Reactor Hazard Identification Case Study

Hazard Identification and Risk Analysis using RAST

Version: 1.0
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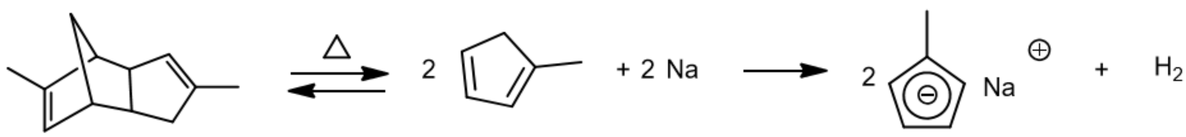
Process Description

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.

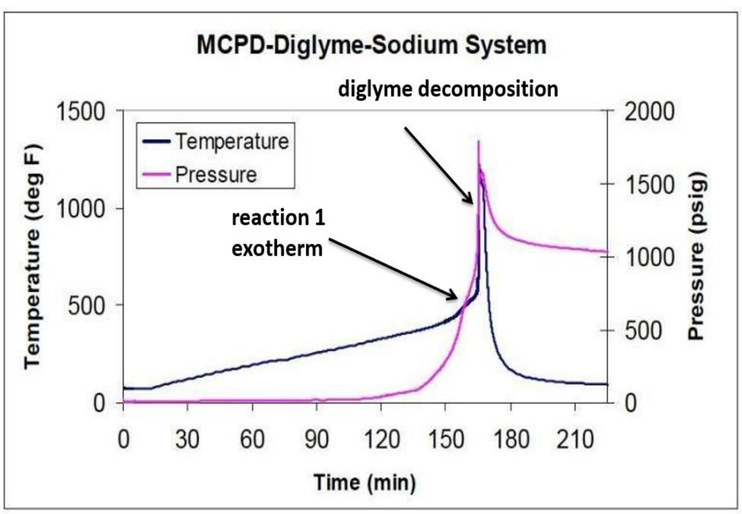
Intended Reaction



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.

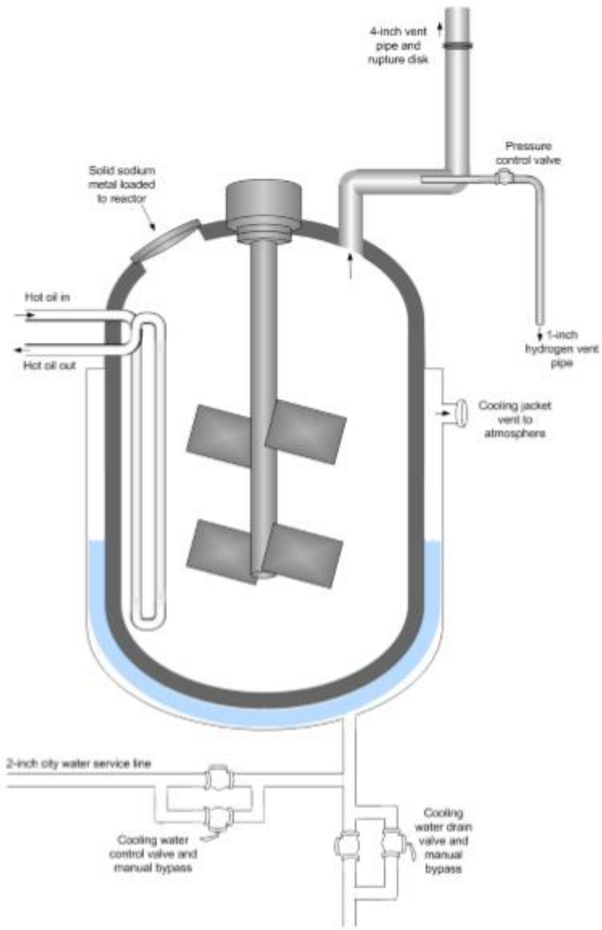
In addition to the intended reaction, a solvent (diglyme) decomposition occurs at elevated temperature. This reaction was unknown to operations personnel. VSP (Vent Sizing Package) tests was run for the typical recipe in a sealed system with results used to better understand decomposition kinetics. Test results indicated a maximum temperature rate of 1300°C/min and maximum pressure rate of 2200 bar/min with maximum temperature of 650°C at which point the test cell ruptured (such that the reaction may not have been complete). The overall heat of decomposition from the experiment is greater than -1110 J/g mixture (-260 cal/g) as indicated by the greater than 440 C temperature rise in a nearly adiabatic test apparatus and an average liquid heat capacity of roughly 2.5 J/g C.



Equipment and Site Description

The reaction equipment is a 2450 gallon vessel with a Maximum Allowable Work Pressure (MAWP) of 600 psig (41 barg). Cooling is provided by adding water to the vessel jacket which evaporates and is vented to the atmosphere. The cooling surface area is approximately 160 ft^2 (15 m^2).

The manufacturing facility is located on a 5-acre site in an industrial area and extends approximately 100 m from the reactor. A small control building is located roughly 50 ft (15 m) from the reactor. There is a trucking company and other businesses adjacent to the site with larger buildings/warehouse approximately 460 ft (140 m) away.



Inputs for RAST

Chemical data for the materials used in this example is not in the RAST chemical database as provided from CCPS, but they may be added by the User. Information from the Sigma-Aldrich Safety Data Sheet (SDS), ExxonMobil SDS, Protective Action Criteria (PAC) database Revision 29, and selected properties estimated by group contribution methods will be used. The RAST chemical data input sheets for methylcyclopentadiene and diglyme are shown below.

