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SUPPLEMENTARY INFORMATION

Mechanistic modeling, parametric study, and optimization of immobilization of enzymatic cascades in porous particles

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1 Analytical solutions for the concentration profiles inside pore α-A

Using the methodology first established by Professor Ernst Thiele[1] and presented in detail in Professor Octave Levenspiel's book[2] we derive material balances for the pores. The analytical solutions for the material balances are presented here. The methods we applied to derive the analytical solutions can be found in the book of Professor George Simmons[3]. For substrate S_1, we derive the following material balance around pore α-A.

$$\frac{d^2 S_{1,\alpha-A}}{dx^2} = \frac{k_A \cdot E_{A,\alpha-A}}{D_1} \cdot S_{1,\alpha-A} \tag{1}$$

The following two boundary conditions are considered:

$$S_{1,\alpha-A}|_{x=0} = S_{1,0} \tag{2}$$

$$\left.\frac{dS_{1,\alpha-A}}{dx}\right|_{x=L} = 0 \tag{3}$$

Equation (1) is a second order, linear and homogeneous differential equation with constant coefficients. The general solution is:

$$S_{1,\alpha-A} = c_1 \cdot e^{m_{1,\alpha-A} \cdot x} + c_2 \cdot e^{-m_{1,\alpha-A} \cdot x} \tag{4}$$

with

$$m_{1,\alpha-A} = \sqrt{\frac{k_A \cdot E_{A,\alpha-A}}{D_1}} \tag{5}$$

$$c_1 = \frac{S_{1,0} \cdot e^{-m_{1,\alpha-A} \cdot L}}{e^{m_{1,\alpha-A} \cdot L} + e^{-m_{1,\alpha-A} \cdot L}} \tag{6}$$

$$c_2 = \frac{S_{1,0} \cdot e^{m_{1,\alpha-A} \cdot L}}{e^{m_{1,\alpha-A} \cdot L} + e^{-m_{1,\alpha-A} \cdot L}} \tag{7}$$

For substrate S_2, we derive the following material balance around pore α-A.

$$\frac{d^2 S_{2,\alpha-A}}{dx^2} = -\frac{k_A \cdot E_{A,\alpha-A}}{D_2} \cdot S_{1,\alpha-A} \tag{8}$$

Substituting the solution we obtained for $S_{1,\alpha-A}$ in Equation (8) we get:

$$\frac{d^2 S_{2,\alpha-A}}{dx^2} = -\frac{k_A \cdot E_{A,\alpha-A}}{D_2} \cdot c_1 \cdot e^{m_{1,\alpha-A} \cdot x} + \\ -\frac{k_A \cdot E_{A,\alpha-A}}{D_2} \cdot c_2 \cdot e^{-m_{1,\alpha-A} \cdot x} \tag{9}$$

The following two boundary conditions are considered:

$$S_{2,\alpha-A}|_{x=0} = S_{2,0} \tag{10}$$

$$\left.\frac{dS_{2,\alpha-A}}{dx}\right|_{x=L} = 0 \tag{11}$$

Equation (9) is a second order, linear and heterogeneous differential equation with constant coefficients. The general solution is:

$$S_{2,\alpha-A} = c_3 \cdot x + c_4 + c_5 \cdot e^{m_{1,\alpha-A} \cdot x} + c_6 \cdot e^{-m_{1,\alpha-A} \cdot x} \tag{12}$$

with

$$c_3 = -c_5 \cdot m_{1,\alpha-A} \cdot e^{m_{1,\alpha-A} \cdot L} + c_6 \cdot m_{1,\alpha-A} \cdot e^{-m_{1,\alpha-A} \cdot L} \tag{13}$$

$$c_4 = S_{2,0} - c_5 - c_6 \tag{14}$$

$$c_5 = -\frac{k_A \cdot E_{A,\alpha-A} \cdot c_1}{D_2 \cdot m_{1,\alpha-A}^2} \tag{15}$$

$$c_6 = -\frac{k_A \cdot E_{A,\alpha-A} \cdot c_2}{D_2 \cdot m_{1,\alpha-A}^2} \tag{16}$$

2 Analytical solutions for the concentration profiles inside pore α-B

For substrate S_2, we derive the following material balance around pore α-B.

