

# Problems of Chemical Kinetics using WolframAlpha.

In these problems, you have to:

- Write the *rate matrix* (**K** matrix).
- Find the eigenvalues of the **K** matrix using the `Eigenvalues[]` function of *WolframAlpha*.
- Find the eigendecomposition of the **K** matrix using the `Diagonalize[]` function of *WolframAlpha*. Watch the cases (if any) when the **K** matrix is not diagonalizable.
- Find the matrix exponential  $e^{Kt}$  using the `MatrixExp[]` function of *WolframAlpha*. Make sure you are really calling `MatrixExp[]` rather than `Exp[]`.
- Multiply the resulting  $e^{Kt}$  matrix by an initial-concentration vector. Consider the case when only one reactant [A] is present ( $[A]_0 \neq 0$ ,  $[B]_0 = [C]_0 = \dots = 0$ ) as well as the case when all reactants are present at the beginning:  $[A]_0 \neq 0$ ,  $[B]_0 \neq 0$ ,  $[C]_0 \neq 0, \dots$  *Hint*: this matrix-vector multiplication and the previous step ( $e^{Kt}$  matrix calculation) can be done by *WolframAlpha* in a single step. Figure out yourself how.
- If possible, solve the original system of kinetic equations for the given initial concentrations directly, using the `Solve[]` function of *WolframAlpha*. Compare the results with those obtained previously by the matrix method.

The systems to do are the following ones:

1.  $A \rightarrow B \rightarrow C$  with different rate constants  $k_1 \neq k_2$ .
2.  $A \rightarrow B \rightarrow C$  with identical rate constants  $k_1 = k_2 = k$ .
3.  $A \rightleftharpoons B \rightarrow C$  with rate constants  $k_1, k_{-1}, k_2$ .
4.  $A \rightleftharpoons B \rightarrow C$  with identical rate constants  $k_1 = k_{-1} = k_2 = k$ .
5.  $A \rightarrow B \rightleftharpoons C$  with rate constants  $k_1, k_2, k_{-2}$ .
6.  $A \rightarrow B, A \rightleftharpoons C$  with rate constants  $k_1, k_2, k_{-2}$ .
7.  $A \rightarrow B \rightarrow C \rightarrow D$  with different rate constants  $k_1 \neq k_2 \neq k_3$ .
8.  $A \rightarrow B \rightarrow C$  with identical rate constants  $k_1 = k_2 = k_3 = k$ .