USER GUIDE

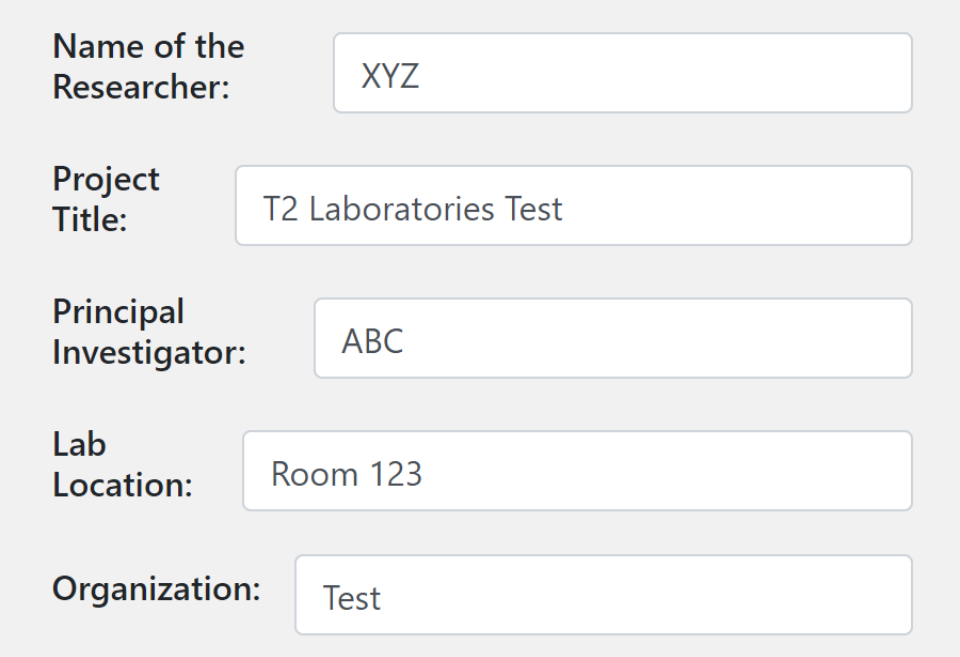
RHEACT (REACTIVE HAZARD EVALUATION AND COMPILATION TOOL)

Welcome to RHEACT!

RHEACT provides the user with a comprehensive initial evaluation of potential hazards and notifies one of any safety-concerns associated with the reaction process before conducting a laboratory experiment. This is achieved by collecting the relevant system information from the user through Safety Data Sheet (SDS) or user-defined inputs. Some of the capabilities provided in the current version of the tool include; 1) parsing multiple Safety Data Sheets (SDSs) for chemical and safety information, 2) creating an operational chemical hazard matrix and providing guidelines for PPE selection, 3) generating a pair-wise chemical compatibility matrix, and 4) calculating adiabatic temperature changes to generate alerts if the final system temperature deviates due to material properties or secondary reaction onsets (based on information provided by the user).

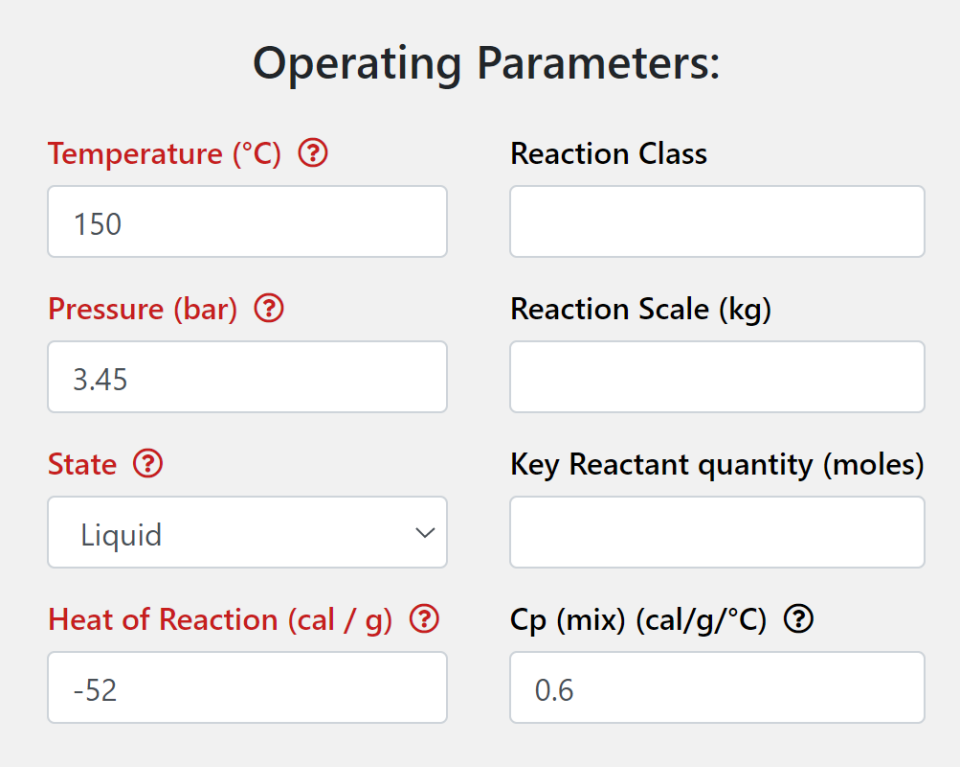
This guide will help the user understand how to run a case study with RHEACT using an example from the runaway reaction explosion at T2 Laboratories. The data for this example has been imported from the case study presented by Center for Chemical Process Safety (CCPS) on the use of Risk Analysis and Screening Tool (RAST) (Reference: https://www.aiche.org/sites/default/files/docs/book-pages/case_study_-_runaway_reaction_t2_industries.pdf). So, let's begin!