< Go To Chemical Data | Clear Chemical Data Inputs

User Chemical Data Input

Save Chemical Data to Chemical Table

Go To Chemical Table to Delete User Chemical >

Chemical Properties	Starting Chemical That is Similar	User Supplied Values	Properties of User Chemical to be Saved
Chemical Name =			Methylcyclopentidiene Dimer
CAS Number =		26472-00-4	26472-00-4
Data Source:		Group Contribution Estimates, Sigma Aldrich/ExonMobil SDS, PAC Database (ERPG)	
Mol Weight =		160.26	160.26
Melting Point, TM (C) =		-51	-51
Boil Point, TB (C) =		200	200
Vap Pres A =			9.261
Vap Pres B =			3982.29
Vap Pres C =			43.0
Dens A =			0.964
Dens B =			0.00091
Liq C A =			0.315
Liq C B =			0.00086
Lat Ht A =			65.9
Lat Ht B =			0.032
Lat Ht C =			0.00000
Flash Pt (C) =		31.8	31.8
LFL (Vol %) =		1	1
UFL (Vol %) =		10	10
AutoIgnition Temperature (C) =		480	480
Ease of Ignition =			
Fuel Reactivity =			
Liquid Conductivity			
Dust Deflagration Class			
Solids Mean Particle Size (micron)			
Solids Part Size at 10% Fract (micron)			
Dust Min Ignition Energy (mJ)			
Dust-Flam Vapor Hybrid?			
ERPG-1 or Odor (ppm) =		0.34	0.34
ERPG-2 (ppm) =		3.7	3.7
ERPG-3 (ppm) =		21	21
NFPA Health =		2	2
NFPA Flammability =		3	3
NFPA Reactivity =		0	0
Dermal Toxicity =			
Aquatic Toxicity =		Very Toxic	Very Toxic
Reactivity Category =			
Good Warning Properties?			

Calculate Physical Property Constants from Data Points

Property	Units	Point 1	Point 2
Temperature	C	25	200
Vapor Pressure (absolute)	mmHg	1.32	760
Liquid Density	gm/ml	0.941	0.781
Liquid Heat Capacity	cal/gm C	0.337	0.488
Heat of Vaporization	cal/gm	65.1	59.5

Estimated Boiling Point, C = 200.0

< Go To Chemical Data | Clear Chemical Data Inputs

User Chemical Data Input

Save Chemical Data to Chemical Table

Go To Chemical Table to Delete User Chemical >

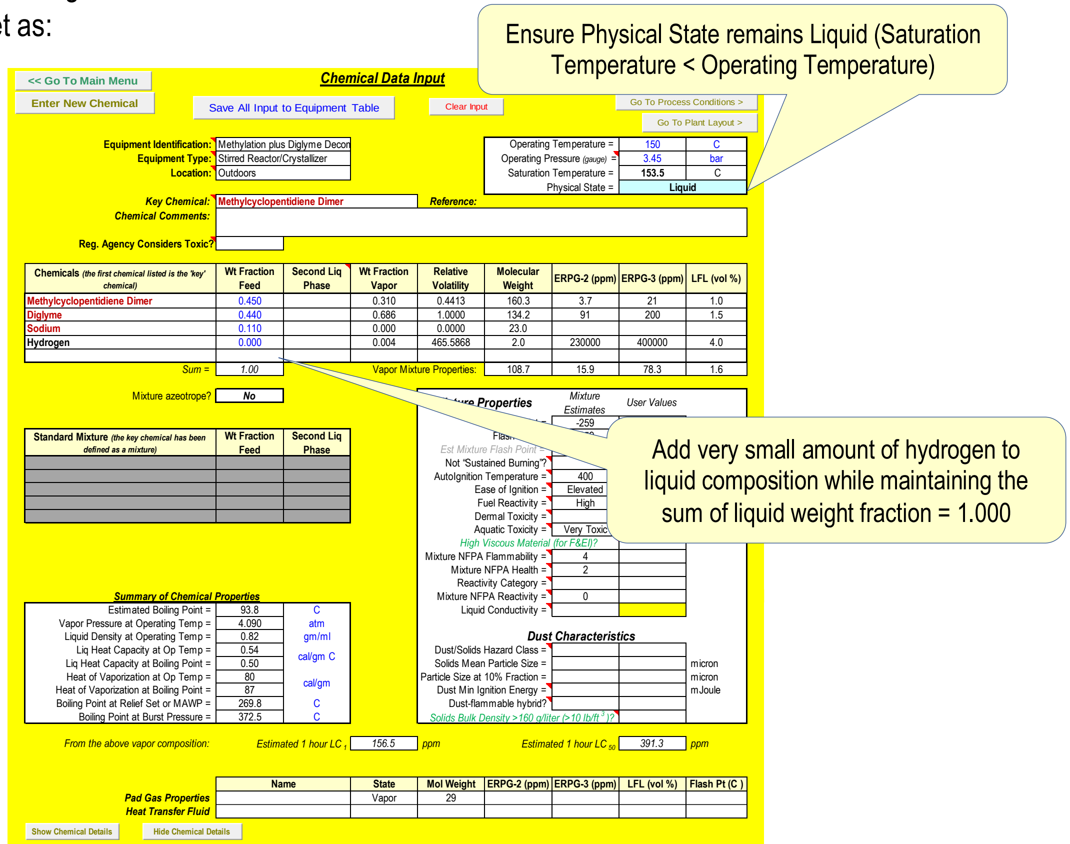
Chemical Properties	Starting Chemical That is Similar	User Supplied Values	Properties of User Chemical to be Saved
Chemical Name =			Diglyme
CAS Number =		111-96-6	111-96-6
Data Source:		Group Contribution Estimates, Sigma Aldrich SDS,PAC Database (ERPG)	
Mol Weight =		134.17	134.17
Melting Point, TM (C) =		-64	-64
Boil Point, TB (C) =		162	162
Vap Pres A =			12.716
Vap Pres B =			4984.70
Vap Pres C =			43.0
Dens A =			0.969
Dens B =			0.00104
Liq C A =			0.569
Liq C B =			0.00086
Lat Ht A =			113.6
Lat Ht B =			0.207
Lat Ht C =			0.00000
Flash Pt (C) =		57	57
LFL (Vol %) =		1.5	1.5
UFL (Vol %) =		17.4	17.4
AutoIgnition Temperature (C) =			
Ease of Ignition =			
Fuel Reactivity =			
Liquid Conductivity			
Dust Deflagration Class			
Solids Mean Particle Size (micron)			
Solids Part Size at 10% Fract (micron)			
Dust Min Ignition Energy (mJ)			
Dust-Flam Vapor Hybrid?			
ERPG-1 or Odor (ppm) =		15	15
ERPG-2 (ppm) =		91	91
ERPG-3 (ppm) =		200	200
NFPA Health =		0	0
NFPA Flammability =		2	2
NFPA Reactivity =		0	0
Dermal Toxicity =			
Aquatic Toxicity =			
Reactivity Category =			
Good Warning Properties?			

