

Risk Analysis Screening Tools (RAST) Case Study – T2 Industries

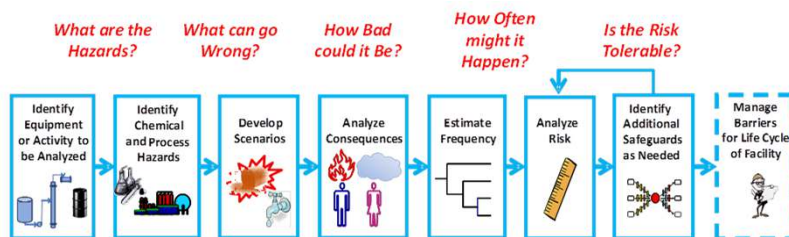


Runaway Reaction and Explosion
 Jacksonville, Florida
 December 19, 2007

March 24, 2022

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Case Study – T2 Industries Hazard Identification and Risk Analysis (HIRA) Study



We begin the study by **Identifying the Equipment or Activity** for which we intend to perform an analysis. RAST uses the operation of a specific equipment item containing a specific chemical or chemical mixture to define the activity. For example, the operation of a storage tank, a reactor, a piping network, etc. Inputs are chemical data, equipment design information, operating conditions, and plant layout.

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Case Study – T2 Industries

Process Description

We have been asked to perform a HIRA study of the MCMT Process. Methylcyclopentadienyl manganese tricarbonyl (MCMT) is an organo-manganese compound used as an octane-increasing gasoline additive. The Ethyl Corporation originally developed MCMT in the late 1950s. T2 manufactured and sold MCMT under the trade name Ecotane.

MCMT is produced in three steps that occur sequentially within a single process reactor. In the first reaction step (called metalation), the process operator feeds a mixture of methylcyclopentadiene (MCPD) dimer and diethylene glycol dimethyl ether (diglyme) solvent into the reactor. An outside operator then hand-loads blocks of sodium metal through a 6-inch gate valve on top of the reactor, closing the valve when complete. The process operator then heats the mixture with the hot oil piping system, setting reactor pressure control at 3.45 bar and hot oil temperature control at 182°C.

Intended Chemistry:



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This is an illustrative example and does not reflect a thorough or complete study.

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Process Description

The initial reaction mixture contains approximately 0.11 weight fraction sodium, 0.45 weight fraction MCPD dimer and 0.44 weight fraction diglyme solvent. Heating this mixture begins the metalation reaction by melting the sodium and splitting each MCPD dimer molecule into two MCPD molecules. The melted sodium then reacts with the MCPD to form sodium methylcyclopentadiene, hydrogen gas, and heat. The hydrogen gas vented to the atmosphere through the pressure control valve and 1-inch vent line.

Once the mixture temperature reaches 99°C, the process operator starts the agitator. The mixing and higher temperature acts to increase the metalation reaction rate. At a reaction temperature of about 149°C, the process operator turns off the hot oil system and heat generated by the metalation reaction continues to raise the mixture temperature. At a temperature of about 182°C, the process operator initiates the control system cooling program, which intermittently injects water into the jacket based on the rate of reaction temperature increase. The heat of reaction for this step is approximately -45.4 kJ/mol sodium, -1975 J/g sodium, or -217 J/g reaction mixture.

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Process Description

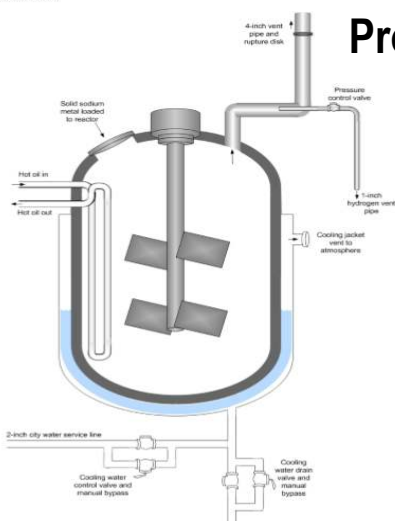
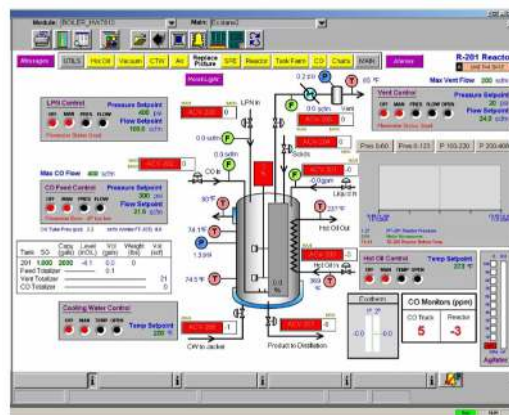


Diagram of MCMT Reactor



T2 screen capture

Process Control Screen for MCMT Reactor

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Risk Analysis Screening Tools (RAST)

Case Study – T2 Industries

We will start by entering information for the MCMT Reactor. At some point, we may decide to include other equipment in the study.

One the Main Menu, enter the equipment identification as the **MCMT Reactor**, equipment type as **Stirred Reactor/Crystallizer** and location as **Outdoors**.

