

## RHEACT Quick Start Guide

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- 1) Go to <https://rheact.github.io/#/>
- 2) In the "Components" tab under Project,
  - a) Upload all SDS files in their respective areas (Reactant, Product, Diluent).
    - i) All SDS must be from Millipore Sigma (Sigma Aldrich, Supelco, Millipore, SAFC). There is a search bar at the top of this page which allows you to query Sigma Aldrich's website for any SDS file. Download the SDS. It is recommended (but not required) that you rename the SDS as the "product#\_ChemicalName" so that you can easily identify which specific SDS on your local computer corresponds to the product. There are typically minor variations in SDS of the same chemical but different product#s. If one SDS does not work for a given chemical, retry with another SDS from a different product# for the same chemical or enter the details manually.
    - ii) For manual entry (assuming failed SDS upload from MilliporeSigma or if you only have SDS from a different source), click "Add Component manually without uploading SDS". Then underneath the Actions, press the edit button. Enter the necessary details from the SDS that you have. Enter H numbers on the same line separated by a comma (e.g. HXXX, HYYY, HZZZ). Enter the rest of the numbers without any unit. Ensure the units of the numbers matches those in brackets. If you don't have some data, enter "No data available" without the quotation marks.
- 3) In the "Details" tab under Project,
  - a) This information is optional and does not impact the calculation.
  - b) The "Project Title" will be the file name of the .rheact file generated by using the "Save" functionality on the "Report" tab in the "Operation" section.
  - c) You can enter the balanced equation using normal text. (e.g.  $A + B \rightarrow C$ )
- 4) In the "Parameters" tab under Operation,
  - a) First, Enter the operating temperature.
    - i) Units can be changed by clicking on the grey box to the right of where numerical values are entered temperature.
  - b) Enter the pressure and heat of reaction.
    - i) Units can be changed by clicking on the grey box to the right of where numerical values are entered for each parameter.
    - ii) We suggest entering the heat of the reaction at operating temperature if you have an easy and accessible way to calculate it or measure it (e.g. by calorimetry). However, since the enthalpy of reaction will only change slightly (typically <20%) with elevated temperatures (relative to the standard conditions), you should be fine to enter the reaction enthalpy calculated by Hess's law using the standard enthalpy of formations (at 298 K and 1 bar). Just make sure that you are using the correct states

(gas, solid, liquid) of your system for the  $\Delta H_{rxn}$  calculations. One can get enthalpy of formation data (and in some cases, enthalpy of reaction) from NIST (<https://webbook.nist.gov/>) or engineering toolbox ([https://www.engineeringtoolbox.com/material-properties-t\\_24.html](https://www.engineeringtoolbox.com/material-properties-t_24.html))

- c) Select the basis for the heat of reaction.
  - i) **Make sure to click “Change Basis” so that your selection is saved.**
  - ii) This basis refers to the normalization for the heat of reaction. For example, a heat of reaction with the basis selected as “total reaction mass” will have units of energy per total reaction mass, whereas if the basis is selected as any specific component (typically limiting reactant), the heat of reaction will have units of energy per amount (mass or mole) of that component.
- d) Enter the mass fractions of all components. You can enter the mass fractions at the initial conditions (batch system) or inlet conditions (flow system). Do not forget to enter the mass fraction of your diluent (e.g. water or Nitrogen gas). If you forgot your diluent, go back to the components tab and upload an SDS or enter information for diluent.
- e) Enter either the mixture heat capacity (“Cp (mix)”) that you have calculated or measured yourself or the component heat capacities that you have obtained.
  - i) A mixture heat capacity will be estimated by the program if all component heat capacities and mass fractions are entered and if the “enter Cp of mixture manually” is unchecked. Multiple units are available for mixture heat capacity.
    - (1) Some heat capacities for ~250 chemicals can be estimated by using parameters from NIST which are stored in the back end of RHEACT. These estimations will be for **liquid phase compounds only**. These parameters are not available for every compound, so some may be left blank. Click “Estimate Cp” only for liquid components. If you change the temperature, make sure to click estimate Cp to update the calculation.
    - (2) For gas-phase compounds, the component heat capacities, if desired, will have to be manually entered. Currently, the program has no way of determining on its own whether a component is a liquid or a gas. You can go to the NIST Webbook or Engineering toolbox to get these component heat capacities.
  - ii) The only units available for component heat capacities is cal/g. See addendum for how RHEACT performs a weight average of component heat capacity to calculate mixture heat capacity.
  - iii) Entering a mixture heat capacity will override any component heat capacities.
  - iv) If the component heat capacities haven’t been estimated, make sure you’ve entered a temperature in the parameters tab.
  - v) At the bottom of the page, in the table containing “component name”, “Mass fraction”, etc., as column headers, you have the option to de-select

components. This will neglect that component during calculation of a mixture heat capacity from the component heat capacities (see calculations in addendum below). Mass fractions will be rescaled appropriately. This will not affect other calculations in the program.

