Chemical Kinetics Library

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CS 207 project

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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

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

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

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

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.