$$\frac{d^2 S_{2,\alpha-\mathrm{B}}}{dx^2} = \frac{k_{\mathrm{B}} \cdot E_{\mathrm{B},\alpha-\mathrm{B}}}{D_2} \cdot S_{2,\alpha-\mathrm{B}} \tag{17}$$

The following two boundary conditions are considered:

$$S_{2,\alpha-\mathrm{B}}|_{x=0} = S_{2,0} \tag{18}$$

$$\frac{dS_{2,\alpha-\mathrm{B}}}{dx}\Big|_{x=L} = 0 \tag{19}$$

Equation (17) is a second order, linear and homogeneous differential equation with constant coefficients. The general solution is:

$$S_{2,\alpha-\mathrm{B}} = d_1 \cdot e^{m_{2,\alpha-\mathrm{B}} \cdot x} + d_2 \cdot e^{-m_{2,\alpha-\mathrm{B}} \cdot x} \tag{20}$$

with

$$m_{2,\alpha-\mathrm{B}} = \sqrt{\frac{k_{\mathrm{B}} \cdot E_{\mathrm{B},\alpha-\mathrm{B}}}{D_2}} \tag{21}$$

$$d_1 = \frac{S_{2,0} \cdot e^{-m_{2,\alpha-\mathrm{B}} \cdot L}}{e^{m_{2,\alpha-\mathrm{B}} \cdot L} + e^{-m_{2,\alpha-\mathrm{B}} \cdot L}} \tag{22}$$

$$d_2 = \frac{S_{2,0} \cdot e^{m_{2,\alpha-\mathrm{B}} \cdot L}}{e^{m_{2,\alpha-\mathrm{B}} \cdot L} + e^{-m_{2,\alpha-\mathrm{B}} \cdot L}} \tag{23}$$

For substrate S_3, we derive the following material balance around pore α-B.

$$\frac{d^2 S_{3,\alpha-\mathrm{B}}}{dx^2} = -\frac{k_{\mathrm{B}} \cdot E_{\mathrm{B},\alpha-\mathrm{B}}}{D_3} \cdot S_{2,\alpha-\mathrm{B}} \tag{24}$$

Substituting the solution we obtained for $S_{2,\alpha-\mathrm{B}}$ in Equation (24) we get:

$$\frac{d^2 S_{3,\alpha-\mathrm{B}}}{dx^2} = -\frac{k_{\mathrm{B}} \cdot E_{\mathrm{B},\alpha-\mathrm{B}}}{D_3} \cdot d_1 \cdot e^{m_{2,\alpha-\mathrm{B}} \cdot x} + -\frac{k_{\mathrm{B}} \cdot E_{\mathrm{B},\alpha-\mathrm{B}}}{D_3} \cdot d_2 \cdot e^{-m_{2,\alpha-\mathrm{B}} \cdot x} \tag{25}$$

The following two boundary conditions are considered:

$$S_{3,\alpha-\mathrm{B}}|_{x=0} = S_{3,0} \tag{26}$$

$$\frac{dS_{3,\alpha-\mathrm{B}}}{dx}\Big|_{x=L} = 0 \tag{27}$$

Equation (25) is a second order, linear and heterogeneous differential equation with constant coefficients. We applied the appropriate methodology by first solving the corresponding homogeneous equation and then solving for the heterogeneous terms. The general solution is:

$$S_{3,\alpha-\mathrm{B}} = d_3 \cdot x + d_4 + d_5 \cdot e^{m_{2,\alpha-\mathrm{B}} \cdot x} + d_6 \cdot e^{-m_{2,\alpha-\mathrm{B}} \cdot x} \tag{28}$$

with

$$d_3 = -(d_5 \cdot m_{2,\alpha-\mathrm{B}} \cdot e^{m_{2,\alpha-\mathrm{B}} \cdot L} - d_6 \cdot m_{2,\alpha-\mathrm{B}} \cdot e^{-m_{2,\alpha-\mathrm{B}} \cdot L}) \tag{29}$$

$$d_4 = S_{3,0} - d_5 - d_6 \tag{30}$$

$$d_5 = -\frac{k_{\mathrm{B}} \cdot E_{\mathrm{B},\alpha-\mathrm{B}} \cdot d_1}{D_3 \cdot m_{2,\alpha-\mathrm{B}}^2} \tag{31}$$

$$d_6 = -\frac{k_{\mathrm{B}} \cdot E_{\mathrm{B},\alpha-\mathrm{B}} \cdot d_2}{D_3 \cdot m_{2,\alpha-\mathrm{B}}^2} \tag{32}$$

