# Mathematical Oncology
Reaction diffusion models: Derivation of reaction terms

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Through two basic examples, we gain an initial understanding of how to derive the (mathematical) reaction terms commonly encountered in Ordinary and Partial Differential Equations. For clarity of presentation, these examples are derived from chemical reactions rather than biological contexts.

Chemical vs Mathematical Reactions — Case I. Consider at first the chemical reaction involving H (Hydrogen) and I (Iodine):

$$H_2 + I_2 \rightarrow 2HI$$
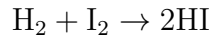
The rate ν at which the reaction takes place is given in two different approaches:

- from the stoichiometry of the chemical reaction, i.e. mass conservation principle expressed through the rate of change of the concentrations of the corresponding chemical substances (denoted here by [ ])

$$\nu = -\frac{d[H_2]}{dt} = -\frac{d[I_2]}{dt} = \frac{1}{2}\frac{d[HI]}{dt}$$

  The $\pm$ sign indicates the production or depletion of the corresponding chemical substance along the "proper" direction of the chemical reaction.

- through experimental observations and measurements, e.g.

$$\nu = k[H_2][I_2]$$

  (or more complicated as we can see in the following example). This is also called *Observed Rate Equation* or <u>Reaction Rate Constant</u>.

When combined, the above approaches yield the following mathematical reactions (!):

$$\begin{cases} -\dfrac{d[H_2]}{dt} = k[H_2][I_2] \\ -\dfrac{d[I_2]}{dt} = k[H_2][I_2] \\ \dfrac{1}{2}\dfrac{d[HI]}{dt} = k[H_2][I_2] \end{cases} \implies \begin{cases} \dfrac{d[H_2]}{dt} = -k[H_2][I_2] \\ \dfrac{d[I_2]}{dt} = -k[H_2][I_2] \\ \dfrac{d[HI]}{dt} = 2k[H_2][I_2] \end{cases}$$

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Chemical vs Mathematical Reactions — Case II. Consider the chemical reaction involving H (Hydrogen) and Br (Bromine):

$$H_2 + Br_2 \rightarrow 2HBr$$
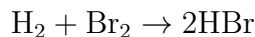
As with the previous example, the rate of the chemical reaction is given by two different approaches: stoichiometry and experimental observations and measurements, i.e.

- stoichiometry of the chemical reaction:

$$\nu = -\frac{d[H_2]}{dt} = -\frac{d[Br_2]}{dt} = \frac{1}{2}\frac{d[HBr]}{dt}$$

- through experimental observations and measurements (hands on), e.g.

$$\nu = k\frac{[H_2][Br_2]^{1/2}}{1 + \tilde{k}\frac{[HBr]}{[Br_2]}}$$

The more complicated result, as opposed to the first example, is just an indication of what could be experimentally observed. (Disclaimer: this reaction rate is completely fictional!)

Never the less, combined, the above yield the following reaction equations:

$$\begin{cases} -\dfrac{d[H_2]}{dt} = k\dfrac{[H_2][Br_2]^{1/2}}{1 + \tilde{k}\frac{[HBr]}{[Br_2]}} \\[2ex] -\dfrac{d[Br_2]}{dt} = k\dfrac{[H_2][Br_2]^{1/2}}{1 + \tilde{k}\frac{[HBr]}{[Br_2]}} \\[2ex] \dfrac{1}{2}\dfrac{d[HBr]}{dt} = k\dfrac{[H_2][Br_2]^{1/2}}{1 + \tilde{k}\frac{[HBr]}{[Br_2]}} \end{cases}$$

or, after using the notations $[H_2] = h$, $[Br_2] = b$, and $[HBr] = r$

$$\begin{cases} \dfrac{dh}{dt} = -k\dfrac{hb^{1/2}}{1 + \tilde{k}\frac{r}{b}} = k\dfrac{hb^{3/2}}{b + \tilde{k}r} \\[2ex] \dfrac{db}{dt} = -k\dfrac{hb^{1/2}}{1 + \tilde{k}\frac{r}{b}} = k\dfrac{hb^{3/2}}{b + \tilde{k}r} \\[2ex] \dfrac{dr}{dt} = 2k\dfrac{hb^{1/2}}{1 + \tilde{k}\frac{r}{b}} = 2k\dfrac{hb^{3/2}}{b + \tilde{k}r} \end{cases}$$