1. Enter general information about the system. This includes:
    a. Name of the researcher
    b. Project title
    c. Name of the principal investigator
    d. Lab location and
    e. Name of the organization



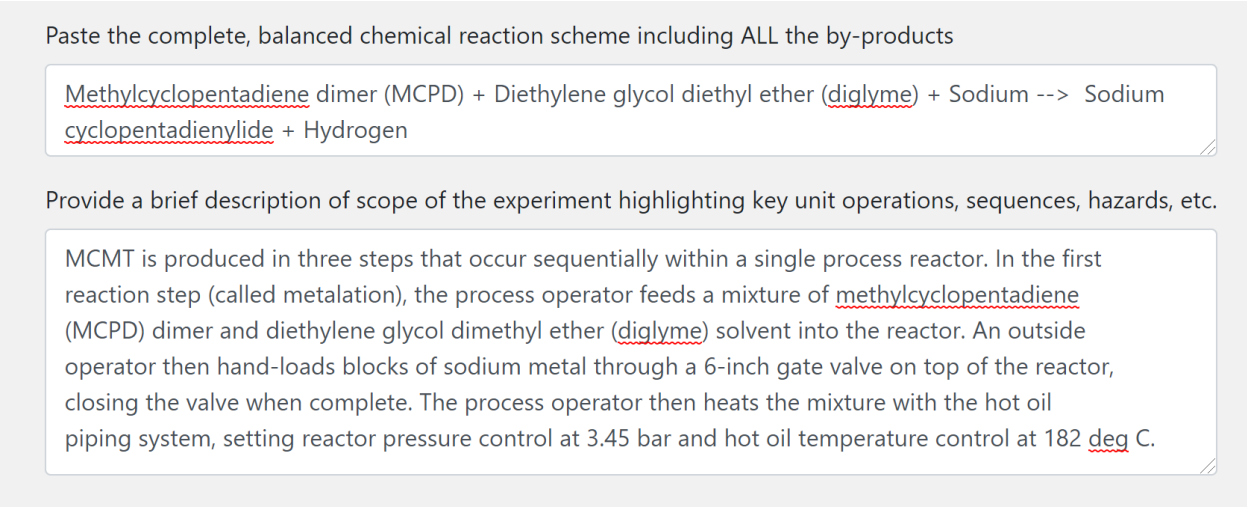
2. Enter the operating conditions for the system. This includes:
   a. Temperature: Enter the operating temperature (in ^{0}C) (mandatory input)
   b. Pressure: Enter the operating pressure (in bar) (mandatory input)
   c. State: Mention whether the system is operated in the gas or liquid state
   d. Heat of reaction: Enter the heat of reaction (in cal/g) at the operating conditions (mandatory input)
   e. Reaction class: Enter the type of reaction being studied (For example: Dehydrogenation, Hydrolysis, Nitration, etc.)
   f. Reaction scale: Enter the value for the scale of the reaction (in kg)
   g. Key reactant quantity: Enter the value for the limiting/key reactant quantity (in moles)
   h. Cp,mix: Enter the value for the specific heat of the reaction mixture (in cal/g/^{0}C) at the operating conditions.

   Note: The user has the option to enter the Cp,mix (if known or calculated) or the specific heat capacity for individual reactants along with the component mole fraction.



Data imported from the RAST Case Study on T2 Laboratories Incident

3. Enter additional information regarding the system (for the purpose of reporting). This includes the reaction scheme and a brief description on the scope of the experiment along with the basic unit operations, sequences, etc. (optional).

