1. Abstract

Chemical Hazard Engineering Fundamentals Screening Tool published by Center for Chemical Process Safety (CCPS) [1] can be used as a screening tool for a variety of situations for example, initial project design (FEL-1), Hazard Identification and Risk Analysis facilitation, or during a Process Safety audit process. The CHEF calculation aid requires minimal inputs which are easy to obtain where Process Safety Information is unavailable or not maintained properly. The CHEF calculation aid has source models, vapor dispersion, explosion, and impact assessments that can be done using an excel file. The file is free and available for download from the CCPS website. This paper explores the versatile use of the CHEF calculation aid in addressing Asset Integrity and Reliability of an internal coil at a petrochemical facility and validation of Process Safety Information during the Hazard Identification and Risk Analysis process.

2. Periodic reactor internal coil failure

Figure 1 is a schematic representation of the reactor where a desired reaction is completed at atmospheric pressure and at an operating temperature of 250 °C. The operating temperature of 250 °C is maintained using a thermic fluid in the jacket. Once the reaction is complete, an internal coil is used for reducing the temperature of the reactor contents. The internal coil is indicated in red color in the schematic diagram in Figure 1. During the reaction stage, the return line of the internal coil is closed, however, the vent line is open and discharges to the top of the building with a weather hood. Normal cooling water is used for the cooling process.

Interview during a process safety audit indicated that there are approximately 10 reactors out of which there are 3 to 4 internal coil failure per year. These failures range from pin hole leaks to a guillotine break across the welded sections of the pipe. As part of the process safety audit, a review of the Hazard Identification and Risk Analysis (HIRA) was performed. A HAZOP was completed in 2020 and the reactor node did not consider an internal failure of the internal coil. In addition, a risk assessment was not performed for the internal coil.

2.1 CHEF Screening tool to address the internal coil failure

The failure rates of the internal coil were high and an investigation was warranted. Process Safety Information (PSI) was provided and found that the design pressure of the internal coil was found to be 5 kg/cm^2 (g). The design pressure of the reactor is 3 kg/cm^2 (g). The volume of the reactor is 10 m^3 and the internal coil is 0.25 m^3. Using the CHEF tool [1], the operating temperature of the reactor was entered, a liquid physical state was assumed for convergence, and the chemical chosen was water with a weight fraction of 1 modelling the cooling water of the internal coil, see Figure 2. The vapor pressure of water is 39.5 kg/cm^2 (g) at 250 °C.

