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 3

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

1. Make an algebraic equation of the 8th degree with respect to the variable y_3:

$$a_8 y_3^8 + a_7 y_3^7 + a_6 y_3^6 + a_5 y_3^5 + a_4 y_3^4 + a_3 y_3^3 + a_2 y_3^2 + a_1 y_3 + a_0 = 0, \qquad (1)$$

where

$$a_8 = -3K_7^2, \quad a_7 = -2K_7\left[3K_7(x_2 - x_3) + 2K_7(K_2 + K_m) + (K_1K_m - K_2K_3)\right],$$

$$a_6 = K_7\left[K_2K_3(K_2 + K_m) + K_1K_m(K_2 - 3K_m) - (x_2 - x_3)(8K_7K_m - 5K_2K_3 + 7K_1K_m)\right] + \\ + K_2K_7^2(11x_3 - 6K_m - K_2 - 2x_2),$$

$$a_5 = K_2^2\left[2K_7K_3(2x_2 - 2x_3 - K_m) + 2K_mK_3^2 + 2K_7^2(3x_3 - K_m)\right] + 2K_2K_3K_7(x_3 - x_2)^2 + \\ + K_1\left[2K_2K_3K_m(x_2 - x_3 - K_2 - K_m) + 10K_mK_7(K_2x_3 + K_mx_3 - K_mx_2) + 2K_2K_mK_7(2K_2 + x_2)\right] + \\ + 2K_m\left[K_2K_7(2K_7(4x_3 - x_2) - (K_m + x_2 + 2x_3)K_3) + K_1^2K_m(x_3 - x_2 + K_2)\right],$$

$$a_4 = K_2K_3\left[K_2(5K_3K_m(x_2 - x_3) + K_2(K_7x_2 - K_1K_m)) + (K_1K_m + K_2K_7)(x_2 - x_3)^2\right] - \\ - K_1K_m^2\left[K_2K_3(6K_2 + 3K_m + 4x_2) + ((3K_m - 2K_2)(x_2 + x_3 + K_2) - 6K_m(x_3 + K_2))K_1\right] + \\ + K_2^2\left[5K_mK_7(2K_7x_3 - K_3K_m) + 2K_3K_m(K_7x_2 + 2K_3K_m) + (K_3 - K_7)(K_3K_m - K_7x_3)K_2\right] + \\ + K_2K_mK_7\left[(x_2 + 5K_m)(K_1K_2 - 2K_3x_2) + K_1(K_2^2 + 3K_2x_3 + 17K_mx_3) + K_3x_3(3K_m + x_2 + x_3)\right],$$

$$a_3 = 2K_2K_m^3\left[K_3(K_2(K_3 - 3K_1) + (2x_3 - 5x_2)K_1) + (2x_3 + x_2 + 2K_2)K_1^2\right] + \\ + 2K_2K_3K_m\left[K_2(2K_3(x_3 - x_2)^2 - K_7(x_3^2 - x_2^2)) - K_m(x_3 - x_2)(K_7x_3 - K_1x_2 - 2K_7x_2)\right] + \\ + 2K_2^2K_m^2\left[K_7(K_1(4x_3 + x_2) + (4x_3 - 3x_2)K_3) - K_3(5K_3x_3 - 2K_1x_3 - 3K_3x_2)\right] + \\ + 2K_2^3K_m\left[K_m(K_3 - K_1)(K_3 - K_7) - (K_3 + K_7)(K_3x_3 - K_3x_2 - K_7x_3)\right],$$

$$a_2 = K_2^2K_m^2\left[K_1^2K_m(x_2 + x_3 + K_2) + K_3^2K_m(x_2 + K_2 - 5x_3) + 2K_1K_3(K_2x_2 - x_3^2 + x_2^2)\right] + \\ + K_2^2K_3^2K_m\left[(x_2 - x_3)^2(x_2 - x_3 + K_2) + 2K_m(x_2 - 2x_3)(x_2 - 2x_3 + K_2)\right] + \\ + K_2K_3K_m^2x_3\left[K_2(2K_7x_2 - 2K_3x_2 - 5K_7x_3) - 2K_1K_m(x_2 - x_3)\right] + \\ + K_2^3K_mK_7x_3\left[K_1K_m + K_3(x_2 - x_3 + 3K_m)\right] - 2K_1K_2K_3K_m^3\left[K_2(K_2 + 3x_2 - 4x_3) + 2(x_2 - x_3)^2\right],$$