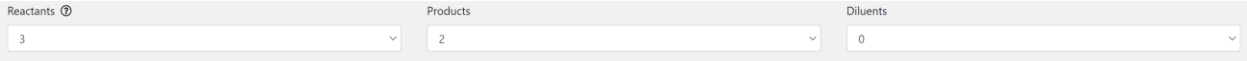


Data imported from the RAST Case Study on T2 Laboratories Incident

4. Enter known information on any side reactions associated with the system. This can be done by selecting the number of reactions from the drop-down list and populating information such as the reaction description, reaction onset temperature and pressure.

Data imported from the RAST Case Study on T2 Laboratories Incident

5. Select the number of reactants, products and diluent associated with the system. The user can select up to 4 reactants, 4 products and 2 diluents using the drop-down list.



Note: The '?' provides additional information for the input.

6. Once you have selected the number of reactants, products and the diluents, the corresponding tabs for these reagents would appear on the screen. The user can upload the Safety Data Sheet (SDS) for individual components using the 'Upload SDS' tab.

Note: Currently the tool only accepts SDS upload from Sigma Aldrich (Sigma Aldrich has SDSs available for over 300,000 chemicals). For SDSs not available on Sigma Aldrich, the user can manually input the field values.

7. Once the user uploads the SDS, the data parsing module extracts the required chemical and hazard related information and displays it on the interface for user

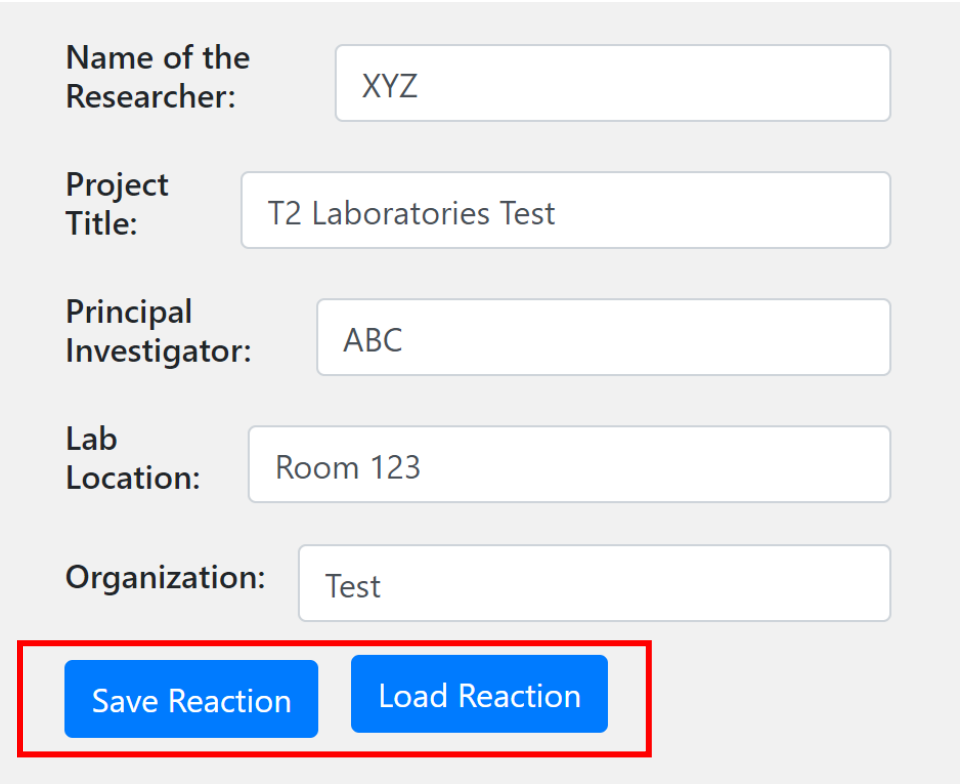
review. Additional inputs such as the mole fraction and specific heat capacity (in cal/g/^{0}C) (mandatory input) for individual components can be added at this point.