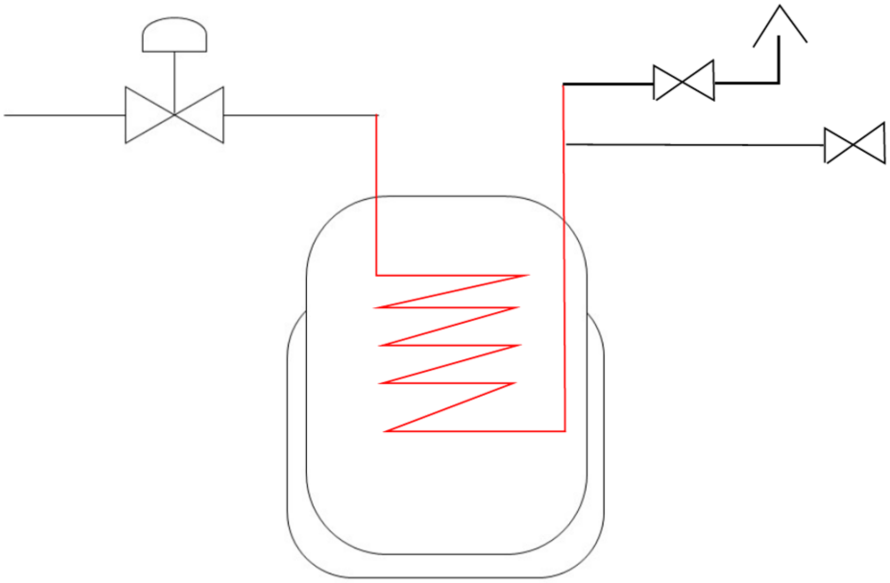
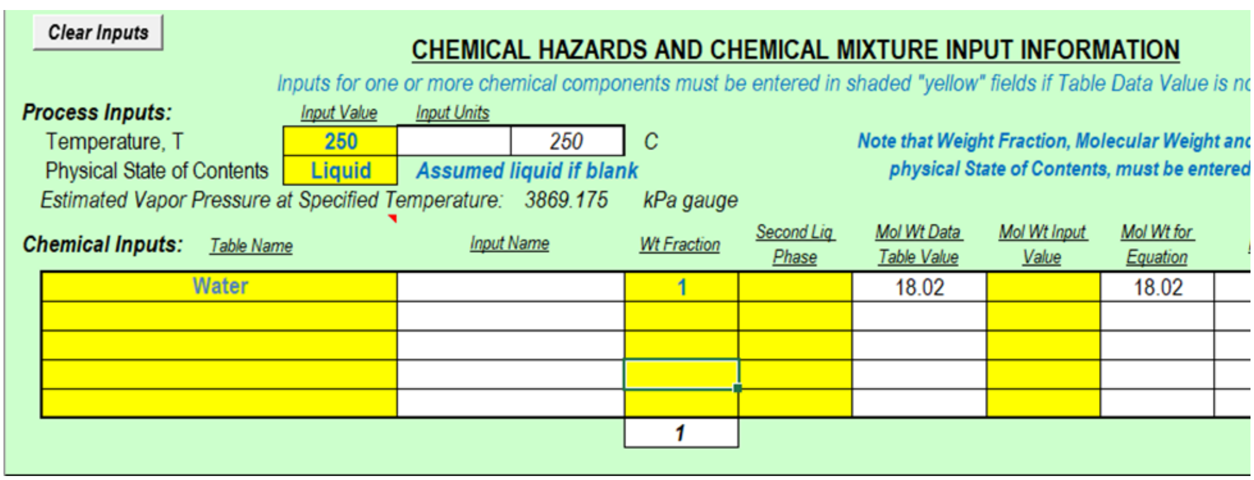


Figure 1 Schematic Diagram of Reactor



Clear Inputs

CHEMICAL HAZARDS AND CHEMICAL MIXTURE INPUT INFORMATION

Inputs for one or more chemical components must be entered in shaded "yellow" fields if Table Data Value is nc

Process Inputs: Input Value | Input Units

Temperature, T | 250 | | 250 | C

Physical State of Contents | Liquid | Assumed liquid if blank

Estimated Vapor Pressure at Specified Temperature: 3869.175 kPa gauge

Note that Weight Fraction, Molecular Weight and
physical State of Contents, must be entered

Chemical Inputs:

Table Name	Input Name	Wt Fraction	Second Liq Phase	Mol Wt Data Table Value	Mol Wt Input Value	Mol Wt for Equation
Water		1		18.02		18.02
		1				

Figure 2 CHEF Screening tool Snip 1

The bubble point pressure of water at 250 °C is 39.5 kg/cm^2 (g) which is 13 times the design pressure. Such pressure excursion occurs if the vent valve is not fully open during introduction of cooling water when the operator wants to begin the cooling process. Upon further investigation and interview with the process engineer, it was found that water hammering was observed whenever the operator opened the cooling water control valve. The hammering caused damage to the internal coil and for reducing the hammering effect, the operations team designed an installation of a 1/2" by pass valve. This reduced the failure rates of the internal coil damage was not sufficient to eliminate the issue. The Leidenfrost temperature of water is at 200 °C, therefore film boiling takes place resulting in rapid phase transition and hammer. The opening of the bypass valve only reduced the shockwave in the coil but did not eliminate the pressure excursion. Here is a summary of the deficiencies and failure mechanisms identified during the audit:

- The cooling water is of low quality that will result in scaling of the pipe and these deposits can result in further deterioration of piping
- The pipe can catastrophically rupture and Section 2.2 has a discussion on how to estimate the hazard distances due to an overpressure excursion
- Thermal stress cracking when cooling water is introduced as part of the cooling process
- Vibration fatigue due to overpressurization
- Process Hazard Analysis ranks the blocked cooling water outlet with a low consequence