Chemical Data – RAST requires a chemical or chemical mixture that is representative of the hazards. RAST does not perform time-dependent or location-dependent composition changes (such as within a reactor or distillation column). Where hazards may be significantly different between reactor feed and products, or distillation overheads versus bottoms; evaluation of the equipment may be repeated using different composition (such as Reactor A with feed composition and Reactor B with products composition).

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Risk Analysis Screening Tools (RAST) Case Study – T2 Industries

Begin by entering
information on the
Main Menu worksheet.
Start with the MCMT
Reactor

Enter Equipment Identification,
Equipment Type and Location

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Risk Analysis Screening Tools (RAST) Case Study – T2 Industries

Diglyme solvent and Methylcyclopentadiene Dimer (MCPD) are major components of the feed but not listed in the RAST chemical data table, so we will enter this as a new chemical. Many companies have access to large chemical property databases that contain the information we will need. In other cases, vendor Safety Data Sheets, Cameo Chemicals (US National Oceanic and Atmospheric Administration), or literature references may be used. It is good to look for agreement among multiple sources.

Diamond	Hazard	Value	Description
1	Health	1	Can cause significant irritation.
3	Flammability	3	Can be ignited under almost all ambient temperature conditions.
0	Instability	0	Normally stable, even under fire conditions.

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Case Study – T2 Industries Chemical Data

Risk Analysis Screening Tools (RAST) Overview / Demonstration

Select “Add New Chemical” from the Chemical Data worksheet to access the “New Chemical” worksheet. Start with “Diglyme”

Since the information available from common sources is very limited, we will start with data from a chemical with nearly the same molecular weight and boiling point (2-butoxyethanol), then update with what little we know.

Save as “diglyme”. RAST uses relatively simple correlations for chemical properties that require only one or two data points.

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Go To Chemical Table | New Chemical Data | **User Chemical Data Input** | Save Chemical Data to Chemical Table

Go To Chemical Table to Delete User Chemical

Starting Chemical That is Similar: Diglyme

User Supplied Values: Diglyme

Chemical to be Saved: Diglyme

Chemical Properties	Starting Chemical That is Similar	User Supplied Values	Properties of User Chemical to be Saved
Chemical Name	Diglyme (Dibutyl ether)		Diglyme
CAS Number	111-96-2	111-96-2	111-96-2
Data Source		Cameo Chemicals, Volume 100 and Thermoflex Scientific SDS	
Mol Weight	118.2	118.2	118.2
Melting Point, T _m (C)	-77	-64	-64
Boiling Point, T _b (C)	170.7	162	162
Vap. Press. A	10.876	10.302	10.302
Vap. Press. B	4183.21	4018.32	4018.32
Vap. Press. C	29.3	28.0	28.0
Dens. A	0.821	0.864	0.864
Dens. B	0.00094	0.00094	0.00094
U.S.C. A	0.844	0.844	0.844
U.S.C. B	0.00084	0.00084	0.00084
Lat. Heat A	119.3	119.3	119.3
Lat. Heat B	0.185	0.185	0.185
Lat. Heat C	0.00018	0.00018	0.00018
Flash Pt. (C)	68	68	68
U.S. Vol. %	1.5	1.5	1.5
U.S. Vol. %	17.4	17.4	17.4
Autoignition Temp. (C)	170	170	170
State of Ignition	Normal	Normal	Normal
Flam. Reactivity	Medium	Medium	Medium
Liquid Conductivity			
Heat of Vaporization			
Solub. Max. (g/100g Solvent)			
Solub. Part. Size at 10% (nm)			
Heat of Vaporization (J/mol)			
ERPG-1 (or Odor) ppm	20	91	91
ERPG-2 (ppm)	20	130	130
ERPG-3 (ppm)	2	0	0
NFPA Health	2	0	0
NFPA Reactivity	0	0	0
NFPA Instability	0	0	0
Chemical Toxicity			
Acute Toxicity			
Respiratory Corrosion			
Good Laboratory Practices?			

Calculate Physical Properties, Correlate from Data Points

Property	Units	Point 1	Point 2
Temperature 1 and 2	C	25	162
Vapor Pressure (atmos)	atmos	0	162
Liquid Density	g/cm ³		
Liquid Heat Capacity	J/gm C		
Heat of Vaporization	J/gm		

Estimated Boiling Point, C = 162.0

Information Sources may be noted

The normal boiling point and vapor pressure at 25 C from Molbase SDS

Liquid density, liquid heat capacity and heat of vaporization for 2-butoxyethanol were used

Flash Point, Flammable Limits, NFPA Ratings and ERPG (in this case PAC) concentrations are from Cameo Chemicals

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Case Study – T2 Industries Chemical Data

Risk Analysis Screening Tools (RAST) Overview / Demonstration

Select “Add New Chemical” from the Chemical Data worksheet to access the “New Chemical” worksheet.

Since the information available from common sources is very limited, we will start with data from a chemical with nearly the same molecular weight and boiling point (triethyl benzene), then update with what little we know.

Save as “Methylcyclopentadiene Dimer”. RAST uses relatively simple correlations for chemical properties that require only one or two data points.