Property	Reactant 1	Reactant 2	Reactant 3	Product 1	Product 2
	Upload SDS	Upload SDS	Upload SDS	Upload SDS	Upload SDS
Product Name	Methylcyclopentadiene di	Diethylene glycol diethyl e	Sodium	Sodium cyclopentadienyli	Hydrogen
Initial Weight Fraction	0.45	0.44	0.11	0	0
Mol. Weight (g/mol)	160.26	162.23	22.99	88.08	2.02 g
CAS-No.	26472-00-4	112-36-7	7440-23-5	4984-82-1	1333-74-0
Physical and Chemical Properties					
pH at 20°C (g/l)	No data available	No data available	No data available	No data available	No data available
Initial boiling point (°C)	200	180	883	65	252.8
Flash point (°C)	31.8	67	No data available	-17	150
Upper explosion limit (% V)	No data available	No data available	No data available	No data available	74.2
Lower explosion limit (% V)	No data available	No data available	No data available	No data available	4
Vapour pressure at 20°C (hPa)	No data available	0.7	No data available	No data available	No data available
Vapour density (Air = 1.0)	No data available	5.6	No data available	No data available	0.08
Relative density at 25°C (g/cm3)	0.941	0.909	No data available	0.946	No data available
Auto ignition temperature (°C)	No data available	174	No data available	No data available	400
Decomposition temperature (°C)	No data available	No data available	No data available	No data available	No data available
Viscosity	No data available	No data available	No data available	No data available	No data available
Thermal Conductivity - k	No data available	No data available	No data available	No data available	No data available
Specific heat capacity - Cp (cal/g/°C)					

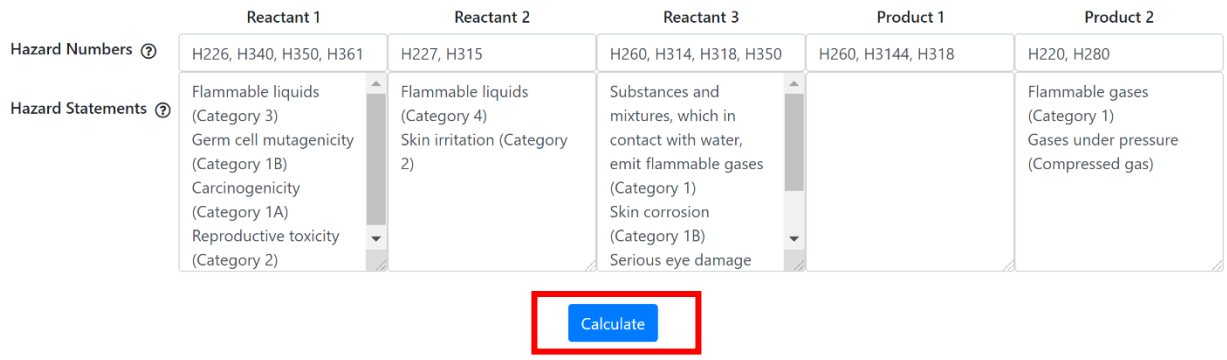
	Reactant 1	Reactant 2	Reactant 3	Product 1	Product 2
Hazard Numbers	H226, H340, H350, H361	H227, H315	H260, H314, H318, H350	H260, H3144, H318	H220, H280
Hazard Statements	Flammable liquids (Category 3) Germ cell mutagenicity (Category 1B) Carcinogenicity (Category 1A) Reproductive toxicity (Category 2)	Flammable liquids (Category 4) Skin irritation (Category 2)	Substances and mixtures, which in contact with water, emit flammable gases (Category 1) Skin corrosion (Category 1B) Serious eye damage		Flammable gases (Category 1) Gases under pressure (Compressed gas)

Note: The values for specific heat capacity for individual components should be at the operating conditions (in cal/g/^{0}C). The tool assumes no change in the values for Cp and heat of reaction when performing adiabatic change calculations.

8. The user can now verify the information on the interface. Once done, before generating the report, the user can save the system progress by clicking on the 'Save Reaction' tab available at the top of the webpage. This tab saves the webpage progress through a downloadable .json file. The system can be studied again later by uploading the .json file using the 'Load Reaction' tab.



9. Once the system information has been verified the user can click on the 'Calculate' for the tool to generate a hazard summary report



10. The system processes the information and generates a hazard summary report. The progress on the steps involved are displayed to the user. The user can press 'Okay' to continue and view the report.

Note: The tool generates the chemical compatibility matrix (CAMEO Table) by submitting a query to the CAMEO Chemicals webpage (Reference: https://cameochemicals.noaa.gov/) with the necessary information (Chemical name and CAS number). **In a system where one (or more) of the components are not available on the CAMEO database, the tool generates a chemical compatibility matrix with that one (or more) component less.**

11. As mentioned earlier, the hazard summary reports: (a) adiabatic change calculations, (b) hazard matrix and (c) chemical compatibility matrix. The adiabatic change calculations assume contributions from the heat of reaction alone (additional contributions from pooling, fire, misloading are not calculated in RHEACT). The final system temperature is compared with the reagent properties (flash point, boiling point, autoignition and decomposition temperature) to generate alerts for deviation from the input. The tool also compares the final system temperature with the secondary reaction onset temperature (added as an input by the user) and generates alerts accordingly. These system alerts can help predict thermal runaway events.

