

CHEMICAL KINETICS LIBRARY

HARVARD UNIVERSITY

CS 207 PROJECT

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Contents

| | | |
|----------|--|----------|
| 1 | Introduction | 2 |
| 1 | Reaction Rates | 2 |
| 1.1 | Constant Reaction Rate Coefficient | 2 |
| 1.2 | Arrhenius Reaction Rate Coefficient | 2 |
| 1.3 | Modified Arrhenius Reaction Rate Coefficient | 2 |
| 2 | Progress Rate and Reaction Rate | 2 |
| 2 | Installation | 3 |
| 3 | Basic Usage and Examples | 4 |

Chapter 1

Introduction

Chemical kinetics is the study of chemical reactions with respect to reaction rates, effect of various variables, re-arrangement of atoms, formation of intermediates etc.

1 Reaction Rates

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

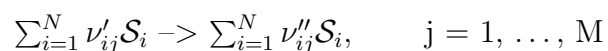
$$k_{modarr} = AT^b \exp\left(-\frac{E}{RT}\right)$$

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



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

$$f_i = \sum_{j=1}^M \nu_{ij} \omega_j, \quad i = 1, \dots, N$$

where the progress rate for each reaction is given by

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

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

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

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

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

```
1 [ 1.20000000e+04 -1.85794997e-09 -1.20000000e+04 -1.20000000e+04
2  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

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

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

```
1 [ 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.