Calculate Physical Property Constants from Data Points

Property	Units	Point 1	Point 2
Temperature	C	25	162
Vapor Pressure (absolute)	mmHg	0.82	760
Liquid Density	gm/ml	0.943	0.8
Liquid Heat Capacity	cal/gm C	0.591	0.709
Heat of Vaporization	cal/gm	108.4	80

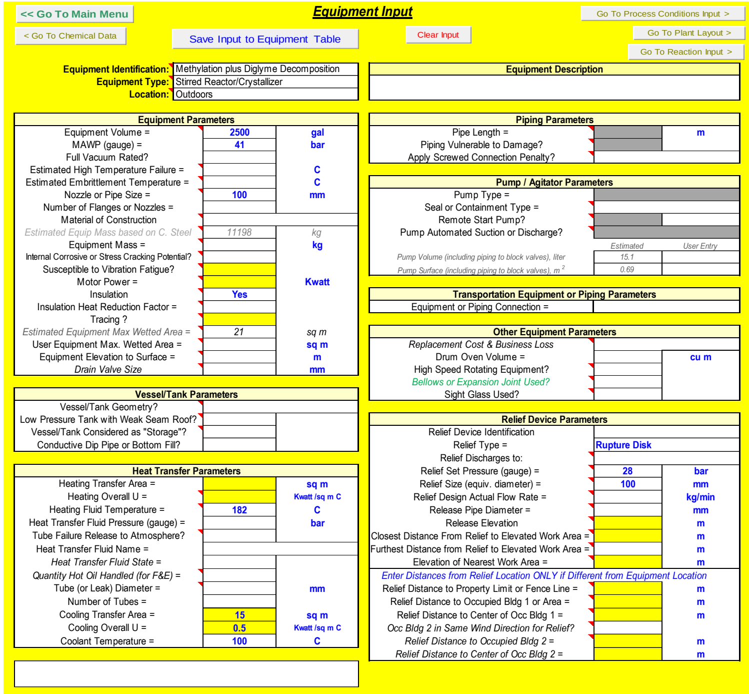
Estimated Boiling Point, C = 162.0

Sodium was entered as a generic dissolved solid. The final chemical mixture from the RAST Chemical Data Input worksheet as:

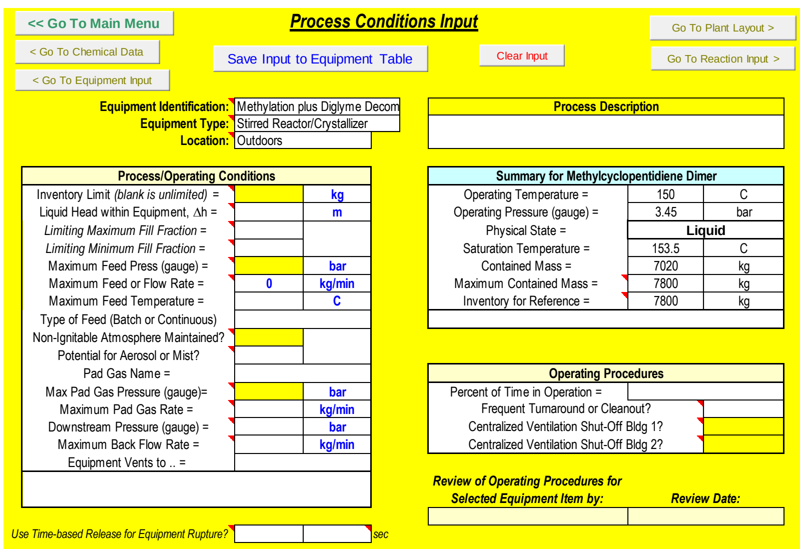


RAST <u>does not</u> account for changing composition during reaction. The liquid composition entered is intended to represent the Chemical Hazards for the equipment. Consider adding small quantity of dissolved gas or evaluation of multiple cases of different composition.

Equipment Data Entry is entered on the Equipment Input worksheet. Note that there are few required fields and information may be added later to improve results.



Since the reactor is operated batch-wise, the feedrate may be set to zero on the Process Conditions worksheet. A separate case to evaluate overfill of the reactor during the fill steps could be also be run.



Plant and Site Layout information is entered on the Plant Layout worksheet. For this example, we have assumed 3 occupants in the control building and 20 in the warehouse as a daytime value.

Plant Layout Input

<< Go To Main Menu

< Go To Chemical Data

< Go To Equipment Input

Save Input to Equipment Table

Clear Input

Go To Reaction Input >

< Go To Process Conditions

Equipment Identification:	Methylation plus Diglyme Decon
Equipment Type:	Stirred Reactor/Crystallizer
Location:	Outdoors

Layout Description

Location Information		
Distance to Property Limit 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?		
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 =		
Quantity of "Other" Flammables in Immediate Area		kg
Quantity of Flammables in Adjacent Area		kg
Adjacent Containment or Dike Surface Area =		sq m
Automated EBVs 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 =		m
Distance to Center of Occupied Bldg 1 =		m
Occupied Bldg Type =		
Occupied Bldg Ventilation Rate =		changes/hr
Number of Building Occupants =	3	
Occ Bldg 2 in Same Wind Direction?	No	
Occupied Building 2 Name =	Warehouses	
Distance to Occupied Bldg 2	140	m
Elevation of Occ Bldg 2 Ventilation Inlet =		m
Distance to Center of Occ Bldg2 =		m
Occupied Bldg 2 Type =		
Occupied Bldg 2 Ventilation Rate =		changes/hr
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		

As this example is for a reactor system, reaction information is added to the Reaction Input worksheet which also serves to provide high level reaction hazard screening. Limited kinetic information is needed which will provide a simple first order reaction model (shown graphically on the Reaction Input worksheet) used in the evaluation. As the kinetic information is not well known and the test container ruptured in both sealed experiments, one might assume a potential for deflagration or detonation. An activation energy of 20 kcal/mole is assumed to approximate the maximum temperature rate in the 600 to 650 C range as noted in the CSB report. It would be very important to obtain a good kinetic model, particularly in sizing of a pressure relief device to protect the equipment during a runaway reaction.

