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

Journal of Mathematical Chemistry

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Online Resource 5

Algorithm for calculating the point of x_3^* in which the maximum initial rate $v = v(x_1, x_2, x_3)$ is reached with fixed values of variables x_1, x_2 $(0 < x_1, x_2 < \infty)$

1. Make an algebraic equation of the 7th degree with respect to the variable y_3:

$$a_7 y_3^7 + a_6 y_3^6 + a_5 y_3^5 + a_4 y_3^4 + a_3 y_3^3 + a_2 y_3^2 + a_1 y_3 + a_0 = 0\,, \tag{1}$$

where $$a_7 = K_7^2\,, \quad a_6 = K_7\left[K_m\left(2K_7 + K_1\right) + \left(K_3 + K_2\right)K_7\right],$$

$$a_5 = \frac{1}{4}\left[K_7\left(K_3 + K_2\right) + K_1 K_m\right]\left[K_7\left(K_2 + K_3\right) + \left(10K_7 + K_1\right)K_m\right],$$

$$a_4 = \left[\frac{3}{4}\left(K_7(K_3 + K_2) + K_1 K_m\right)^2 + K_7\left(K_1 K_m (K_3 + K_2) + (K_7 - K_1)K_3 K_2\right)\right]K_m\,,$$

$$a_3 = \frac{1}{2}K_m[K_1^2 K_m^2\left(K_3 + K_2\right) + \left(K_1 K_7 (K_3 + K_2)^2 - \left(K_7(x_1 + x_2) + K_1^2\right)K_3 K_2\right)K_m +$$
$$+ \left(K_7 - K_1\right)\left(K_3 + K_2\right)K_7 K_3 K_2]\,,$$

$$a_2 = -\frac{1}{2}K_m^2 K_3 K_2\left(K_1 + x_2 + x_1\right)\left[K_7(K_3 + K_2) + K_1 K_m\right],$$

$$a_1 = -\frac{1}{4}K_m^2 K_2 K_3[2\left(K_1 + x_2 + x_1\right)\left(K_1 K_m (K_3 + K_2) + K_7 K_2 K_3\right) +$$
$$+ \left(x_1 - x_2 - K_1\right)\left(x_1 - x_2 + K_1\right)K_2 K_3]\,,$$

$$a_0 = -\frac{1}{4}\left[\left(K_1 + x_2 + x_1\right)^2 - 4x_2 x_1\right]K_3^2 K_2^2 K_m^3\,.$$

2. Solve equation (1) with respect to y_3. This equation with fixed values of coefficients can have no more than 7 real positive roots. For each of these roots, calculate the x_3 value using the formula:

$$x_3 = \frac{A y_3}{B}\,, \tag{2}$$

where $$A = b_5 y_3^5 + b_4 y_3^4 + b_3 y_3^3 + b_2 y_3^2 + b_1 y_3 + b_0\,,$$

$$b_5 = K_7\,, \quad b_4 = \frac{1}{2}\left[K_7\left(K_2 + K_3 + 4K_m\right) + K_1 K_m\right],$$

$$b_3 = K_m\left[2K_7\left(K_2 + K_3\right) + K_1 K_m\right] + K_2 K_3\left(K_m - K_7\right),$$

$$b_2 = \frac{1}{2} K_m K_2 K_3 \left[2\left(K_m + K_3 + K_2\right) + \left(x_1 + x_2 - K_1\right) \right] -$$
$$- \frac{1}{2} \left[K_7 \left(K_3 + K_2\right) + K_1 K_m \right] \left[K_2 K_3 - \left(K_3 + K_2\right) K_m \right],$$

$$b_1 = K_m K_2 K_3 \left[K_m \left(K_2 + K_3 - K_1\right) + \left(K_2 x_1 + K_3 x_2 + K_2 K_3\right) \right],$$

$$b_0 = \frac{1}{2} K_m K_2 K_3 \left[\left(x_2 + x_1 + K_1\right)\left(K_2 K_3 - (K_2 + K_3) K_m\right) + 2K_m \left(K_2 x_1 + K_3 x_2 + K_2 K_3\right) \right],$$

and $B = K_m K_2 K_3 (K_m + y_3)(K_2 + y_3)(K_3 + y_3)$

3. Among the roots of equation (1) there is only one positive root y_3, in which the values x_3, y_1 and y_2 calculated by the formulas (2) and (3.1), respectively, will be positive. Select this root y_3 and calculate the value of x_3 by formula (2). Then $x_3^* = x_3$ is the point at which the maximum initial rate $v = v\left(x_1, x_2, x_3\right)$ is reached with fixed values of variables x_1, x_2 ($0 < x_1, x_2 < \infty$).