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Go To Chemical Table | New Chemical Data | **User Chemical Data Input** | Save Chemical Data to Chemical Table

Go To Chemical Table to Delete User Chemical

Starting Chemical That is Similar: Methylcyclopentadiene Dimer

User Supplied Values: Methylcyclopentadiene Dimer

Chemical to be Saved: Methylcyclopentadiene Dimer

Chemical Properties	Starting Chemical That is Similar	User Supplied Values	Properties of User Chemical to be Saved
Chemical Name	Methylcyclopentadiene Dimer		Methylcyclopentadiene Dimer
CAS Number	2080-18-5	2080-18-5	2080-18-5
Data Source		Cameo Chemicals, Volume 100, Thermoflex Scientific SDS	
Mol Weight	152.28	152.28	152.28
Melting Point, T _m (C)	-61	-61	-61
Boiling Point, T _b (C)	218.4	200	200
Vap. Press. A	10.039	8.430	8.430
Vap. Press. B	4781.94	3024.76	3024.76
Vap. Press. C	42.3	43.0	43.0
Dens. A	0.860	0.860	0.860
Dens. B	0.00078	0.00078	0.00078
U.S.C. A	0.860	0.860	0.860
U.S.C. B	0.00078	0.00078	0.00078
Lat. Heat A	90.3	90.3	90.3
Lat. Heat B	0.081	0.081	0.081
Lat. Heat C	0.00080	0.00080	0.00080
Flash Pt. (C)	83	26	26
U.S. Vol. %	1	1	1
U.S. Vol. %	5.6	10	10
Autoignition Temp. (C)			
State of Ignition			
Flam. Reactivity			
Liquid Conductivity			
Heat of Vaporization			
Solub. Max. (g/100g Solvent)			
Solub. Part. Size at 10% (nm)			
Heat of Vaporization (J/mol)			
ERPG-1 (or Odor) ppm	3	0.34	0.34
ERPG-2 (ppm)	33	3.7	3.7
ERPG-3 (ppm)	195	21	21
NFPA Health	0	0	0
NFPA Reactivity	2	3	3
NFPA Instability	0	0	0
Chemical Toxicity			
Acute Toxicity			
Respiratory Corrosion			
Good Laboratory Practices?			

Calculate Physical Properties, Correlate from Data Points

Property	Units	Point 1	Point 2
Temperature 1 and 2	C	25	200
Vapor Pressure (atmos)	atmos	7.8	200
Liquid Density	g/cm ³		
Liquid Heat Capacity	J/gm C		
Heat of Vaporization	J/gm		

Estimated Boiling Point, C = 200.0

Information Sources may be noted

The normal boiling point and vapor pressure at 25 C from Molbase SDS

Liquid density, liquid heat capacity and heat of vaporization for triethyl benzene were used

Flash Point, Flammable Limits, NFPA Ratings and ERPG (in this case PAC) concentrations are from Cameo Chemicals

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Case Study – T2 Industries

Chemical Data

A composition (weight fraction):
0.45 Methylcyclopentadiene Dimer
0.44 Diglyme
0.11 Dissolved Solids
(representing Sodium metal)
was used as representative of the initial charge to the reactor.
The operating pressure was entered as 3.45 barg and the operating temperature was entered as 150 C.

The operating pressure entered as the initial pressure set pressure.

Saturation temperature is estimated and physical state as "liquid"

RAST allows up to 5 components.

Hydrogen as the Pad Gas is entered on the Process Conditions worksheet

Chemical details may be shown or hidden

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Equipment Input

The reaction equipment is a 2450 gallon vessel with a Maximum Allowable Work Pressure (MAWP) of 600 psig (41 bar). The cooling surface area is approximately 160 ft² (15 m²) and cooled with evaporating water at 100 C. Assume a heat transfer coefficient for the jacketed of 0.2 kwatt/m² C. The hot oil heating media temperature is 182 C and the vessel is insulated.

Only minimal data will be entered at this time.

The equipment volume and maximum allowable working pressure

A 4 inch (100 mm) nozzle is assumed the largest liquid connection to the vessel.

The reactor was equipped with a 4 inch (100 mm) rupture disk set at 28 barg (400 psig)

Information related to heat transfer of the equipment

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Process Conditions

The maximum flowrate during the methylation reaction step is zero (all is added batchwise at the start of reaction). We can evaluate the loading step by entering the equipment information with a separate identification (such as MCMT Reactor-loading). The temperature and pressure conditions during this step would be different from the reaction step.

Hydrogen has been entered as the pad gas since it is a reaction product not present initially. (Also, the flash routines in RAST do not handle trace amounts of highly volatile component in the liquid phase.)

Process Conditions Input

Equipment Identification: MCMT Reactor
Equipment Type: Stirred Reactor/Crystallizer
Location: Outdoors

Process Description

Summary for Methylcyclopentadiene Dimer

Operating Temperature =	150	C
Operating Pressure (gauge) =	3.45	bar
Physical State =	Liquid	
Saturation Temperature =	256.3	C
Contained Mass =	6357	kg
Maximum Contained Mass =	7946	kg
Inventory for Reference =	7946	kg

Operating Procedures

Percent of Time in Operation =
Frequent Turnaround or Cleanout?
Centralized Ventilation Shut-Off Bldg 1?
Centralized Ventilation Shut-Off Bldg 2?

Review of Operating Procedures for Selected Equipment Item by: Review Date:

Use Time-based Release for Equipment Rupture? sec

Note that with an entry of zero federate, no overflow scenario will be suggested.