Reaction Data Input and Evaluation

<< Go To Main Menu | < Go To Chemical Data | < Go To Equipment Input | Save Input to Equipment Table | Save Reaction Data to Chemical Table | < Go To Process Conditions | < Go To Plant Layout

Equipment Tag =	Methylation plus Diglyme Decomposit	
Key Chemical =	Methylcyclopentidiene Dimer	
Physical State =	Liquid	
Reactivity Data Input		
Assess Reactive Scenarios Only?	No	
	Table / User	User Value
Data Reference:		
Reaction Parameters based on VSP exper	Reaction Parameters based on VSP experiment in CSB report	
Heat of Reaction, ΔHR (cal/g mix) =	-300	-300
Activation Energy, ΔE (Kcal/g mole) =	18.1	18.1
Detected Onset, T_0 (C) =	190	190
Detected Rate, R_0 (C/min) =	1.3	1.3
Gas Generation, k (g mole/cc mix) =	0.0024	2.40E-03
Gas Generation precedes Exotherm?		
Inhibited Monomer?		
Thermal Inertia (ARC or other), ϕ =		
Test Method =	Theoretical	Theoretical
Limiting Reaction Rate =		cal/g mix-min
Intended reaction for this Equipment?		
Potential Catalyzed Reaction?		
~~Potential for "Pooling" of Reactants?~~		
~~Reactants in Separate Liquid Phase?~~		
~~Fraction of Reaction Heat for "Pooling"~~		Typically < 1.0
Potential Mis-Loading of Reactants?		
Multiple of Reaction Heat for Mis-Loading		Typically > 1.0
Potential for Mixing Incompatible Materials?		
Intended Exothermic Reaction (for F&EI)		
Intended Endothermic Reaction (for F&EI)		
Considered Condensed Phase Explosive?	Yes	

Potential for Insulation or Packing Fire			
Britton's Method, Z =	0.61	Potential =	LOW

Estimation of Frank-Kamenetskii Critical Diameter (Slab)		
Material Thermal Conductivity		watt / m C
F-K Critical Diameter at 150 deg C		cm

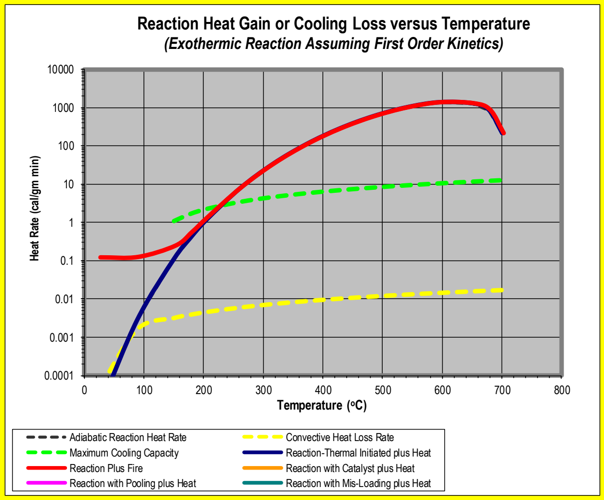
Estimation of Activation Energy from ARC Data		
Temperature, C	280	650
Observed Rate, C/min	3	1300
Fraction Conversion	0.1619	0.5000
Activation Energy =	18.1	Kcal/gm mole

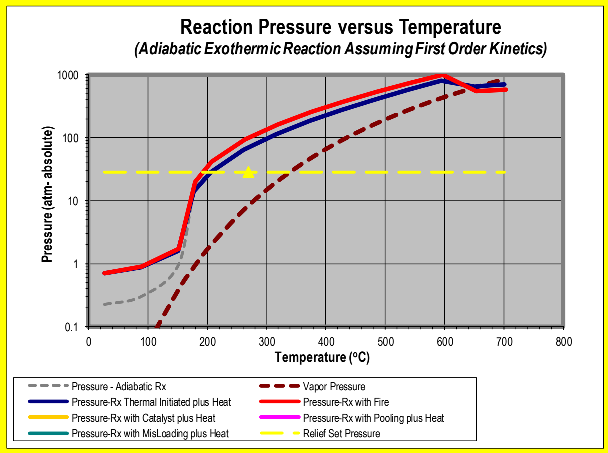
Estimation of Gas Generation		
Observed Press (atm abs) and Temp (C)		
Estimated Vapor Pressure + Inert Pad	0.92	atm
Estimated Gas Generation, k =		gm mole/cc mix

Time to Maximum Rate at Specified Starting Temperatures

Reaction Scenario Type = Reaction

Temperature (C)	TMR	Time to Relief at	269.8 deg C
100	22.6	>Relief Temp	Hours
125	5.5	>Relief Temp	Hours
150	97.1	>Relief Temp	Minutes
200	12.5	>Relief Temp	Minutes





Reaction Screening Calculations					
Initial Temperature =	150.0	C	Rate at Initial Temp =	0.1091	cal/gm-min
Max Adiabatic Temp =	700.5	C	Reactivity Parameter =	10.0	
Max Adiabatic Pressure =	794.92	atm	Insulated?	Fireproof	
Temp of No Return, TNR =	>TNR	C	Convective HT Coefficient =	0.0005	Kwatt/sq m C
TNR with Cooling =	223.627601	C			
Potential for Detonation Conditions - Consider Shock Sensitivity in Addition to Other Hazards					

Notice the green line on the heat rate graph. This indicates that the cooling system is capable of maintaining temperature control as long as the system is below 200 C (which is noted in the screening criteria, Temperature of No Return (TNR) with Cooling is estimated to be 200 C.

Reports

Following entry of the input information, several reports may be run to summarize hazards and risks. A good report to start with is the **Hazard Summary**. Based on the input information, RAST suggests considering flammable hazards due to the hydrogen present and that maximum temperatures during an upset are above the mixture flash point. The estimated Emergency Response Planning Guideline – Level 3 (ERPG-3) concentrations indicated toxic hazards to be considered. The reaction information also suggested significant reaction hazards exist.