$$a_1 = -2x_3K_2^2K_3K_m^2\left[K_m(K_3 - K_1)(x_2 + K_2 - 2x_3) + K_2(K_3x_2 - K_3x_3 + K_7x_3) + K_3(x_2 - x_3)^2\right],$$

$$a_0 = -K_2^2K_3K_m^3x_3^2\left[K_3(K_2 + x_2 - x_3) - K_1K_2\right].$$

2. Solve equation (1) with respect to y_3. This equation with fixed values of coefficients can have no more than 8 real positive roots. For each of these roots, calculate the x_1 value using the formula:

$$x_1 = \frac{A}{B}, \tag{2}$$

where $A = b_7 y_3^7 + b_6 y_3^6 + b_5 y_3^5 + b_4 y_3^4 + b_3 y_3^3 + b_2 y_3^2 + b_1 y_3 + b_0$,

$$b_7 = -K_7, \quad b_6 = -K_7\left(2x_2 - 2x_3 + 3K_2\right),$$

$$b_5 = K_m\left[2K_m\left(K_1 + K_7\right) - K_2\left(K_1 + K_3\right) - \left(x_2 - x_3\right)\left(3K_7 + K_1\right)\right] + \\ + K_7\left[2K_m\left(K_3 - 2K_2\right) - K_2\left(x_2 + K_2 + 2K_3 - 4x_3\right)\right],$$

$$b_4 = K_m\left[K_2\left(2K_1(x_3 - K_3) - (K_2 - 2x_3 - 2K_m + 2x_2)K_3\right) + K_1K_m\left(2K_3 + x_3 + 3K_m - x_2\right)\right] + \\ + \left(x_2 - x_3\right)\left(K_3K_m - 2K_2K_m - K_2K_3\right) - 2K_2K_m\left(K_3 - 3x_3\right) + K_2^2\left(x_3 - K_3 - 2K_m\right) + K_m^2\left(K_2 + 3K_3\right)$$

$$b_3 = K_2K_mx_3\left[2K_mK_7 + 4K_1K_m + K_3K_m + 3K_2K_7 + K_2K_3\right] + \\ + K_m\left[K_3K_m\left(2K_7 + K_1\right)\left(x_2 - x_3\right) - K_2K_3\left(3K_1K_m + (x_2 - x_3)^2\right) + K_1K_m^2\left(x_2 - x_3 + 3K_2 + 3K_3\right)\right] + \\ + K_2K_3K_m\left[\left(2K_7 + K_1 - K_m\right)\left(K_m - K_2 - x_2 + x_3\right) - 4K_m\left(x_2 - x_3 + K_2\right) + K_2\left(K_m - x_2 + x_3\right)\right]$$

$$b_2 = K_m^2\left[2K_1K_3\left(K_m - K_2\right)\left(K_2 - x_3 + x_2\right) - K_2\left(K_m - K_1\right)\left(K_2K_m + K_mx_2 + K_2x_3\right)\right] + \\ + K_2K_3K_m\left[x_3\left(2K_m^2 + K_2x_2 + K_m(4K_2 + 3x_2)\right) - x_3^2\left(K_2 + 2K_m\right) - K_m\left(K_m + x_2\right)\left(K_2 + x_2\right)\right] + \\ + K_2K_m\left[K_m^3\left(K_2 + x_2\right) + K_mK_7x_3\left(K_2 - K_3\right) + K_2x_3\left(K_3K_7 + K_m^2\right)\right]$$

$$b_1 = K_2K_3K_m^2x_3\left[K_2\left(x_2 + 2K_m + K_1 - 2x_3\right) - \left(x_3 + x_2 - K_1\right)K_m\right], \quad b_0 = -K_2^2K_3K_m^3x_3^2,$$

and

$$B = y_3\left(-K_m + K_2\right)[K_7y_3^2\left(K_2K_m + K_2y_3 + y_3^2 + K_my_3\right) - K_3K_m\left((x_3 - y_3)(y_3 + K_m) - x_2y_3\right) + \\ - K_2 + y_3\left(K_7y_3 + K_1K_m\right)\left(K_2K_m + 3K_my_3 + 2y_3^2\right).$$

3. Among the roots of equation (1) there is only one positive root y_3, in which the values x_1, 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_1 by formula (2). Then $x_1^* = x_1$ is the point at which the maximum initial rate $v = v(x_1, x_2, x_3)$ is reached with fixed values of variables x_2, x_3 ($0 < x_2, x_3 < \infty$).