3 Macro kinetic expressions for the single immobilization case

The macro kinetics or apparent reaction rates, v_k, for the single immobilization case can then be calculated by applying Fick's law at the start ($x = 0$) of the corresponding pore. Since the concentration profiles were calculated analytically, we can also derive analytical expressions for the concentration gradient at the beginning of the pores and use this to get an analytical expression of the apparent reaction rates. For the single immobilization case, these are presented below.

$$v_{\mathrm{I}} = p_{1,\alpha-\mathrm{A}} \cdot S_{1,0} \tag{33}$$

$$v_{\mathrm{II}} = p_{2,\alpha-\mathrm{B}} \cdot S_{2,0} \tag{34}$$

with

$$p_{1,\alpha-\mathrm{A}} = N_{\alpha-\mathrm{A}} \cdot A \cdot D_1 \cdot m_{1,\alpha-\mathrm{A}} \cdot \tanh(m_{1,\alpha-\mathrm{A}} \cdot L) \tag{35}$$

$$p_{2,\alpha-\mathrm{B}} = N_{\alpha-\mathrm{B}} \cdot A \cdot D_2 \cdot m_{2,\alpha-\mathrm{B}} \cdot \tanh(m_{2,\alpha-\mathrm{B}} \cdot L) \tag{36}$$

4 Analytical solutions for the concentration profiles inside pore β

For substrate S_1, we derive the following material balance around pore β.

$$\frac{d^2 S_{1,\beta}}{dx^2} = \frac{k_A \cdot E_{A,\beta}}{D_1} \cdot S_{1,\beta} \tag{37}$$

The following two boundary conditions apply:

$$S_{1,\beta}|_{x=0} = S_{1,0} \tag{38}$$

$$\left.\frac{dS_{1,\beta}}{dx}\right|_{x=L} = 0 \tag{39}$$

Equation (37) is a second order, linear and homogeneous differential equation with constant coefficients. The general solution is:

$$S_{1,\beta} = e_1 \cdot e^{m_{1,\beta} \cdot x} + e_2 \cdot e^{-m_{1,\beta} \cdot x} \tag{40}$$

with

$$m_{1,\beta} = \sqrt{\frac{k_A \cdot E_{A,\beta}}{D_1}} \tag{41}$$

In order to find the particular solution we use the two boundary conditions given in Equations (38) and (39).

$$e_1 = \frac{S_{1,0} \cdot e^{-m_{1,\beta} \cdot L}}{e^{m_{1,\beta} \cdot L} + e^{-m_{1,\beta} \cdot L}} \tag{42}$$

$$e_2 = \frac{S_{1,0} \cdot e^{m_{1,\beta} \cdot L}}{e^{m_{1,\beta} \cdot L} + e^{-m_{1,\beta} \cdot L}} \tag{43}$$

For substrate S_2, we can write the following material balance around pore β.

$$\frac{d^2 S_{2,\beta}}{dx^2} - \frac{k_B \cdot E_{B,\beta}}{D_2} \cdot S_{2,\beta} = -\frac{k_A \cdot E_{A,\beta}}{D_2} \cdot S_{1,\beta} \tag{44}$$

Substituting the solution we obtained for $S_{1,\beta}$ in Equation (44) we get:

$$\frac{d^2 S_{2,\beta}}{dx^2} - \frac{k_B \cdot E_{B,\beta}}{D_2} \cdot S_{2,\beta} = -\frac{k_A \cdot E_{A,\beta}}{D_2} \cdot e_1 \cdot e^{m_{1,\beta} \cdot x} + \\ -\frac{k_A \cdot E_{A,\beta}}{D_2} \cdot e_2 \cdot e^{-m_{1,\beta} \cdot x} \tag{45}$$