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HAZARD SUMMARY

RAST Version 1.1 *Date:*

Summary of Chemical Information **for Process Unit: Stirred Reactor/Crystallizer; Methylation plus D**

Physical State at Operating Conditions for Methylcyclopentidiene Dimer = Liquid and Feed of:

Weight Fraction Methylcyclopentidiene Dimer	0.45
Weight Fraction Diglyme	0.44
Weight Fraction Sodium	0.109994
Weight Fraction Hydrogen	0.000006

Normal Boiling Point, C	93.8	**Hazard Screening**
Flash Point, C	**-259.0**	*Note Chemical Information in Bold*
Lower Flammable Limit at Initial Composition, vol %	2.2	
Combustible Dust?	No	*Flammability Hazard Sufficient for Further Consideration*
ERPG-2 at Initial Composition, ppm	13.7	
ERPG-3 at Initial Composition, ppm	**72.4**	
Dermal Toxicity Classification *(or Corrosive to Human Tissue)*		*Toxicity Hazard Sufficient for Further Consideration*
Aquatic Toxicity Classification	**Very Toxic**	
Considered Toxic by a Regulatory Agency?	No	
Heat of Reaction, kJoule/kg (Exothermic)	**-1256.1**	*Reactivity Hazard Sufficient for Further Consideration*
Highly Volatile or Gaseous Products Generated?	**Yes**	
Potential for Mixing Incompatible Materials?	No	
Considered Condensed Phase Explosive?	Yes	*Process Equipment is Considered in Hazardous Service*

Summary of Equipment and Process Conditions

Equipment or Vessel Volume 2500 gal

	Temperature C	Pressure bar gauge	*Pressure Exceeds Relief Device Set Pressure?*
Normal Operating Conditions	**150**	**3.45**	
Relief Device Set Pressure	269.8	**28.00**	
Catastrophic Failure/Burst Pressure	372.5	**82.00**	
Full Vacuum Rated? Not Entered			
Catastrophic Failure Higih Temperature	**600.0**		
Temperature where Low Temp Embrittlement may Occur?	*Not Entered*		
Maximum Feed Pressure		Not Entered	
Maximum Gas Pad Pressure		Not Entered	
Maximum Downstream Equipment Pressure		Not Entered	
Maximum from Liquid Displacement *(based on 9 X compression or feed pressure)*		2.29	**No**
Estimated Maximum Headspace Deflagration Pressure		10.13	**No**
Maximum Pressure from Hydraulic Surge (Piping Only)			
Maximum Ambient Conditions	25	-0.71	**No**
Maximum Feed Temperature			
Minimum Coolant Temperature	100	0.48	**No**
Normal Boiling Point of Equipment Contents	93.8		
Maximum from Heating Media Temperature	182	7.11	**No**
Estimated time to Relief Set Pressure or MAWP from Heat Transfer at Low Level, min			
Estimated time to Relief Set Pressure or MAWP from Heat Transfer at High Level, min			
Heating Media Source Pressure		0.00	**No**
Max from Mechanical Energy at Low Level: Insulated			
Estimated time to Relief Set or MAWP from Mechanical Energy at Low Level, min			
Max from Mechanical Energy at High Level: Insulated			
Estimated time to Relief Set or MAWP from Mechanical Energy at High Level, min			

		Max. Temperature Exceeds High Temperature Failure
Maximum Temperature , C	**706.1**	**Yes**
		Min Temperature less than Embrittlement Temperature
Minimum Temperature, C	**25**	**No**

Potential for Uncontrolled Reaction **Yes**

Reaction Temperature of No Return is Less Than: Ambient Temperature, Operating Temperature, Heating Media Temperature,

		With Gas Genera	Pressure Exceeds Relief Device Set Pressure?
Exothermic Reaction Temperature of No Return	>TNR		
Maximum Reaction based on Adiabatic and Initial Temperature as Operating Temperature	*Temperature, C* 706.1	*Pressure, barg* **794.92**	**Yes**

Max Reaction Temp Exceeds High Temperature Failure? **Yes**

Potential for Pool Fire Yes

The Flash Point is Less Than: 60 C, Ambient Temperature + 5 C, Operating Temperature + 5 C, Heating Media Temperature + 5 C, Max Mechanical Energy Temperature + 5 C

Quantity Flammable Available based on System Inventory	5000.0	kg
Maximum Pool Fire Duration based on Direct Fire	187.6	minutes
Fire Heat Input per API 521 for Process Vessel or Equipment with Credit for Insulation	145449.6	Kwatt

Contents Reach Temperature of No Return at Pool Fire Duration
Contents Do Not Reach Relief Conditions at Pool Fire Duration
Contents Do Not Reach Failure or Rupture Conditions at Pool Fire Duration

Another very useful report is the **Scenario List.** Deviations of common Parameters for a Stirred Reactor that could lead to an unintended loss of hazardous material or energy along with the most common causes are listed. The list also contains comments why the scenario was selected. Scenarios in gray were not selected. The comments may explain why which may indicate a missing input. This table provides a "starting point" for identifying scenarios to consider for Risk Analysis. Note that "Uncontrolled Reaction – Adiabatic" cased by loss of cooling is one of the scenarios suggested for consideration.

<< Go To Main Menu | Update | ***Suggested Scenarios from the RAST Library*** | Go To Scenario Results >

Create User Scenario

HAZOP Node:
Plant Section = Stirred
Equipment Type = Reactor/Crystallizer
Equipment Tag = Methylation plus

HAZOP Design Intent
Methylation plus Diglyme Decomposition is a Stirred Reactor/Crystallizer containing Methylcyclopentidiene Dimer Mix that operates at 150 C and 3.45 bar. The volume is 2500 gal with a design pressure of 41 bar. The maximum feed or flow rate is 0 kg/min

Scenarios in gray were considered but are excluded for reason noted

LOPA Menu Filters:

Scenarios with NO IPL's Required will NOT be reported.