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Site Layout

The manufacturing facility is located on a 5 acre site north of a Jacksonville, Florida industrial area. A small control building is located roughly 50 ft (15 m) from the reactor with up to 10 occupants. There is a trucking company and other businesses adjacent to the T2 site, roughly 140 m away with possibly 20 occupants.

Plant Layout Input

Equipment Identification: MCMT Reactor
Equipment Type: Stirred Reactor/Crystallizer
Location: Outdoors

Layout Description

Location Information

Distance to Property Line or Fence Line =	100	m
Furthest Distance to Fence Line (> 100 m) =		m
Max. Onsite Outdoor Population Density		people/m ²
Personnel Routinely in Immediate Area?		
Distance to end of Offsite Zone 1		m
Offsite Population Density within Zone 1		people/m ²
Offsite Population Density Beyond Zone 1		people/m ²
Effective Egress from Work Area?		
Access for Emergency Services?		
Degree of Equipment Congestion in Area?		sq m
Containment or Dike Surface Area =		sq m
Consider Dike or Bund Failure for Vessel Rupture?		
Credit Fire Heat Adsorption for Drainage/Indirect?		
Distance to Nearest Fired Equipment =		kg
Quantity of Other Flammables in Immediate Area		kg
Quantity of Flammables in Adjacent Area		kg
Adjacent Containment or Dike Surface Area =		sq m
Automated ERVs to limit spill quantity?		

Enclosed Process Area Data

Enclosed Process Volume =		cu m
Enclosed Process Ventilation =		changes/hr
No. Enclosed Area Personnel =		

Occupied Building Data

Occupied Building 1 Name =	Control Room
Distance to Occupied Bldg 1 or Area =	15 m
Elevation of Occ Bldg 1 Ventilation Inlet =	
Distance to Center of Occupied Bldg 1 =	
Occupied Bldg Type =	
Occupied Bldg Ventilation Rate =	
Number of Building Occupants =	10
Occ Bldg 2 in Same Wind Direction?	No
Occupied Building 2 Name =	Warehouses and Adjacent
Distance to Occupied Bldg 2	140 m
Elevation of Occ Bldg 2 Ventilation Inlet =	
Distance to Center of Occ Bldg 2 =	
Occupied Bldg 2 Type =	
Occupied Bldg 2 Ventilation Rate =	
Number of Occupants Bldg 2 =	20

Environmental Inputs

Spills to Soil Require Remediation?	
Potential for Water Contamination?	
High Population Downstream of Facility?	

Note that Environmental Scenarios are Excluded

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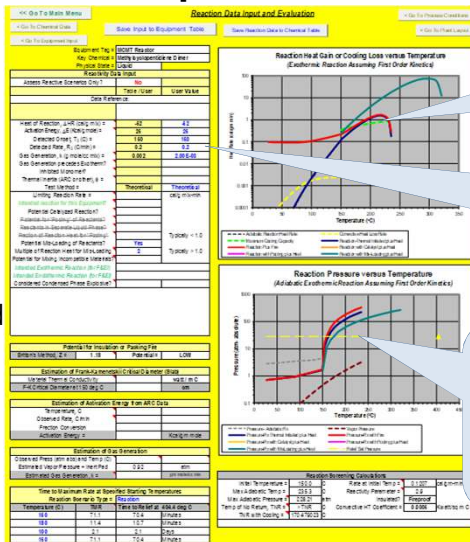
Reaction Input

Each ml of reaction mixture contains 0.84 g and roughly 0.09 g sodium or 0.004 gmole. From the reaction stoichiometry, 0.5 mole hydrogen is evolved per mole of sodium or 0.002 gmole hydrogen per ml of reaction mixture.

The known heat of reaction for the methylation step is -217 J/g or -52 cal/g reaction mixture. The activation is assumed a typical value of 25 to 30 kcal/gmole.

Finally at temperature rise rate of 0.2 C/min is assumed at 150 C such that it would take approximately 60 minutes for the reaction mass to heat from 150 to 180 C.

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Dashed green line is the cooling capability of the reactor jacket

Reaction parameters are entered. Ideally, experimental values or a kinetic model would be available.

The maximum reaction pressure far exceeds the MAWP of the reactor. However, the rate of pressure rise would be such that the vent system would normally be capable of handling it.

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Case Study – T2 Industries

Reaction Evaluation

In addition to the chemical hazards of flammability and toxicity, there are significant hazards associated with the methylation reaction. It is exothermic such that loss of temperature control will allow the reaction to proceed more quickly than the equipment may be designed for. Secondly, the reaction includes a gaseous product (hydrogen) such that extremely high pressure could be attained (far greater than the design limits of the equipment) if the system is not properly vented.

Another process upset to consider would be misloading of the initial materials, particularly the diglyme solvent. If there is less solvent to adsorb the reaction heat, the maximum reaction temperature would be higher with a corresponding higher reaction rate. (Note the “yes” to misloading with a multiple of 2 on the heat as solvent is nearly 50% of the initial charge.)

There is very little reaction information available to better understand what might happen under upset conditions suggesting that additional reactive chemicals testing should be done.

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Risk Analysis Screening Tools (RAST)

Case Study – T2 Industries

Select **Save Inputs to Equipment Table** (blue macro button). All Input Information will be stored in the Equipment Table in a single row identified by a unique Equipment Identification or Tag.