2.2 Overpressure excursion due to closure of vent isolation valve

During the start of the new batch, the reactor is visually observed and materials are charged. After charging the materials, the contents are heated using thermic fluid in the jacket up to 250 °C. The internal coils most often are liquid filled at the time of the charging inside the internal coil due to cooling operations from the previous batch. The operator closes the isolation valve in the cooling water supply and return line and opens the vent line before the batch begins. The internal coil will catastrophically explode if all cooling water supply and return valves are closed when the batch begins. The manual opening of the vent isolation valve is the only safeguard identified during the time of the audit. It is always good to understand the consequence of misoperation of the isolation valve that can lead to a pressure excursion inside the internal coils thereby an overpressure inside the reactor. Assuming a liquid filled volume of 0.25 m^3 for the internal coil,

Specific Volume of Water at 250 °C = 1.25173E-03 m^3/kg [2]

Specific Volume of Steam at 250 °C = 0.0500829 m3/kg [2]

Volume of steam occupied after expansion will be 12.52 m^3 due to a ratio of volume expansion of water to steam of 40. The settle out pressure after internal coil failure will most likely be 17.5 kg/cm^2 (g) by using the ASME Safety Factor of 3.5.

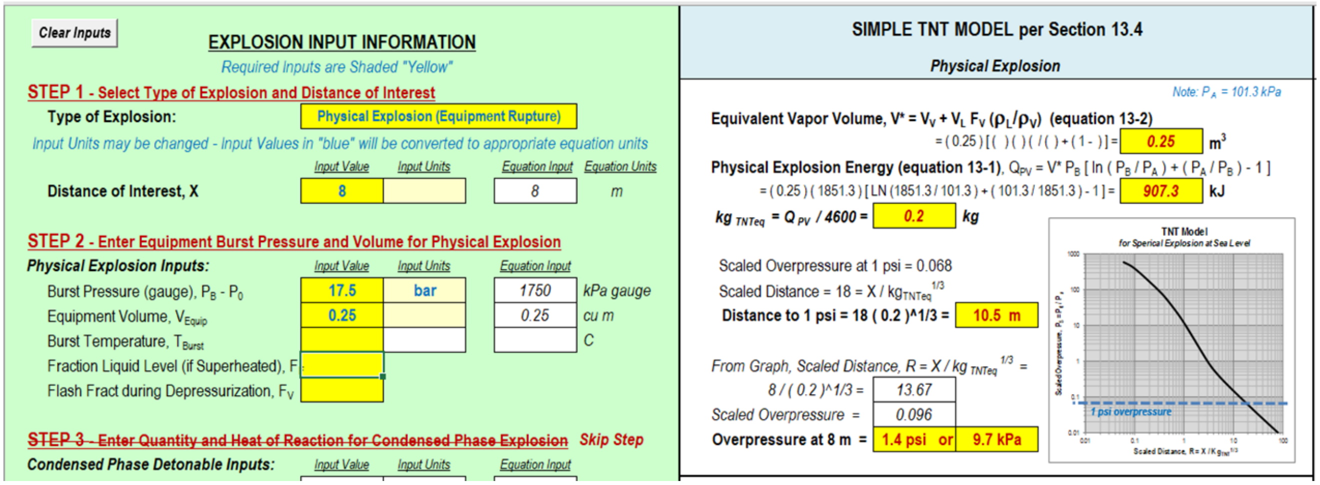


Figure 3 CHEF Screening Tool Snip 2

A screening model for equipment rupture is considered for an internal volume of 0.25 m^3 and Figure 3 is a screen shot from the CHEF tool. A cabin and a break room are present 8 m from the reactor and is distance of interest that is entered in the CHEF Tool. The overpressure observed at 8 m is 1.4 psi. The distance to 1 psi is 10.5 m indicating potential for injuries. However, the internal coils is going to most likely damage most of the reactor internals and create an overpressure excursion inside the reactor. The reactor is equipped with a combination relief device and has an open path to a scrubber system.

In summary, the CHEF tool was used as a screening tool to understand the process safety issues. In addition, the high failure rates of internal coil resulting in a guillotine break or other punctures were validated using the simple screening tools available in the CHEF excel sheet. The failure rates were high since the thermal and vibration fatigues was high due to water hammer, plus using low quality water accelerates the deterioration of the pipe.