Scenario Type	Scenario Comments	Parameters and Deviation	Initiating Event (Cause)	Initiating Event Description	Incident	Outcome
Drain or Vent Valve Open	Drain or Vent Valve left open following infrequent maintenance, purging or cleaning	Flow-Loss of Containment	Human Failure Action once per quarter or less	Operator leaves Drain or Vent Open following infrequent maintenance	Drain or Vent Leak	Off-Site Toxic Release, On-Site Toxic Release, Toxic Infiltration, Chemical Exposure, Flash Fire or Fireball, Vapor Cloud Explosion
Mechanical Integrity Failure - Medium	Mechanical Integrity Loss of Containment for Medium Hole Size	Flow-Loss of Containment	IEF=4 as determined by Process Safety	Failure from corrosion, fatigue, etc.	Medium Hole Size Leak	Off-Site Toxic Release, On-Site Toxic Release, Toxic Infiltration, Chemical Exposure, Flash Fire or Fireball, Vapor Cloud Explosion
Mechanical Integrity Failure - Very Large	Mechanical Integrity Loss of Containment for Very Large Hole Size	Flow-Loss of Containment	IEF=4 as determined by Process Safety	Failure from corrosion, fatigue, etc.	Very Large Hole Size Leak	Off-Site Toxic Release, On-Site Toxic Release, Toxic Infiltration, Chemical Exposure, Flash Fire or Fireball, Vapor Cloud Explosion
Mechanical Integrity Failure - Very Small	Mechanical Integrity Loss of Containment for Very Small Hole Size	Flow-Loss of Containment	IEF=3 as determined by Process Safety	Failure from corrosion, fatigue, etc.	Very Small Hole Size Leak	On-Site Toxic Release
Seal Leak	No Agitator Seal indicated	Flow-Loss of Containment	Single Mechanical Seal Failure	Failure from corrosion, alignment, low flow, etc.	Mechanical Seal Failure above Liquid Level	On-Site Toxic Release, Toxic Infiltration, Flash Fire or Fireball
Uncontrolled Reaction - Adiabatic	Noted as a Condensed Phase Detonable Material	Reaction-High Rate	BPCS Instrument Loop Failure	Loss of Cooling results in Uncontrolled Exothermic Reaction	Vapor Relief Vent - Reaction	Off-Site Toxic Release, On-Site Toxic Release, Toxic Infiltration, Flash Fire or Fireball, Vapor Cloud Explosion
					Equipment Rupture - Detonation	Off-Site Toxic Release, On-Site Toxic Release, Toxic Infiltration, Chemical Exposure, Flash Fire or Fireball, Vapor Cloud Explosion, Equipment Explosion
Excessive Heat Input - Heat Transfer	Vapor Pressure plus pad gas Does Not exceed Maximum Allowable Working Pressure or Relief Set Pressure at Ambient or Heating Media Temperature	Pressure-High	BPCS Instrument Loop Failure	Failure of Flow Control	Criteria for Triggering Incidents Not Met	
Excessive Heat Input - Pool Fire Exposure	Fire duration is insufficient to heat equipment contents to Relief Set or Burst Pressure	Pressure-High	IEF=2 as determined by Process Safety	Leak of Flammable Material or Material above its Flash Point which may ignite	Criteria for Triggering Incidents Not Met	
Excessive Pad Gas Pressure	Maximum Pad Gas Pressure Does Not Exceed the Maximum Allowable Working Pressure or Relief Set Pressure	Flow-High	Regulator Failure	Regulator Fails causing high flow or pressure	Criteria for Triggering Incidents Not Met	
High Temperature Failure	Maximum Feed Temperature Exceeds Temperature limits of Equipment	Temperature-High	BPCS Instrument Loop Failure	Failure of Temperature Control	Criteria for Triggering Incidents Not Met	
Ignitable Headspace	Chemical is handled/stored above at sufficently high temperature such that vapor composition is above the flammable limits or fuel rich	Composition-Wrong Concentration	BPCS Instrument Loop Failure	Failure of Pressure or NonCombustible Atmosphere Control	Criteria for Triggering Incidents Not Met	
Overfill, Overflow, or Backflow	Maximum Feed Pressure or Downstream Equipment Pressure is not sufficient to active Relief Device resulting in Overfill	Level-High or Flow-Backflow	BPCS Instrument Loop Failure	Failure of Level Indication with continued addition of material	Criteria for Triggering Incidents Not Met	
Pad Gas Compression	Maximum Feed or Downstream Pressure does not exceed the Maximum Allowable Working Pressure or Relief Set Pressure	Pressure-High	BPCS Instrument Loop Failure	Failure of Pressure Control	Criteria for Triggering Incidents Not Met	
Piping or Equipment Leak - Small	Motor below Vibration Power Limit for Potential for Vibration Fatigue Failure of Rotating Equipment	Flow-Loss of Containment	Mechanical Failure	Loss of Alignment or Equipment Support causing Vibration or Excessive Movement	Criteria for Triggering Incidents Not Met	
Rotating Equipment Damage	Motor Power below Rotating Equipment Vibration or Damage Limit	Composition-Contaminants	Mechanical Failure	Breakage of rotating blade or internal parts due to alignment, wear,or fatigue	Criteria for Triggering Incidents Not Met	
Uncontrolled Reaction - Fire Induced	Maximum Temperature at Relief Set Pressure is less than the Temperature of No Return or Fire Duration Not Sufficient to Reach Reaction Conditions	Reaction-High Rate	IEF=2 as determined by Process Safety	Leak of Flammable Material or Material above its Flash Point which may ignite	Criteria for Triggering Incidents Not Met	
Vacuum Damage	Equipment is rated for Full Vacuum	Pressure-Low	BPCS Instrument Loop Failure	Failure of Pressure Control	Criteria for Triggering Incidents Not Met	

RAST also performs **Consequence Analysis** on each of the scenarios suggested (in addition to any scenarios the User adds). A summary of this analysis is found on the Consequence Summary worksheet. For example, the Incident Type suggested for the Uncontrolled Reaction scenario listed above is Rupture at Saturation Temperature.

