Chemical Kinetics Library

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CS 207 project

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Contents

Chapter 1

Introduction

Chemical kinetics is the study of rates of chemical processes. Different experiment settings and conditions, such as temperature or concentration of reactants, can influence the speed of chemical reactions as well as the yield of products.

The library *chemkin* we wrote aims to make such calculation in chemical kinetics easier.

1 Reaction Rate Coefficients

There are several kinds of reaction rates, and here we are introducing three types of reaction rate coefficients:

1.1 Constant Reaction Rate Coefficient

$$k_{const} = k$$

1.2 Arrhenius Reaction Rate Coefficient

$$k_{arr} = A \exp\left(-\frac{E}{RT}\right)$$

1.3 Modified Arrhenius Reaction Rate Coefficient

$$k_{modarr} = AT^b \exp\left(-\frac{E}{RT}\right)$$

Note:

- The Arrhenius prefactor A is strictly positive.
- The modified Arrhenius parameter b must be real.
- R=8.314 is the ideal gas constant. It should never be changed (except to convert units)
- The temperature T must be positive (assuming a Kelvin scale)

2 Progress Rate and Reaction Rate

Consider a system consisting of N species undergoing M irreversible, elementary reactions of the form

$$\sum_{i=1}^{N} \nu'_{ij} \mathcal{S}_i \text{ -> } \sum_{i=1}^{N} \nu''_{ij} \mathcal{S}_i, \qquad \text{j} = 1, \ldots, \text{M}$$

the rate of change of specie i (the reaction rate) can be written as

$$f_i = \sum_{j=1}^{M} \nu_{ij} \omega_j, \qquad \text{i} = 1, \ldots, \text{N}$$

where the progress rate for each reaction is given by

$$\omega_j = k_j \prod_{i=1}^{N} x_i^{\nu'_{ij}}, \qquad \text{j} = 1, \ldots, \text{M}$$

Symbol Notes

Symbol	Meaning
$\mathcal{S}_i$	Chemical symbol of specie i
ν'_{ij}	Stoichiometric coefficients of reactants
ν''_{ij}	Stoichiometric coefficients of products
N	Number of species in system
M	Number of elementary reactions
f_i	Rate of consumption or formation of specie i (reaction rate)
ω_j	Progress rate of reaction j
x_i	Concentration of specie i
k_j	Reaction rate coefficient for reaction j

Chapter 2

Installation

At the moment, this is a partially implemented Module. Thus it can be downloaded by downloading a zip of the module from github.

- Download instruction:
  - Go to https://github.com/cs207G6/cs207-FinalProject
  - Click the clone or download button on the right side.
  - Click Download as zip!
- Using the Zip:
  - Unzip the file.
  - Import the module into your code
  - Now you can use the module.

  See "Basic Usage and Examples" below for how to use the module.

Chapter 3

Basic Usage and Examples

- Get Progress Rate

```
import chemkin

data_parser = chemkin.DataParser() # create a data parser class
reaction_data = data_parser.parse_file("data/rxns.xml") # parse the data
    file and return an instance of ReactionData class
progress_rates = reaction_data.get_progress_rate([1,2,3,4,5,6],100)
print(progress_rates)
```

  where the arguments of *get_progress_rate* are chemical concentrations for each of the six species, ordered as specified in the *.xml* file ([1,2,3,4,5,6] in the example above) and reaction temperature (100 in the example above).

  output:

```
[   1.06613928e-26    1.85794997e-09    1.20000000e+04]
```

  where each value above is corresponding to the progress rate of each elementary reaction.

- Get Reaction Rate

```
reaction_rates = reaction_data.get_reaction_rate(progress_rates)
print(reaction_rates)
```

  where the arguments of *get_reaction_rate* is the result of *get_progress_rate* we got above. output:

```
[   1.20000000e+04   -1.85794997e-09   -1.20000000e+04   -1.20000000e+04
    1.20000000e+04   -1.06613928e-26]
```

  where each value above is the reaction rate of each species in the order given in the *.xml* file.

- Get Reaction Rate Coefficient

```
ks = reaction_data.get_k(20)
print(ks)
```

  where the argument of *get_k* is the temperature (20 in the example above) of the reaction. output:

```
[   1.15383261e-176    3.35659594e-067    1.00000000e+003]
```

  where each value above is the reaction rate coefficient calculated based on the type specified in the *.xml* file.