# The CHEMKIN User Manual

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1 Introduction

CHEMKIN is a Python library that computes the reaction rates of all species participating in a system of elementary, irreversible reactions.

1.1 Key chemical concepts and terminology

A system consisting of M elementary reactions involving N species has the general form

$$\sum_{i=1}^{N} \nu'_{ij} \mathcal{S}_i \longrightarrow \sum_{i=1}^{N} \nu''_{ij} \mathcal{S}_i, \qquad j = 1, \ldots, M. \tag{1}$$
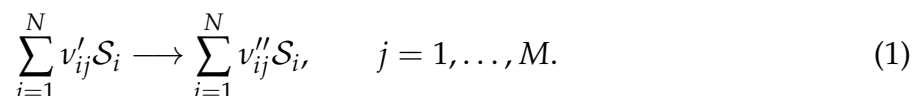
$\mathcal{S}_i$ is the ith specie in the system, ν'_{ij} is its stoichiometric coefficient (dimensionless) on the reactants side of the jth reaction, and ν''_{ij} is its stoichiometric coefficient (dimensionless) on the product side for the jth reaction.

Each specie is characterized by a concentration x_i, in units of [mol/vol]. The **reaction rate** of each specie is the time rate of change of its concentration, $\frac{dx_i}{dt}$. The reaction rate is usually represented by the symbol f_i, such that

$$f_i = \sum_{j=1}^{M} (\nu''_{ij} - \nu'_{ij})\omega_j = \sum_{j=1}^{M} \nu_{ij}\omega_j, \qquad i = 1, \ldots, N. \tag{2}$$

ω_j is the **progress rate** of the jth reaction,

$$\omega_j = k_j \prod_{i=1}^{N} x_i^{\nu'_{ij}}, \qquad j = 1, \ldots, M. \tag{3}$$

1.2 Features

The package can solve for the reaction rates of a system with an arbitrary number of species and elementary reactions. The reaction rate coefficient k for each reaction is assumed to take one of three possible forms:

1. $k = \text{constant}$

2. Arrhenius: $k = A \exp(-\frac{E}{RT})$, where A is the pre-factor, E is the activation energy, R is the universal gas constant, and T is the temperature.

3. Modified Arrhenius: $k = AT^b \exp(-\frac{E}{RT})$, where A is the pre-factor, E is the activation energy, R is the universal gas constant, T is the temperature, and b is the temperature scaling parameter.

1.2.1 Input

1.2.2 Output

1.2.3 Installation

Describe where the code can be found and downloaded. Tell the user how to run the test suite. We are not releasing this code as a package yet, but when we do that this section will include instructions how how to install the package.

2 Basic Usage and Examples

2.1 Input format

Provide a few examples on using your software in some common situations. You may want to show how the code works with a small set of reactions.