CONSEQUENCE SUMMARY

RAST Version 1.1 *Date:*

glyme De **Incident Type for: Stirred Reactor/Crystallizer; Methylation plus Diglyme Decomposition Containing** — Equipment Rupture at Detonation/Deflagration

Equipment Rupture Modeled as Catastrophic Failure (Instatnaneous)

Release Location — Outdoors

Prob of Exposure (proximity based) with Personnel Not in Immediate Area

Airborne Quantity Summary:		
Release Temperature, C	372.5	
Release Pressure, barg	82.000	
Physical State at Release Conditions	Liquid	
Heat Input, Kcal/min		
Equivalent Hole Size, cm		
Release Rate, Kg/sec	Instantaneous	
Release Duration, min		
Spray Distance, m	74.0	
Flash + Aerosol Evaporation Fraction	0.673	
Estimated Aerosol Droplet Diameter, *micron*	175	
Pool Area, sq m	186.0	
Estimated Pool Temperature, C	61.5	
Maximum Pool Evaporation Rate, kg/sec	0.0031	
Total Airborne Rate, kg/sec		
Total Airborne Quantity, Kg	2185.4	

	Factor	*Probability*
On-Site Toxic POE		
Flash Fire POE		
Chemical Exposure POE		
Physical Explosion POE		

Airborne Quantity Composition:	
Mole Fraction Methylcyclopentidiene Dimer	0.393
Mole Fraction Diglyme	0.606
Mole Fraction Sodium	0.000
Mole Fraction Hydrogen	0.001
Mole Fraction Pad Gas (at Mw = 29)	
ERPG-2 for Vapor Composition, ppm by volume	67.0
ERPG-3 for Vapor Composition, ppm by volume	347.6
LFL for Vapor Composition, % by volume	1.25

Fence Line Concentration Exceeds ERPG-2

Ground or Work Area Exceeds 1/2 LFL or Multiple of ERPG-3

Dispersion Summary:	
Max Distance to Time-Scaled ERPG-2, m	1209.4
Max Distance to Time-Scaled ERPG-3, m	530.8
Max Distance to 1% Lethality for 1.5 F weather, m	1267.4
Max Distance to ERPG-3 multiple, m	283.2
Max Distance to 1/2 LFL, m	176.4
Maximum Ground Elevation Concentration, ppm	1000000.0
Concentration at Distance to Fence Line, ppm	9700.0
Concentration at Distance to Unrestricted Work Area, ppm	1000000.0
Concentration at Distance to Occupied Bldg 1, ppm	303297.9
Concentration at Distance to Occupied Bldg 2, ppm	4972.6
Concentration within Enclosed Process Area, ppm	
Conc within Enclosed Process Area w/Ventilation, ppm	

Potential Flamm Impact to Occupied Building (Conc > 1/2 LFL)

Potential Toxic Impact to Occupied Building (Conc > ERPG-3)

Explosion Summary:	
VCE or Building Explosion Distance to 1 psi Overpressure, m	638.9
Overpressure at Distance to Occupied Building, psi	294.0
Overpressure at Center of Occupied Building, psi	294.0
Distance to Severe Thermal Radiation Impact, m	
Distance to Direct Blast Impact (10 psi), m	29.4
Maximum Fragment Range, m	932.9
Rupture Distance to 1 psi Overpressure, m	138.4
Rupture Overpressure at Distance to Occupied Building, psi	35.2
Ruture Overpressure at Center of Occupied Building, psi	35.2

Probability of Ignition (POI):

Potential Explosion Impact to Occupied Building

Probability of Explosion (POX):

Potential Equip Rupture Impact to Occupied Building

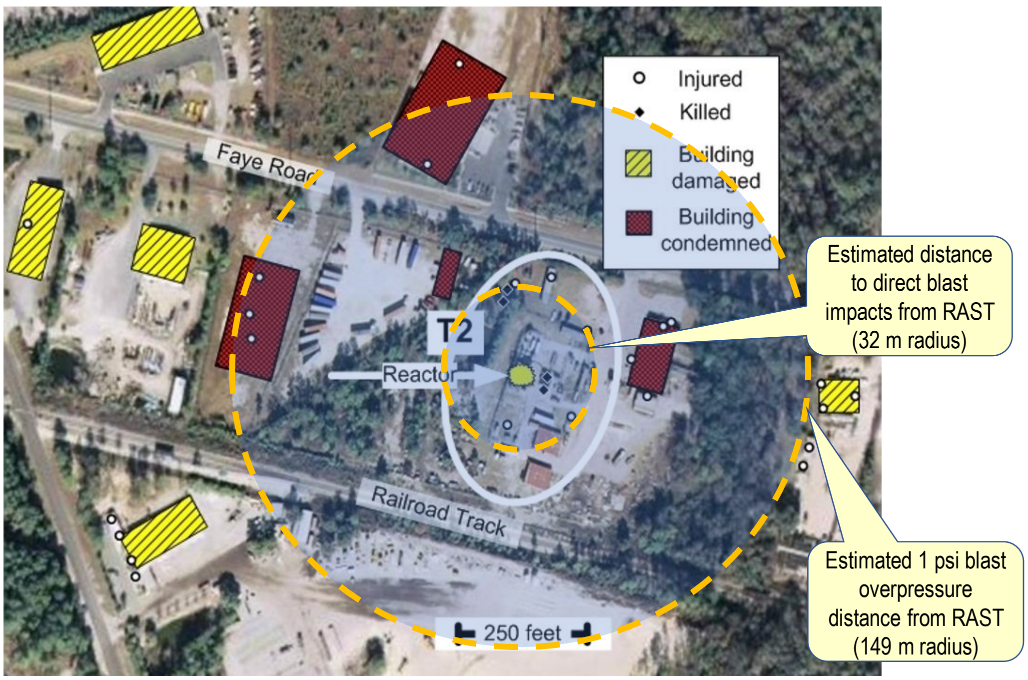
Consequences:

Impact Assessment with Personnel routinely in the immediate area	Exceeds Threshold Criteria	**LOPA Tolerable Frequency Factors**
Offsite Toxic Impact based on 100 m to Fence Line	Yes	**7**
Onsite Toxic Impact with 200 people/sq km outdoors	Yes	**5**
Outdoor Toxic Exposure Duration 63 sec		
Onsite Flammable Impact with 200 people/sq km outdoors	Yes	**4**
Onsite Chemical Exposure with 200 people/sq km outdoors		**4**
Onsite Direct Blast Impact with 200 people/sq km outdoors		**6**
Onsite Therm Rad Impact with 200 people/sq km outdoors		
Occupied Building Toxic Impacts	Yes	**5**
Number of Potential Serious Impacts for Building 1: 3 people		
Number of Potential Serious Impacts for Building 2: 0.6 people		
Occupied Building Explosion Impacts	Yes	**6**
Number of Potential Serious Impacts for Building 1: 3 people		
Number of Potential Serious Impacts for Building 2: 9.6 people		
1 psi Blast Overpressure Distance exceeds the Fence Line, Consider additional Offsite Impacts		
Occupied Building Physical Explosion Impacts	Yes	**6**
Number of Potential Serious Impacts for Building 1: 3 people		
Number of Potential Serious Impacts for Building 2: 0 people		
1 psi Blast Overpressure or Max Fragment Distance exceeds the Fence Line, Consider additional Offsite Impacts		
Environmental Impact:		**NA**

The analysis provides tolerable frequency for the various incident outcome based on the company's risk criteria. In this example, Offsite toxic represents a very high consequence scenario. This may prompt the User to check the location and population density of offsite personnel and enter additional information. The explosion impacts are also significant with the occupants for both building entered at risk. The damage distance to 1 psi from the rupture is estimated at 149 m with fragments to 1004 m. If the released vapor forms a large cloud before ignition, RAST estimates a vapor cloud explosion may also occur with 1 psi blast overpressure to 682 m.