3. Process Safety Information Validation

Isopropanol (IPA) is a widely used solvent in the chemical process industry, and there have been several incidents in India in the year 2020 and 2021 that have resulted in large scale fire and explosions. Understanding the inherent hazards of IPA is imperative to have an appropriate safeguard strategy. Adequate layers of protection are necessary to prevent explosion and fire as it is a highly flammable fluid. The independent safeguards are to be validated to ensure they work on demand. The flash point is 12 °C and the boiling point 82.5 °C obtained from CHEF Calculation Aid [1]. The vapor pressure of isopropanol at 30 °C storage temperature is 7.3 kPa (absolute), Figure 4. The maximum volume of IPA in mL per cubic meter of air at 30 °C will be 72,063 mL/m^3 which equals 7.2% [vol basis]. Isopropanol has LEL of 2% and UEL of 12% per Cameo Chemicals [3].

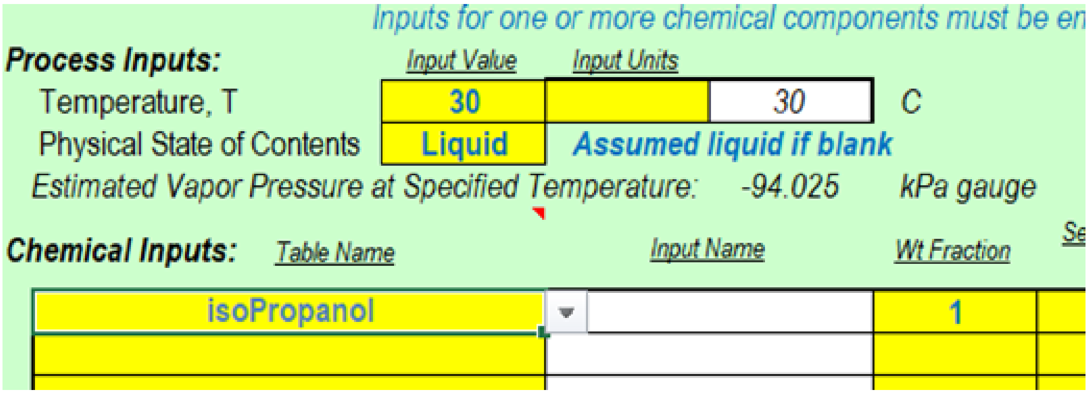


Figure 4 CHEF Screening Tool Snip 3

The simple operation of storing IPA in an atmospheric storage tank can result in an explosive condition. At an ambient storage temperature of 30 °C, the contents are within the explosive range and an internal deflagration, resulting in loss of containment and secondary domino effects are possible.

3.1 Internal deflagration of IPA storage tank

A 50 m^3 storage tank stores IPA with an average void space volume of 15 m^3. The storage temperature is 30 °C and the CHEF calculation aid is used for determining the consequence of the internal deflagration inside the storage tank. It is an open to atmosphere storage tank with a flame arrestor installed on the top nozzle. Internal deflagration due to flash back in to the tank was considered as part of the process safety audit. The source of ignition was considered lightning during the monsoon season. The flame arrester is sized and selected in accordance with the explosive group of gas [4]. Lightning protectors are designed and installed using the collection volume method. Lightning protection for the specific IPA tank was not validated during the time of the audit. Validation of the lightning arrestor design and flame arrestor is part of disciplined adherence to standard and was recommended to the user. The following inputs were added to the CHEF calculation aid explosions tab, see Figure 5. Building or Head Space Explosion model was considered in Step 1 with a distance of interest of 15 m to see the overpressure effects of a nearby high foot traffic area.

