Evolving Python coding in lab classes to enhancing student understanding of key kinetic concepts in tutorials

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`https://github.com/bjmorgan/ViCEPHEC17`

The following are questions taken from our first year tutorials. Model answers are shared to tutors and provided to students on the Monday the week following the tutorial.

We propose that a deeper level of student understanding is provided by engagement with provided coding models.

1.

For the following reaction derive an expression for the steady state of the intermediate.

$$\mathrm{A} \underset{k_{-1}}{\overset{k_1}{\leftrightarrows}} \mathrm{B} \overset{k_2}{\rightarrow} \mathrm{C}$$

Under what conditions does the steady state approximation hold?

`Notebook: SSA simulation.ipynb`

2.

One of the ways that ozone is destroyed in the upper atmosphere is by reaction with halogen gases such as chlorine. Part of the reaction pathway is (treat equations as elementary):

$$\mathrm{Cl_2} \underset{k_{-1}}{\overset{k_1}{\leftrightarrows}} \mathrm{2Cl^\bullet}$$

$$\mathrm{Cl^\bullet + O_3} \overset{k_2}{\rightarrow} \mathrm{ClO^\bullet + O_2}$$

$$\mathrm{ClO^\bullet + O_3} \overset{k_3}{\rightarrow} \mathrm{Cl^\bullet + 2O_2}$$

(i) Write an expression for the rate of consumption of Cl_2.
(iii) Write an expression for the rate of production of ClO•
(iv) Write an expression for the rate of production of Cl•

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Notebook: This question does not have an associated notebook, but is left as an open
programming exercise, where interested students can extend the approach from the SSA
simulation example.
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3.

For the following pair of reversible reactions:

$$\mathrm{A} \underset{k_{-1}}{\overset{k_1}{\leftrightarrows}} \mathrm{B} \qquad \mathrm{A} \underset{k_{-2}}{\overset{k_2}{\leftrightarrows}} \mathrm{C}$$

deduce and expression for the ration of [B]/[C] at equilibrium.

If the rate constants for the various processes are:

$k_1 = 1\ \mathrm{s}^{-1}$
$k_{-1} = 10^{-7}\ \mathrm{s}^{-1}$
$k_2 = 10^{-2}\ \mathrm{s}^{-1}$
$k_{-2} = 10^{-12}\ \mathrm{s}^{-1}$

which of the two products would be under “thermodynamic control” and which under “kinetic control”?

`Notebook: Competing Equilibria.ipynb`

4.

(i) Sketch the velocity probability distribution of a light, medium and heavy molecule at a single temperature.

(ii) Which (light, medium, heavy) has the most kinetic energy for 1 mole of gas?

(iii) How would these distributions change if the temperature was increased?

(iv) Describe what is meant by each of the following terms:

- mean speed
- most probable speed
- root mean squared speed

Which is highest for molecular hydrogen at 298 K?

`Notebook: Maxwell-Boltzmann.ipynb`

All of the Python materials from Dr Benjamin Morgan can be found at
https://github.com/bjmorgan/ViCEPHEC17