- f) Details of any important side reactions can also be entered at the bottom of the screen in the "Side Reactions" box. Some reactions typically have some decomposition or over-oxidation side reactions that can onset at varying conditions. Ensure that you perform appropriate literature searches for any possible side reactions.
- 5) In the "Report" tab in the "Operation" section,
- a) Click on the "Click here to generate report" button at the top of the screen.
    - i) This will generate an estimate of the adiabatic temperature rise for the system, as well as a list of hazards associated with each chemical, a chemical compatibility matrix, and a hazard matrix. There are also several resource links at the bottom of this page.
  - b) The report can be saved by selecting the "Print" button at the top left of the screen.
- 6) In the "Questionnaire" tab,
- a) Select "Yes" for any situations which apply to your specific system.
- 7) In the "Report" tab in the "PPE" section,
- a) This automatically updates based on the uploaded SDS files and your selections in the "Questionnaire" tab.
  - b) The typical minimum PPE required for any lab work is listed at the top of the page.
  - c) The additional PPE recommendations based on your selections in the "Questionnaire" tab are listed below the minimum PPE.
  - d) The SDS recommendation section (section 8.2) from each uploaded SDS are then displayed one after another.
  - e) The report can be saved by using your computer's print screen (Ctrl + P) or screenshot functionality.
- 8) Finally, you can save your work as a .rheact file. Click Save and enter the file name (without extension) and file type will be RHEACT File.

### **Details on Adiabatic Temperature Change calculations ( $\Delta T_{ad}$ )**

1-4 are calculations for the  $\Delta T_{ad}$  when all required inputs are in cal, g, °C;

5-6 are unit conversions that convert other input units (e.g. J, mol, °F) to cal, g, °C

7 is rescaling mass fraction

#### **1) Final temperature**

- a) Variable:  $T_{final}$
- b) Equation:  $T_{final} = T_{initial} + \Delta T_{ad}$
- c) Desired Units for variable: °C
- d) Pre-requisites
  - i) Initial temperature,  $T_{initial}$  [=] °C
  - ii) Adiabatic temperature change,  $T_{ad}$  [=] °C
    - Note "[=]" means units while "=" means equation

#### **2) Adiabatic temperature change**

- a) Variable:  $\Delta T_{ad}$
- b) Equation:  $\Delta T_{ad} = \frac{-\Delta H_{rxn}}{C_{p,mix}} * X_i$
- c) Desired Units for variable: °C [=]  $\frac{cal}{g_i} * \frac{g_{total}}{cal} * \frac{g_i}{g_{total}}$
- d) Pre-requisites
  - i) Heat of reaction,  $\Delta H_{rxn}$  [=] cal/g<sub>i</sub>  
Where i is the basis; **g<sub>i</sub>** can either be g<sub>A</sub> or g<sub>total</sub>
    - (a) Where g<sub>A</sub> is the mass of some species A (if the basis of  $\Delta H_{rxn}$  is an individual component).
    - (b) Where g<sub>total</sub> is the total reaction mass (if the basis of  $\Delta H_{rxn}$  is the total reaction mass).
  - ii) Mixture heat capacity,  $C_{p,mix}$  [=] cal/g<sub>total</sub>/°C
  - iii) Mass fraction of basis for  $\Delta H_{rxn}$ ,  $X_i$  [=] g<sub>i</sub>/g<sub>total</sub>  
**g<sub>i</sub>** can either be g<sub>A</sub> or g<sub>total</sub>
    - (a) Where g<sub>A</sub> is mass of some species A (if the basis of  $\Delta H_{rxn}$  is an individual component)  $\Rightarrow X_i = X_j$
    - (b) Where g<sub>total</sub> is the total reaction mass (if the basis of  $\Delta H_{rxn}$  is the total reaction mass).  $\Rightarrow X_i = 1$

#### **3) Heat capacity of the mixture**

- a) Variable:  $C_{p,mix}$
- b) Equation:  $C_{p,mix} = \sum_j^{# components} X_j * C_{p,j}$ 
  - i) Ignore calculation if  $C_{p,mix}$  specified by the user
- c) Desired Units for variable: cal/g<sub>total</sub>/°C
- d) Pre-requisites
  - i) Component heat capacity,  $C_{p,j}$  [=] cal/g<sub>j</sub>/°C
    - (1) Can be specified by the user OR calculated from information in the database (**only for liquid phase**)
  - ii) Mass fraction of species j,  $X_j$  [=] g<sub>j</sub>/g<sub>total</sub> (this is unitless)
    - (1) Mass fraction of species is provided by user but not calculated

#### **4) Component heat capacity**

- a) Variable:  $C_{p,j}$
- b) Equation (for liquid  $C_p$  only):  $C_{p,j} = A + B*T$

- i) Can also be specified by the user (no need to calculate)
  - ii) Do not perform this calculation if not liquid phase; instead user has to provide component  $C_{p,j}$  for gas phases (This has not been implemented yet)
- c) Desired Units for variable:  $\text{cal/g}_j/^{\circ}\text{C}$
- d) Pre-requisites
  - i) Heat capacity constant 1,  $A [=] \text{cal/g}_j/^{\circ}\text{C}$ 
    - (1) Found in back-end database (for liquid phase only)
  - ii) Heat capacity constant 2,  $B [=] \text{cal/g}_j/^{\circ}\text{C}^2$ 
    - (1) Found in back-end database (for liquid phase only)
  - iii) Operating temperature,  $T [=] ^{\circ}\text{C}$ 
    - (1) Specified by user