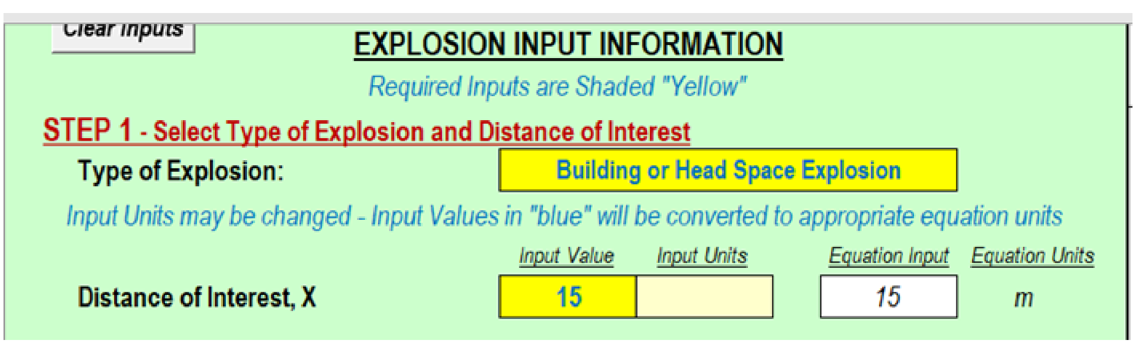


Figure 5 CHEF Screening Tool Snip 4

The isopropanol is selected from the chemical list and the LEL of 2%, molecular weight, and fuel reactivity of medium is automatically populated with the internal chemical database of the CHEF Calculation Aid. The head space volume inside the storage tank is 15 m^3, Figure 6. The advantage of the CHEF calculation aid is to make screening evaluation of process safety events with limited inputs. This is especially advantageous during initial project design (or) PHA facilitator trying to determine consequence (or) auditors who are identifying major accident risk potential with limited information.

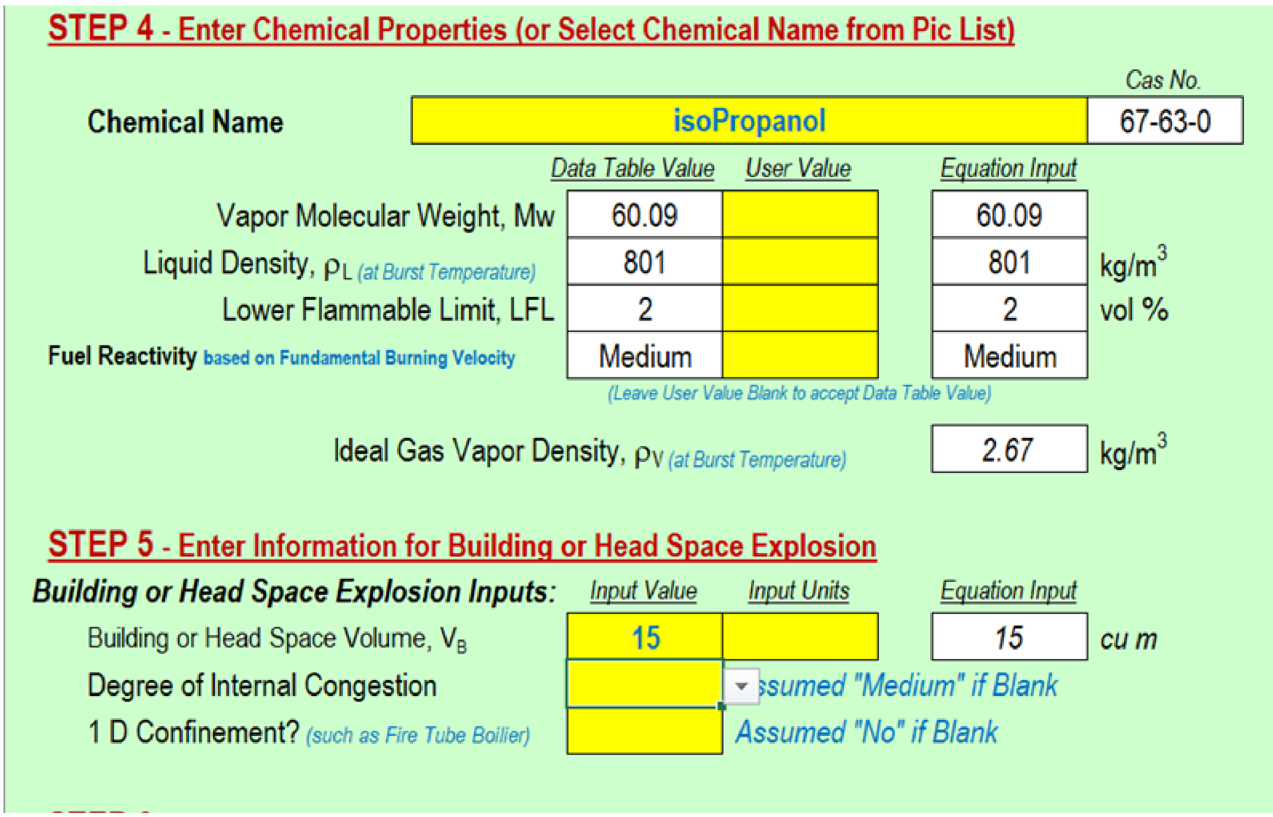


Figure 6 CHEF Screening Tool Snip 5

The Baker-Strehlow-Tang Model is used for computing hazard distances due to internal deflagration, see Figure 7. The distance to 1 psi is 25.2 m and the overpressure at the walkway present 15 m from the storage tank is 1.7 psi.