Retrieve Information for an Equipment Item by selecting any cell in the desired row and entering **Load Selected**

Input Data for an Equipment Item stored in one row by Equipment Tag

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Risk Analysis Screening Tools (RAST)

Risk Matrix

To understand the Consequence Severity and Tolerable Frequency, the values for key Study Parameters and a Risk Matrix may be viewed on the Workbook Notes worksheet. These values may be updated on hidden worksheets and should reflect the company's specific risk criteria.

For this case study, the Risk Matrix (right) has been used. The Human Harm criteria is based on an estimated number of people severely impacted (severe injury including fatality).

Risk Matrix: Risk = Consequence Severity times Frequency									
Description	Consequence Severity Description			Frequency					
	Human Harm	Environment	Business Loss	10 ⁻¹ /Year	10 ⁻² /Year	10 ⁻³ /Year	10 ⁻⁴ /Year	10 ⁻⁵ /Year	10 ⁻⁶ /Year
Severity Level 1	Minor Injury Occurs (or 0.01 Person Severely Impacted Off-site) Potential for Adverse Local Publicity	Releasable Incident to Environmental Agency OR < 10 kg Very Toxic to Waterway OR < 100 kg NFPA-H to Soil < 100 kg Toxic to Waterway OR < 1000 kg NFPA-H to Soil < 1000 kg Hazard to Waterway OR < 10000 kg NFPA-H to Soil	Property Damage and Business Loss < \$50M	High	High	High	High	High	High
Severity Level 2	Major Injury Occurs (or 0.01 to 0.1 Person Severely Impacted Off-site) Public Reported to State or Federal (or Minor Injury Off-site)	Environmental Contamination Confirmed to State OR < 100 kg Very Toxic to Waterway OR < 1000 kg NFPA-H to Soil < 1000 kg Toxic to Waterway OR < 10000 kg NFPA-H to Soil < 10000 kg Hazard to Waterway OR < 100000 kg NFPA-H to Soil	Property Damage and Business Loss \$50 M to \$500 M	High	High	High	High	High	High
Severity Level 3	Potential Fatality Occurs (or 0.1 to 1 Person Severely Impacted Off-site) or Potential Major Injury Off-site	< 1000 kg Very Toxic to Waterway OR < 10000 kg NFPA-H to Soil < 10000 kg Toxic to Waterway OR < 100000 kg NFPA-H to Soil < 100000 kg Hazard to Waterway OR < 1000000 kg NFPA-H to Soil	Property Damage and Business Loss \$500 M to \$500 MM	High	High	High	High	High	High
Severity Level 4	1 to 10 People Severely Impacted Off-site 0.1 to 1 People Severely Impacted Off-site	Incident Requiring Significant Off-Site Remediation OR < 10000 kg Very Toxic to Waterway OR < 100000 kg NFPA-H to Soil < 100000 kg Toxic to Waterway OR < 1000000 kg NFPA-H to Soil < 1000000 kg Hazard to Waterway OR < 10000000 kg NFPA-H to Soil	Property Damage and Business Loss \$500 MM to \$500 MM	High	High	High	High	High	High
Severity Level 5	> 10 People Severely Impacted Off-site > 1 Person Severely Impacted Off-site	Incident with Significant National Media Attention OR > 100000 kg Very Toxic to Waterway OR > 1000000 kg NFPA-H to Soil > 1000000 kg Toxic to Waterway OR > 10000000 kg NFPA-H to Soil	Property Damage and Business Loss > \$500 MM	High	High	High	High	High	High

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Risk Analysis Screening Tools (RAST) Overview / Demonstration

CPS
Center for Chemical Process Safety

Case Study – T2 Industries

Suggested Scenarios for the MCMT Reactor

Additional Scenarios are Added using "Create User Scenario"

The high consequence severity for the uncontrolled reaction scenarios also suggest that additional reactive chemicals testing and/or evaluation is warranted.

Once Inputs are Entered use "Update Input this Worksheet" to Save

Analysis Team captures which Scenarios warrant more Detailed Evaluation (Layers of Protection Analysis)

Analysis Team captures Existing Safeguards and Recommendations for Scenarios Identified

Evaluation Date(s) and Participant Names are entered on the Main Menu

A very serious scenario is overpressure and rupture of the MCMT Reactor from an uncontrolled reaction. Even if the vent system can prevent the rupture, venting flammable and toxic gases may also be an issue.

RAST is also suggesting the Vapor Cloud explosion may be a concern from the sudden release of flammable material if the vessel ruptures. However, the vapor may immediately ignite if the release is above the Autoignition temperature or from sparks emitted during rupture leading to fire rather than explosion.

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Risk Analysis Screening Tools (RAST) Overview / Demonstration

CPS
Center for Chemical Process Safety

Case Study – T2 Industries

Suggested Scenarios for MCMT Reactor

WORKING WITH YOUR EVALUATION TEAM:

- ☐ Review the suggested list of scenarios. Do these represent what you would expect for a batch reactor?
- ☐ Are there scenarios that have been "screened out" (shown in gray) that should be considered?
- ☐ Are there scenarios missing? (Possibly similar scenarios with different Initiating Events)
- ☐ Do you agree with the "worst" Consequence (Tolerable Frequency Factor) for the scenario listed?