## UNIT CONVERSIONS

### 5) Heat of reaction

- a) Variable:  $\Delta H_{\text{rxn}}$
- b) Desired units for variable:  $\text{cal/g}_i$
- c) Unit conversion strategy:
  - If** (units are  $\text{cal/g}_i$ )
  - { Do nothing }
  - Else if** (other units)
  - { Used specified unit conversion }

(y is  $\Delta H_{\text{rxn}}$  in units of  $\text{cal/g}$ )

(x is original value of  $\Delta H_{\text{rxn}}$  in original units)

(M.W. is the molecular weight of the basis for  $\Delta H_{\text{rxn}}$ )

**Note:** Since, there is no such thing as per mole of reaction, if the user selects any of the energy per mole units, they cannot select total reaction mass anymore as basis of heat of reaction.

### 6) Heat capacity

- a) Variable:  $C_{p,\text{mix}}$
- b) Desired units for variable:  $\text{cal/g}_{\text{total}}/^{\circ}\text{C}$
- c) Unit conversion strategy:
  - If** (units are  $\text{cal/g}_{\text{total}}/^{\circ}\text{C}$ )
  - { Do nothing }
  - Else if** (other units)
  - { Use specified unit conversion }

### Heat capacity

- d) Variable:  $C_{p,j}$
- e) Desired units for variable:  $\text{cal/g}_j/^{\circ}\text{C}$
- f) Unit conversion strategy (currently, only flexible units are allowed for  $cp_{\text{mix}}$ ):
  - If** (units are  $\text{cal/g}_j/^{\circ}\text{C}$ )
  - { Do nothing }
  - Else if** (units are  $\text{J/g}_j/^{\circ}\text{C}$ )
  - { Use unit conversion }

(y is  $\Delta H_{\text{rxn}}$  in units of  $\text{cal/g}$ )

(x is original value of  $\Delta H_{\text{rxn}}$  in original units)

(M.W. is the molecular weight of the basis for  $\Delta H_{\text{rxn}}$ )

**Note:** there is no such thing as per mole of reaction. Thus if the user selects any of the energy per mole units, they cannot select total reaction mass anymore as basis of heat of reaction.

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### RESCALING MASS FRACTIONS

#### 7) Rescaling mass fractions in the case of some components being neglected due to unavailability of Cp data or if they are minor components in the mixture (for heat capacity of reaction mass calculation only)

Rescale each mass fraction,  $x_i$ , by dividing  $x_i$  by the sum of the remaining mass fractions

$$\text{a) Equation: } C_{p,\text{mix}} = \sum_{j \neq m}^{\text{\# components not neglected}} \frac{x_j}{\sum_{k \neq m} x_k} * C_{p,j}$$

Where  $m$  is the neglected component(s)

b) Units for variable [=] cal/g<sub>total</sub>/°C

**Example:** If  $x_A = 0.33$ ,  $x_B = 0.33$ , and  $x_C = 0.34$ , and  $x_C$  is neglected,  $x_A$  and  $x_B$  will be rescaled as  $0.33/(0.33+0.33)=0.5$  for only the cp mix calculations. The rest of the code after will still use the unscaled mass fraction

#### **Potential Future feature:**

Consistency check: Prompt user to select if reaction is endothermic or exothermic reaction.

Then check if the sign is consistent with what they entered

Allow for mole fraction ( $y_j$ ) input and convert to mass fraction

$$X_j = \frac{MW_j * y_j}{\sum_k MW_k * y_k}$$

### **UNIT CONVERSIONS**

	<b>Unit</b>	<b>Conversion to base unit used in calculations</b>
<b>Temperature</b>	°C	Used in calculations
	K	$x - 273.15$
	°F	$(x - 32) * 5/9$
<b>Pressure</b>	<b>bar</b>	Used in calculations
	kPa	$x/100$
	atm	$x*1.01325$
	Torr (mmHg)	$(x/760)*1.01325$
	psia (absolute)	$(x/14.6959)*1.01325$
	<b>psig (gauge)</b>	$(1 + x/14.6959)*1.01325$
<b>Heat of Reaction (can take positive or negative values). Usually in per g or per mol of specified substance (usually major product or limiting reactant) in a balanced reaction stoichiometry</b>	<b>cal/g</b>	Used in calculations
	kcal/g	$x*1000$
	kJ/g	$(x/4.184)*1000$
	btu/lb	$(x*252.164)/453.592$
	kcal/mol	$x*1000/M.W.$
	kJ/mol	$(x/4.184)*1000/M.W.$
<b>Heat capacity</b>	<b>cal/g/°C</b>	Used in calculations
	kcal/g/°C	$x*1000$
	kJ/g/°C	$(x/4.184)*1000$
	kcal/mol/°C or kcal/mol/K	$x*1000/M.W.$
	kJ/mol/°C or kJ/mol/K	$(x/4.184)*1000/M.W.$