Two different types of kinetics, where the initial rate increases faster or slower than the reactant concentration, can coexist on bell-shaped kinetic dependencies

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Online Resource 1

Calculating the Jacobian Mapping $F_+ : \mathbb{R}^3_+ \to \mathbb{R}^3_+$ (Theorem 1)

Let us calculate the Jacobian mapping $F_+ : \mathbb{R}^3_+ \to \mathbb{R}^3_+$:

$$\Im = \frac{D(x_1, x_2, x_3)}{D(y_1, y_2, y_3)} = \det\left(\frac{\partial x_i}{\partial y_j}\right)_{i,j=1,2,3}.$$

Mapping

$$x = F_+ y, \quad x = (x_1, x_2, x_3) \in \mathbb{R}^3_+, \quad y = (y_1, y_2, y_3) \in \mathbb{R}^3_+$$

is specified by the formulas

$$x_1 = y_1\left(1 + \frac{y_3}{K_3} + \frac{(K_m + y_3)y_2}{K_1K_m + K_7y_3}\right), \tag{1}$$

$$x_2 = y_2\left(1 + \frac{y_3}{K_2} + \frac{(K_m + y_3)y_1}{K_1K_m + K_7y_3}\right), \tag{2}$$

$$x_3 = y_3\left(1 + \frac{y_1}{K_3} + \frac{y_2}{K_2} + \frac{y_1y_2}{K_1K_m + K_7y_3}\right). \tag{3}$$

Finding partial derivatives

$$\frac{\partial x_i}{\partial y_j}, \quad i, j = 1,2,3.$$

From the formula (1) follows

$$\frac{\partial x_1}{\partial y_1} = 1 + \frac{y_3}{K_3} + \frac{(K_m + y_3)y_2}{K_1K_m + K_7y_3}, \quad \frac{\partial x_1}{\partial y_2} = \frac{(K_m + y_3)y_1}{K_1K_m + K_7y_3},$$

$$\frac{\partial x_1}{\partial y_3} = y_1\left(\frac{1}{K_3} + \frac{y_2}{K_1K_m + K_7y_3} - \frac{K_7(K_m + y_3)y_2}{(K_1K_m + K_7y_3)^2}\right).$$

From the formula (2) we find

$$\frac{\partial x_2}{\partial y_1} = \frac{(K_m + y_3)y_2}{K_1K_m + K_7y_3}, \quad \frac{\partial x_2}{\partial y_2} = 1 + \frac{y_3}{K_2} + \frac{(K_m + y_3)y_1}{K_1K_m + K_7y_3},$$

$$\frac{\partial x_2}{\partial y_3} = y_2\left(\frac{1}{K_2} + \frac{y_1}{K_1K_m + K_7y_3} - \frac{K_7(K_m + y_3)y_1}{(K_1K_m + K_7y_3)^2}\right).$$

Similarly, from formula (3), we obtain

$$\frac{\partial x_3}{\partial y_1} = y_3\left(\frac{1}{K_3} + \frac{y_2}{K_1K_m + K_7y_3}\right), \quad \frac{\partial x_3}{\partial y_2} = y_3\left(\frac{1}{K_2} + \frac{y_1}{K_1K_m + K_7y_3}\right),$$

$$\frac{\partial x_3}{\partial y_3} = 1 + \frac{y_1}{K_3} + \frac{y_2}{K_2} + \frac{y_1 y_2}{K_1 K_m + K_7 y_3} - \frac{K_7 y_1 y_2 y_3}{\left(K_1 K_m + K_7 y_3\right)^2}.$$