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Case Study – T2 Industries

Consequence Analysis

What was unknown to the T2 owners is that the diglyme solvent decomposes exothermally at elevated temperature in the presence of sodium or possibly sodium methylcyclopentadiene. The heat of reaction and reaction rate at elevated temperature is such that the normal hydrogen vent, cooling capability and the relief device are not effective. The uncontrolled reaction scenario considering decomposition is a much higher risk as the heat generated in the methylation reaction will cause the system temperature to reach that where the decomposition proceeds at a very significant rate – only a loss of cooling is needed.

Heat of diglyme decomposition ~ -320 kJ/mol diglyme or -1050 J/g reaction mixture. This may have sufficient energy for deflagration or detonation depending on peak reaction rate. The activation energy from modeling is roughly 19 kcal/mol.

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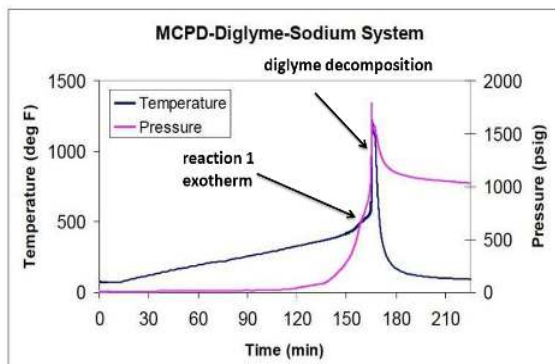
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Consequence Analysis

Following the incident at T2 Industries, a VSP test was run for the typical recipe with results used to create a kinetic model. Test results indicated a maximum temperature rate of 1300°C/min and maximum pressure rate of 2200 bar/min with maximum temperature of 650°C. **These conditions are well above the design limits of the equipment. In addition, the higher reaction rate evolves hydrogen at a rate which likely far exceeds the design of the vent system.**

Adiabatic Reaction Calorimetry used for kinetic constants estimates



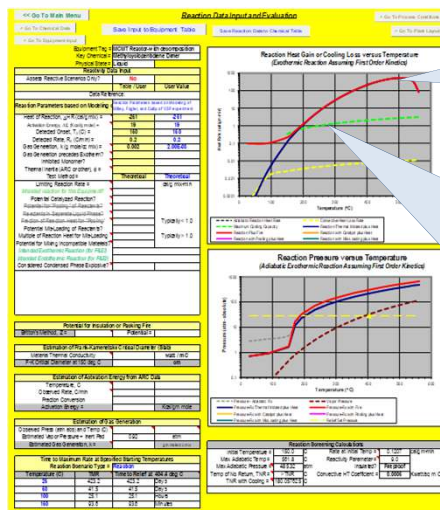
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Case Study – T2 Industries Updated Reaction Input

The VSP experimental data was fit to a kinetic model to better understand the behavior of the reaction during process upsets. Reference Willey, Fogler and Cutlip; "The Integration of Process Safety into a Chemical Reaction Engineering Course: Kinetic Modeling of the T2 Incident", Process Safety Progress 30 (2010).

A key finding is that if the rupture disk had been set to a much lower pressure (maybe 100 psig), it may have had sufficient capacity to prevent the rupture.



Note the much higher reaction rate and final temperature than from the intended reaction only.

Note the estimated point where the reaction rate exceeds the cooling capability is 180 C. The plant routinely operated without cooling to 190 C, so the kinetic parameters or jacket heat transfer coefficient may be low. However, this indicates that normal operation was very close to the estimated "temperature of no return".

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Case Study – T2 Industries Updated Reaction Input

The MCMT reaction including the decomposition reaction information may be easily saved as an additional equipment item. On the Main Menu, change the equipment ID to **MCMT Reactor –with decomposition**. Then use the **Save Inputs to Equipment Table** macro button.

Enter the updated Equipment Identification

Note an addition input line on the Equipment Table worksheet which contains the data for the decomposition reaction while retaining the initial equipment item with the intended reaction data.

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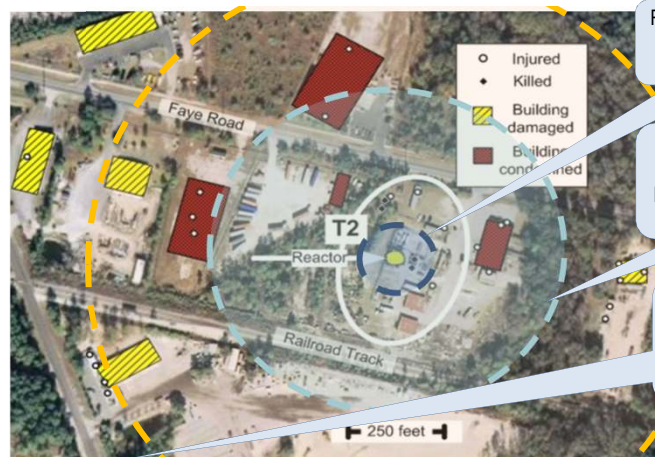
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Case Study – T2 Industries

Consequence Analysis – Physical Explosion

RAST estimated a maximum fragment range of 876 m (2870 ft). The reactor head was found 400 ft away, the agitator 350 ft away, and support columns 1000 ft from the original location.

