As an example of a simple chemical reaction that is in fact quite complicated, we consider hydrogen and oxygen which combine to make water. The basic process is summarized as

$$2\text{H}_2 + \text{O}_2 \rightarrow 2\text{H}_2\text{O}$$

where the 2’s appearing in front of $\text{H}_2$ and $\text{H}_2\text{O}$ have been added so that the total number of atoms balance on either side of the arrow.

However this is not how the reaction actually proceeds - the fundamental inorganic chemical reaction involves two reactants combining into one product or one reactant falling apart into two products ($A + B \rightarrow C$ or $C \rightarrow A + B$). We will consider a simplified model for this process, which includes the following basic reactions:

\begin{align*}
\text{H}_2 + \text{O}_2 & \rightarrow 2\text{OH} & \text{Rate} = k_0[\text{H}_2][\text{O}_2], \\
\text{OH} + \text{H}_2 & \rightarrow \text{H}_2\text{O} + \text{H} & \text{Rate} = k_1[\text{OH}][\text{H}_2], \\
\text{H} + \text{O}_2 & \rightarrow \text{OH} + \text{O} & \text{Rate} = k_2[\text{H}][\text{O}_2], \\
\text{O} + \text{H}_2 & \rightarrow \text{OH} + \text{H} & \text{Rate} = k_3[\text{O}][\text{H}_2], \\
\text{H} + \text{H} & \rightarrow \text{H}_2 & \text{Rate} = k_4[\text{H}]^2,
\end{align*}

where note that all $k_i > 0$. Thus we have five species taking part in five reactions; using the Law of Mass Action, we will write down five coupled ODEs in terms of five unknowns representing the concentrations of the various chemical species. Note that a fuller model of this process, the Baldwin-Walker mechanism, has 32 reactions!

We will define the concentration variables: $X = [\text{H}_2]$, $Y = [\text{O}_2]$, $Z = [\text{H}_2\text{O}]$, $W = [\text{OH}]$, $U = [\text{H}]$, and $V = [\text{O}]$. The 5 reactions can then be translated into:

\begin{align*}
\frac{dX}{dt} &= -k_0XY - k_1XW - k_3XV + k_4U^2, \\
\frac{dY}{dt} &= -k_0XY - k_2UY, \\
\frac{dZ}{dt} &= k_1XW, \\
\frac{dW}{dt} &= 2k_0XY - k_1XW + k_2UY + k_3XV, \\
\frac{dU}{dt} &= k_1XW - k_2UY + k_3XV - k_4U^2, \\
\frac{dV}{dt} &= k_2UY - k_3XV,
\end{align*}
Notice that all individual atoms ($H$ and $O$) are conserved; they are neither created nor destroyed, just shuffled around. The net result of this is that

\[
\frac{dX}{dt} + \frac{dY}{dt} + \frac{dZ}{dt} + \frac{dW}{dt} + \frac{dU}{dt} + \frac{dV}{dt} = 0
\]

You should check this. What is the quantity which is conserved?

Note that because of this conservation law, we don’t need to solve for all five concentrations - obtaining 4, we can add them up and determine the fifth...

We will discuss methods of simplifying these ODEs in class. Later we will treat such systems qualitatively in state space, and also numerically.