Using the partial derivatives $\frac{\partial x_i}{\partial y_j}$, $i, j = 1,2,3$ found above, we directly calculate the Jacobian mapping $F_+ : \mathbb{R}^3_+ \to \mathbb{R}^3_+$:

$$\Im = \frac{D\left(x_1, x_2, x_3\right)}{D\left(y_1, y_2, y_3\right)} = \det\left(\frac{\partial x_i}{\partial y_j}\right)_{i,j=1,2,3} = \frac{A}{B},$$

where the numerator is:

$$\begin{aligned}
A = {} & K_3 K_7^2 y_3^3 + K_1 K_2 K_3 K_m^2 y_1 + K_7^2 y_1 y_3^3 + K_1 K_3 K_m^2 y_2^2 + 2K_1 K_2 K_3 K_7 K_m y_3 + K_2 K_7^2 y_3^3 + \\
& + K_7^2 y_2 y_3^3 + K_3 K_7 y_2 y_3^3 + 2K_1 K_7 K_m y_3^3 + K_2 K_3 K_m y_1 y_2^2 + K_3 K_7^2 y_2 y_3^2 + K_2 K_3 K_m y_1^2 y_2 + \\
& + K_1 K_2 K_m y_1^2 y_3 + K_2 K_7 K_m y_1 y_3^2 + 2K_2 K_7 K_m y_1 y_2 y_3 + K_1^2 K_3 K_m^2 y_2 + 2K_7 y_1 y_2 y_3^3 + \\
& + K_3 K_7 y_2^2 y_3^2 + K_3 K_7 K_m y_2^2 y_3 + K_3 K_2 K_7 y_2 y_3^2 + K_1^2 K_3 K_m^2 y_3 + K_1^2 K_m^2 y_1 y_3 + K_2 K_7 K_m y_1^2 y_3 + \\
& + K_1^2 K_2 K_m^2 y_1 + K_1 K_2 K_m^2 y_1^2 + 2K_1 K_7 K_m y_1 y_3^2 + K_1^2 K_2 K_3 K_m^2 + K_1 K_3 K_m^2 y_2 y_3 + K_1 K_3 K_m y_2^2 y_3 + \\
& + K_2 K_3 K_7 K_m y_2 y_3 + K_1 K_3 K_m^2 y_1 y_2 + K_2 K_7 y_1^2 y_3^2 + 2K_1 K_3 K_7 K_m y_2 y_3 + K_2 K_3 K_7 y_1 y_3^2 + \\
& + K_1^2 K_2 K_m^2 y_3 + K_3 K_7 K_m y_2 y_3^2 + K_1 K_2 K_m^2 y_1 y_3 + K_1 K_3 K_m y_2 y_3^2 + K_3 K_m y_1 y_2^2 y_3 + K_1^2 K_m^2 y_3^2 + \\
& + 6K_7 K_m y_1 y_2 y_3^2 + K_1 K_2 K_m^2 y_1 y_2 + K_2 K_3 K_7 K_m y_1 y_3 + K_2 K_7^2 y_1 y_3^2 + K_1 K_2 K_m y_1 y_3^2 + \\
& + 4K_1 K_m^2 y_1 y_2 y_3 + 2K_1 K_7 K_m y_2 y_3^2 + 2K_1 K_3 K_7 K_m y_3^2 + K_2 K_m y_1^2 y_2 y_3 + K_1 K_2 K_3 K_m y_2 y_3 + \\
& + 2K_1 K_2 K_7 K_m y_1 y_3 + K_1^2 K_m^2 y_2 y_3 + K_1 K_2 K_3 K_m y_1 y_2 + 2K_3 K_7 K_m y_1 y_2 y_3 + K_1 K_m y_1 y_2 y_3^2 + \\
& + K_2 K_7 y_1 y_3^3 + K_1 K_2 K_3 K_m^2 y_2 + K_1 K_2 K_3 K_m y_1 y_3 + 2K_1 K_2 K_7 K_m y_3^2 + K_7^2 y_3^4 + K_2 K_3 K_7^2 y_3^2
\end{aligned}$$

and the denominator is:

$$B = K_2 K_3 (K_1 K_m + K_7 y_3)^2.$$

Since the constants K_1, K_2, K_3, K_m, K_7 are positive, it is obvious that Jacobian $\Im$ of the mapping $F_+ : \mathbb{R}^3_+ \to \mathbb{R}^3_+$ is also positive on octant $\mathbb{R}^3_+$.