RAST estimated a blast energy equivalent to 900 lb TNT (and assumes $\frac{1}{2}$ this energy is consumed in rupturing the vessel) versus CSB estimate of 1400 lb TNT equivalent.



RAST estimate of Direct Blast Impacts (10 psi overpressure)

RAST estimate of 1 psi Blast Overpressure Damage to Conventional Constructed Buildings

RAST estimate of 0.5 psi Blast Overpressure Damage to Low Strength Buildings

REPORT NO. 2008-3-1-FL, US Chemical Safety Board,
Figure 4. Injury and business locations.

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Case Study – T2 Industries

Risk Analysis / Layers of Protection Analysis (LOPA)

CW10									
Scenario	Equipment	Initiating Event	Consequence	LOPA Worksheet	LOPA Worksheet	LOPA Worksheet	LOPA Worksheet	LOPA Worksheet	LOPA Worksheet
1	142.01	LOPA Reactor with scenario	Uncontrolled Reaction - Adiabatic	IPPC instrument loop failure	IPPC instrument loop failure	IPPC instrument loop failure	IPPC instrument loop failure	IPPC instrument loop failure	IPPC instrument loop failure
2	142.01	LOPA Reactor with scenario	Uncontrolled Reaction - Adiabatic	IPPC instrument loop failure	IPPC instrument loop failure	IPPC instrument loop failure	IPPC instrument loop failure	IPPC instrument loop failure	IPPC instrument loop failure
3	142.01	LOPA Reactor with scenario	Uncontrolled Reaction - Adiabatic	IPPC instrument loop failure	IPPC instrument loop failure	IPPC instrument loop failure	IPPC instrument loop failure	IPPC instrument loop failure	IPPC instrument loop failure
4	142.01	LOPA Reactor with scenario	Uncontrolled Reaction - Adiabatic	IPPC instrument loop failure	IPPC instrument loop failure	IPPC instrument loop failure	IPPC instrument loop failure	IPPC instrument loop failure	IPPC instrument loop failure
5	142.01	LOPA Reactor with scenario	Uncontrolled Reaction - Adiabatic	IPPC instrument loop failure	IPPC instrument loop failure	IPPC instrument loop failure	IPPC instrument loop failure	IPPC instrument loop failure	IPPC instrument loop failure
6	142.01	LOPA Reactor with scenario	Uncontrolled Reaction - Adiabatic	IPPC instrument loop failure	IPPC instrument loop failure	IPPC instrument loop failure	IPPC instrument loop failure	IPPC instrument loop failure	IPPC instrument loop failure
7	142.01	LOPA Reactor with scenario	Uncontrolled Reaction - Adiabatic	IPPC instrument loop failure	IPPC instrument loop failure	IPPC instrument loop failure	IPPC instrument loop failure	IPPC instrument loop failure	IPPC instrument loop failure
8	142.01	LOPA Reactor with scenario	Uncontrolled Reaction - Adiabatic	IPPC instrument loop failure	IPPC instrument loop failure	IPPC instrument loop failure	IPPC instrument loop failure	IPPC instrument loop failure	IPPC instrument loop failure
9	142.01	LOPA Reactor with scenario	Uncontrolled Reaction - Adiabatic	IPPC instrument loop failure	IPPC instrument loop failure	IPPC instrument loop failure	IPPC instrument loop failure	IPPC instrument loop failure	IPPC instrument loop failure
10	142.01	LOPA Reactor with scenario	Uncontrolled Reaction - Adiabatic	IPPC instrument loop failure	IPPC instrument loop failure	IPPC instrument loop failure	IPPC instrument loop failure	IPPC instrument loop failure	IPPC instrument loop failure
11	142.01	LOPA Reactor with scenario	Uncontrolled Reaction - Adiabatic	IPPC instrument loop failure	IPPC instrument loop failure	IPPC instrument loop failure	IPPC instrument loop failure	IPPC instrument loop failure	IPPC instrument loop failure
12	142.01	LOPA Reactor with scenario	Uncontrolled Reaction - Adiabatic	IPPC instrument loop failure	IPPC instrument loop failure	IPPC instrument loop failure	IPPC instrument loop failure	IPPC instrument loop failure	IPPC instrument loop failure
13	142.01	LOPA Reactor with scenario	Uncontrolled Reaction - Adiabatic	IPPC instrument loop failure	IPPC instrument loop failure	IPPC instrument loop failure	IPPC instrument loop failure	IPPC instrument loop failure	IPPC instrument loop failure
14	142.01	LOPA Reactor with scenario	Uncontrolled Reaction - Adiabatic	IPPC instrument loop failure	IPPC instrument loop failure	IPPC instrument loop failure	IPPC instrument loop failure	IPPC instrument loop failure	IPPC instrument loop failure
15	142.01	LOPA Reactor with scenario	Uncontrolled Reaction - Adiabatic	IPPC instrument loop failure	IPPC instrument loop failure	IPPC instrument loop failure	IPPC instrument loop failure	IPPC instrument loop failure	IPPC instrument loop failure
16	142.01	LOPA Reactor with scenario	Uncontrolled Reaction - Adiabatic	IPPC instrument loop failure	IPPC instrument loop failure	IPPC instrument loop failure	IPPC instrument loop failure	IPPC instrument loop failure	IPPC instrument loop failure