BAKER-STREHLOW-TANG MODEL per Section 13.5

Building or Head Space Explosion

Fuel Reactivity	Obstacle Density or Congestion: Low	Medium	High
High	0.5	>1	>1
Low-Medium	0.35	**0.5**	1
Class I Dust		0.35	0.5

Use Mach 0.5 for Low-Medium Fuel Reactivity and Medium Confinement

Potential Explosion Site (PES) Volume, $V_{PES} = V_B =$ **15** m^3

Explosion Energy (equation 13-3), $Q_E = 3500\ V_{PES} =$

3500 (15) = **52500** **kJ**

Note: P_A = 101.3 kPa

Scaled Overpressure at 1 psi = 0.068

Scaled Distance, $R = X / (2\ Q_E / P_0)^{1/3}$ = **2.5**

Distance to 1 psi = $R\ (2\ Q_E / P_0)^{1/3}$ =

2.5 [2 (52500) / 101.3]^1/3 = **25.2 m**

From Graph, Scaled Distance, $R = X / (2\ Q_E / P_0)^{1/3}$ =

15 / [2 (52500) / 101.3]^1/3 = 1.486

Scaled Overpressure = 0.118

Overpressure at 15 m = 1.7 psi or 12 kPa

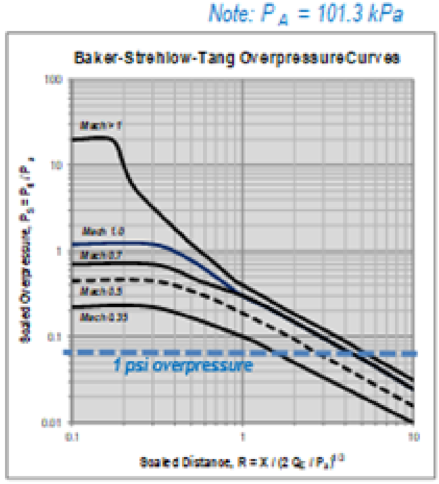


Figure 7 CHEF Screening Tool Snip 6

It was recommended to validate the lightning protection to ensure it is designed adequately and covers the tank farm where the IPA is stored as the consequence of an internal deflagration can impact humans travelling in the walkway. Process Safety Information validation is a corner stone of the PSM program. Additionally, it was recommended to replace the flame arrester open vent with a PVRV.

4. Conclusions

CHEF Calculation aid is versatile and essential tool for Process Safety and Risk Management professionals. The tool has a list of 222 chemicals and process safety models that can be used for screening purposes. It requires limited process safety information for screening purposes. The two examples show the screening capabilities of the CHEF calculation aid to identify the hazards and potential consequence to troubleshoot process safety issues.

5. References

[1] American Institute of Chemical Engineers, "RAST and CHEF Aid," CCPS, 23 April 2021. [Online]. Available: https://www.aiche.org/ccps/resources/tools/risk-analysis-screening-tool-rast-and-chemical-hazard-engineering-fundamentals-chef/rast-user-and-chef-manuals. [Accessed 8 August 2021].

[2] Spirax Sarco, "Spirax Sarco Resources and Design Tools," [Online]. Available: https://www.spiraxsarco.com/resources-and-design-tools. [Accessed 8 August 2021].

[3] US Department of Commerce, "Cameo Chemicals, National Oceanic and Atmospheric Administration," [Online]. Available: https://cameochemicals.noaa.gov/chemical/946. [Accessed 16 August 2021].

[4] American Institute of Chemical Engineers, "Protect your process with proper flame arrestors," *Chemical Engineering Process,* pp. 16-22, 2 December 2013.

[5] Health and Safety Executive, "Methods of approximation and determination of human vulnerability for offshore major accident hazard assessment," [Online]. Available: https://www.hse.gov.uk/foi/internalops/hid_circs/technical_osd/spc_tech_osd_30/spctecosd30.pdf. [Accessed 16 August 2021].