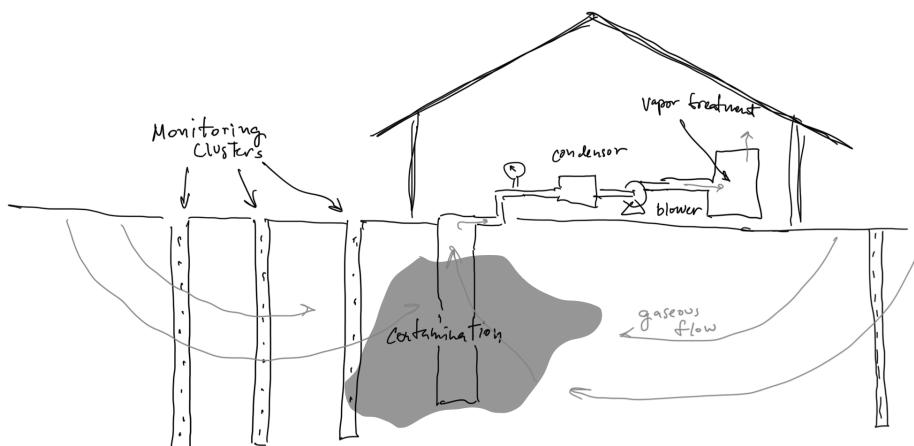


Figure 65: Drawing of a volatilization process.

36.3.9 Bioremediation

Bio-remediation is the use of living organisms to clean up contaminated soil and water. The organisms can be bacteria, fungi, or plants. For example, some bacteria can break down oil into carbon dioxide and water.

36.4 Remediation Example

Mt. Trashmore in Virginia Beach, Virginia, is a former landfill that has been turned into a park. The park is built on top of the landfill, which has been capped with a layer of soil and grass. The park has a lake, playgrounds, and walking trails.

36.5 Example Problems

Which of the following methods would you choose to remediate a gasoline leak from an underground storage tank that has reached a water aquifer? Explain your reasons.

- a. Soil washing
- b. Soil roasting/incineration
- c. Bioremediation/landfarming
- d. Stabilization and solidification, e.g., vitrification
- e. Landfill
- f. Pump and treat
- g. Volatilization (soil vapor extraction or in situ air sparging)

Which of the following methods would you choose to remediate heavy metal contamination of a small volume of soil? Explain your reasons.

- a. Soil washing
- b. Soil roasting/incineration
- c. Bioremediation/landfarming
- d. Stabilization and solidification, e.g., vitrification
- e. Landfill
- f. Pump and treat
- g. Volatilization (soil vapor extraction or in situ air sparging)

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