Report

Calculation

Adiabatic temperature change: 86.667 °C
Calculated final temperature: 236.667 °C
Calculated final pressure: 5.490 bar

Alerts

Reactant Alerts
Final temp exceeds reactant 1 boiling point
Final temp exceeds reactant 1 flash point
Final temp exceeds reactant 2 boiling point
Final temp exceeds reactant 2 flash point

Product Alerts
Final temp exceeds product 1 boiling point
Final temp exceeds product 1 flash point
Final temp exceeds product 2 flash point

Diluent Alerts
Final temp exceeds side reaction 1 temperature onset
Final pressure exceeds side reaction 1 pressure onset

12. The report also generates the hazard statements and hazard matrix using the H-phrases for the reagents, parsed by the tool. The hazard matrix can be used to understand the handling hazards associated with individual components of the system. This information can help guide the PPE selection process.

Hazard Statements

Name	H-Number	H-Statement
Methylcyclopentadiene dimer	H226 H340 H350 H361	Flammable liquids (Category 3) Germ cell mutagenicity (Category 1B) Carcinogenicity (Category 1A) Reproductive toxicity (Category 2)
Diethylene glycol diethyl ether	H227 H315	Flammable liquids (Category 4) Skin irritation (Category 2)
Sodium	H260 H314 H318 H350	Substances and mixtures, which in contact with water, emit flammable gases (Category 1) Skin corrosion (Category 1B) Serious eye damage (Category 1) Carcinogenicity (Category 1A)
Sodium cyclopentadienylide	H260 H3144 H318	
Hydrogen	H220 H280	Flammable gases (Category 1) Gases under pressure (Compressed gas)

Hazard Matrix

Name	Flammability	Reactivity	Skin absorption	Skin contact	Eye contact	Respiratory	Carcinogen	Reproductive hazard	Sensitizer	Other	Ingestion
Methylcyclopentadiene dimer	○	✓	✓	✓	✓	✗	✗	✗	✓	✓	✓
Diethylene glycol diethyl ether	△	✓	✓	△	✓	✓	✓	✓	✓	✓	✓
Sodium	✓	✗	✓	✗	✗	✗	✗	✓	✓	✓	✗
Sodium cyclopentadienylide	✓	✗	✓	✓	✗	✓	✓	✓	✓	✓	✓
Hydrogen	✗	△	✓	✓	✓	✓	✓	✓	✓	✓	✓

Legend: ✓ Safe △ Caution ○ Warning ✗ Danger

The tool also provides web-links to aid the PPE selection process.

The following links can guide the PPE selection process:
https://www.osha.gov/Publications/osha3151.pdf
https://ehs.ucmerced.edu/researchers-labs/ppe/selection
https://www.era-environmental.com/blog/personal-protective-equipment-how-to-read-an-sds
https://www.usf.edu/administrative-services/environmental-health-safety/documents/hazard_control_ppe_guide.pdf
https://www.ehs.washington.edu/system/files/resources/ppeguidelines.pdf
https://www.purdue.edu/ehps/rem/laboratory/Personal/PPE/gloveselection.pdf

Note: These links provide a general guideline for PPE selection based on the nature of the chemical. It is required that the user does thorough research before selecting the appropriate PPE for their system.

13. The tool also generates a chemical compatibility matrix by submitting a query (with all the chemical names and their CAS IDs) to the CAMEO Chemicals online tool. The reactivity predictions are shown in the form of a pair-wise compatibility chart wherein each interaction is marked either as Incompatible, Caution, or Compatible.

Cameo Matrix

	Methylcyclopentadiene dimer		
Diethylene glycol diethyl ether	**Caution** △ Potentially hazardous	Diethylene glycol diethyl ether	
Sodium	**Incompatible** Generates heat Polymerization hazard	**Incompatible** Corrosive Flammable Generates heat	Sodium
Hydrogen	**Caution** △ Generates heat Potentially hazardous	**Compatible**	**Incompatible** Explosive Generates heat Intense or explosive reaction

Note: Currently, the analysis is limited to pair-wise interaction between each chemical. Additional interactions (ternary and above) resulting from the mixture are not predicted by CAMEO Chemicals. Also, RHEACT generates the chemical compatibility matrix based on the database available within CAMEO Chemicals. For reagents not available in CAMEO, the tool returns the compatibility matrix for all the reagents except the ones unavailable. More details about the prediction and estimation of the compatibility can be found on the Cameo website (https://cameochemicals.noaa.gov/).