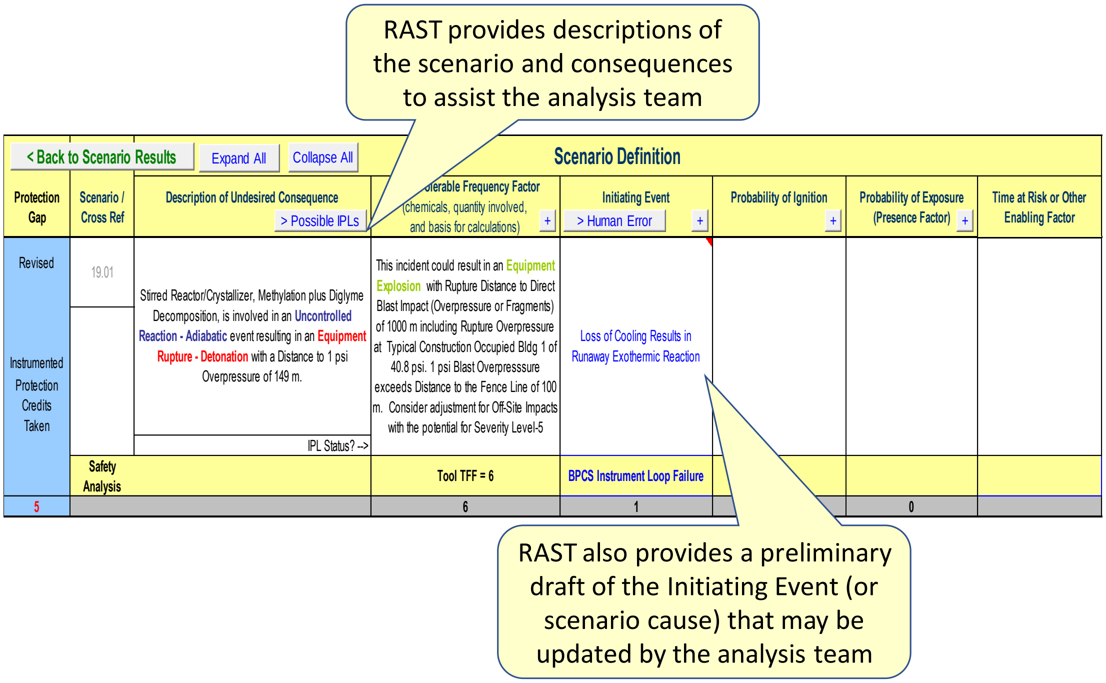
Unfortunately, this incident (Runaway Reaction and Explosion) occurred on December 19, 2007 near Jacksonville, Florida. There were 4 fatalities and 32 injured in the blast. Debris from the explosion was found up to one mile away which is in reasonable agreement with the estimated maximum fragment range of 1004 m (0.62 miles) from RAST.

CSB Final Report – T2 Laboratories Runaway Reaction. Figure 4. Injury and business locations

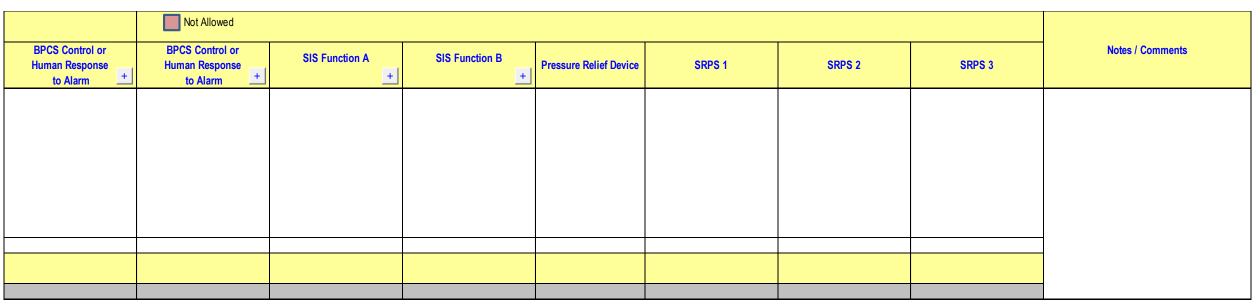


Finally, RAST provides a list of possible cause-consequence scenario cases that may be selected as a starting point for **Layers of Protection Analysis (LOPA)**. In addition to the scenario that occurred at T2 Laboratories, RAST provided an additional 90 cause-consequence pair cases. These cases (in addition to cases the study team identifies) may be evaluated by LOPA to ensure compliance with a company's risk criteria. RAST allows a Technical Administrator to enter a company risk matrix or table of tolerable frequencies for severe consequences. In this example, a tolerable frequency of 10^{-6} / year was entered into RAST for a scenario with the potential to result in multiple fatalities.

RAST contains Initiating Event frequencies and Probability of Failure upon Demand factors for common causes and protective layers used in LOPA analysis. RAST provides a LOPA format that helps to document process risk and the protective layers needed. A description of the scenario and tolerable frequency with key information from the Consequence Analysis is provided.



Information regarding Protective Layers such as instrumented interlocks, pressure relief systems, and other safety related protection systems may be captured by the analysis team in addition to the safety integrity level or probability of failure on demand. Once the mitigated scenario frequency meets the tolerable frequency, the scenario is considered adequately managed.



Reference:

United States Chemical Safety and Hazard Investigation Board (CSB), Investigation Report, "T2 Laboratories, Inc. Runaway Reaction, Jacksonville, Florida December 19, 2007," Report No. 2008-3-I-FL, 2009.