# Theme 1: Markov model

Markov chains can be used to solve problems in chemistry, as here in kinetic chemistry.

## Part I

Suppose we have a homogenous mixture of two chemical components A and B reacting with each other. At the start of the reaction, there is 1.0 mole of component A and 0.2 moles of component B.

Each minute 75% of moles of A are converted to B, and 5% of B are converted to A. We would like to know the following ***(PS: Do not start until you read the rest of the task description!)***

1. How many moles of A and B are present in the mixture at one minute after the process has started?
2. And how much after two minutes?
3. And after 10 minutes?
4. What would be the final composition/stable state/stable equilibrium?

When you solve the task, please consider the following:

1. How to write/draw the model on paper using mathematics/figures? Is there any way to make use of vectors and matrices?
2. How do you code/write the model using Matlab or other tools like Octave online?
3. How many iterations did we perform before we thought we can guess the final state/stable solution/equilibrium?

## Part II

1. In what other way(s) could we calculate the equilibrium? Is there any way to make use of vectors and matrices?
2. Let's have a look at the values we obtained doing iterations. We shall notice that the distances between the states in neighbouring minutes differ, that is, are decreasing in time.

Now imagine that we would like to know how many moles of A and B are present in the mixture after, say, 90 or 150 seconds (1.5 and 2.5 minutes). How could we calculate the state at any time "between the whole minutes"?

# Appendix: Matrix-syntax in Matlab

Please use <http://octave-online.net> if you don’t have Matlab installed on your computer

Example of a 2x2 matrix in Matlab syntax: A = [1 2; 3 4]

Example of a column vector: x = [3;4]