Protection Gap	Scenario / Cause Ref	Description of Undesired Consequence	LOPA Tolerable Frequency Factor (chemicals, quantity involved, and basis for calculations)	Initiating Event (Human Error)	Probability of Ignition	Probability of Exposure (Presence Factor)	Time at Risk or Other Enabling Factor
New	152.01	Stored Reactor/Catalystizer, MOGT Reactor with decomposition, is involved in an Uncontrolled Reaction - Adiabatic event resulting in an Equipment Rupture at Saturation Temperature with a Distance to 1 psi Overpressure of 130 m. Estimated time to rupture is 94 min.	This incident could result in an Equipment Explosion with Rupture Distance to Direct Blast Impact (Overpressure or Fragments) of 876 m including Rupture Overpressure at Typical Construction Occupied Bldg 1 of 31.1 psi. 1 psi Blast Overpressure exceeds Distance to the Fence Line of 100 m. Consider adjustment for Off-Site impacts with the potential for Severity Level-5	Loss of Cooling results in Uncontrolled Exothermic Reaction		Probability of Personnel to be in Close Proximity to Chemical Release based on Physical Expiry	
Safety Analysis			Tolerable Frequency Factor 5	IPPC Instrument Loop Failure		POE Probabi	

Select Loss Event Equipment Rupture at Saturation with Incident Outcome of Equipment Explosion for analysis in LOPA ("Yes"), then select LOPA Worksheet

The initial Initiating Event description may be modified by the study team to more clearly describe what happened

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Case Study – T2 Industries

Risk Analysis / Layers of Protection Analysis (LOPA)

Scenario Definition							
Protection Gap	Scenario / Cross Ref	Description of Undesired Consequence > Possible IPLs	LOPA Tolerable Frequency Factor (chemicals, quantity involved, and basis for calculations)	Initiating Event > Human Error	Probability of Ignition	Probability of Exposure (Presence Factor)	Time at Risk or Other Enabling Factor
New	152.01	Stirred Reactor/Crystallizer, MCMT Reactor with decomposition, is involved in an Uncontrolled Reaction - Adiabatic event resulting in an Equipment Rupture at Saturation Temperature with a Distance to 1 psi Overpressure of 130 m. Estimated time to rupture is 94 min.	This incident could result in an Equipment Explosion with Rupture Distance to Direct Blast Impact (Overpressure or Fragments) of 876 m including Rupture Overpressure at Typical Construction Occupied Bldg 1 of 31.1 psi. 1 psi Blast Overpressure exceeds Distance to the Fence Line of 100 m. Consider adjustment for Off-Site Impacts with the potential for Severity Level-5	Loss of Cooling results in Uncontrolled Exothermic Reaction		Probability of Personnel to be in Close Proximity to Chemical Release based on Physical Explosion Impact Area to 876 m	
Instrumented Protection Credits Taken		IPL Status ? ->					
Safety Analysis			Tolerable Frequency Factor 6	BPCS Instrument Loop Failure		POE Probability Factor 0	
5			6	1		0	

RAST is suggesting that the damage distance is very significant such that a Probability of Exposure enabling condition would not be appropriate.

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Case Study – T2 Industries

Risk Analysis / Layers of Protection Analysis (LOPA)

Not Allowed								Notes / Comments	Issues to Resolve
BPCS Control or Human Response to Alarm	BPCS Control or Human Response to Alarm	SIS Function A	SIS Function B	Pressure Relief Device	SRPS 1	SRPS 2	SRPS 3		
		High temperature activates emergency cooling water addition		Two separate and independent pressure relief devices at a relatively low pressure confirmed by kinetic modeling					
		SIS - SIL 1		Two Independent PRDs on Separate Nodes with Independence Audit					
		1		4					

In addition to a high temperature interlock with an emergency cooling water supply, one of the most cost effective Protective Layers would likely be a second Pressure Relief Device. However, a Relief Device may not be effective for the Diglyme decomposition which would not be predicted in RAST and need to be confirmed by kinetic modeling.

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Risk Analysis Screening Tools (RAST)

Case Study – T2 Industries

Risk Analysis and Incident Investigation often use similar methods to better understand the scenario. Risk Analysis “anticipates” what could go wrong and what the potential consequences may be. For Incident Investigation, the Incident Outcome and Consequences are known in addition to the actual weather conditions and wind direction.

For the MCMT Reactor, RAST did suggest Uncontrolled Reaction as one of many scenarios to consider. RAST also recognized that a Physical Explosion could be a feasible Incident Outcome for the scenario. RAST was in good agreement with the CSB estimate of damage. RAST estimated 10 people severely impacted versus 4 fatalities and 32 injured in the actual incident.

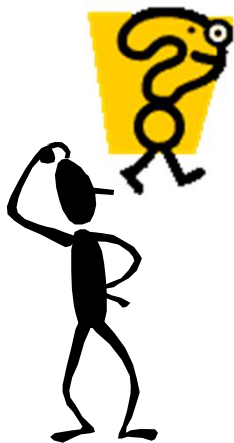
RAST can not predict reaction hazards if the data is not entered (decomposition).

THE USER MUST KNOW THE CHEMISTRY THEY ARE DEALING WITH.

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Questions?



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