The following two boundary conditions are considered:

$$S_{2,\beta}|_{x=0} = S_{2,0} \tag{46}$$

$$\left.\frac{dS_{2,\beta}}{dx}\right|_{x=L} = 0 \tag{47}$$

Equation (45) is a second order, linear and heterogeneous differential equation with constant coefficients. We applied the appropriate methodology by first solving the corresponding homogeneous equation and then solving for the heterogeneous terms. The general solution is:

$$S_{2,\beta} = e_3 \cdot e^{m_{2,\beta} \cdot x} + e_4 \cdot e^{-m_{2,\beta} \cdot x} + e_5 \cdot e^{m_{1,\beta} \cdot x} + e_6 \cdot e^{-m_{1,\beta} \cdot x} \tag{48}$$

with

$$m_{2,\beta} = \sqrt{\frac{k_B \cdot E_{B,\beta}}{D_2}} \tag{49}$$

$$e_3 = S_{2,0} - e_4 - e_5 - e_6 \tag{50}$$

$$e_4 = \frac{m_{2,\beta} \cdot e^{m_{2,\beta} \cdot L} \cdot (S_{2,0} - e_5 - e_6)}{m_{2,\beta} \cdot e^{m_{2,\beta} \cdot L} + m_{2,\beta} \cdot e^{-m_{2,\beta} \cdot L}} + \\ + \frac{m_{1,\beta} \cdot (e_5 \cdot e^{m_{1,\beta} \cdot L} - e_6 \cdot e^{-m_{1,\beta} \cdot L})}{m_{2,\beta} \cdot e^{m_{2,\beta} \cdot L} + m_{2,\beta} \cdot e^{-m_{2,\beta} \cdot L}} \tag{51}$$

$$e_5 = -\frac{k_A \cdot E_A \cdot e_1}{D_2 \cdot (m_{1,\beta}^2 - m_{2,\beta}^2)} \tag{52}$$

$$e_6 = -\frac{k_A \cdot E_A \cdot e_2}{D_2 \cdot (m_{1,\beta}^2 - m_{2,\beta}^2)} \tag{53}$$

For substrate S_3, we derive the following material balance around pore β.

$$\frac{d^2 S_{3,\beta}}{dx^2} = -\frac{k_B \cdot E_{B,\beta}}{D_3} \cdot S_{2,\beta} \tag{54}$$

The following two boundary conditions are considered:

$$S_{3,\beta}|_{x=0} = S_{3,0} \tag{55}$$

$$\left.\frac{dS_{3,\beta}}{dx}\right|_{x=L} = 0 \tag{56}$$

Equation (54) is a second order, linear and heterogeneous differential equation with constant coefficients. We applied the appropriate methodology by first solving the corresponding homogeneous equation and then solving for the heterogeneous terms. The general solution is:

$$S_{3,\beta} = e_7 + e_8 \cdot x + e_9 \cdot e^{m_{2,\beta} \cdot x} + e_{10} \cdot e^{-m_{2,\beta} \cdot x} + e_{11} \cdot e^{m_{1,\beta} \cdot x} \tag{57}$$

with

$$e_7 = S_{3,0} - e_9 - e_{10} - e_{11} - e_{12} \tag{58}$$

$$e_8 = m_{2,\beta} \cdot (-e_9 \cdot e^{m_{2,\beta} \cdot L} + e_{10} \cdot e^{-m_{2,\beta} \cdot L}) + \\ + m_{1,\beta} \cdot (-e_{11} \cdot e^{m_{1,\beta} \cdot L} + e_{12} \cdot e^{-m_{2,\beta} \cdot L}) \tag{59}$$

$$e_9 = -\frac{k_B \cdot E_B \cdot e_3}{D_3 \cdot m_{2,\beta}^2} \tag{60}$$

$$e_{10} = -\frac{k_B \cdot E_B \cdot e_4}{D_3 \cdot m_{2,\beta}^2} \tag{61}$$

$$e_{11} = -\frac{k_B \cdot E_B \cdot e_5}{D_3 \cdot m_{1,\beta}^2} \tag{62}$$

$$e_{12} = -\frac{k_B \cdot E_B \cdot e_6}{D_3 \cdot m_{1,\beta}^2} \tag{63}$$

5 Macro kinetic expressions for the co-immobilization case

The macro kinetics or apparent reaction rates, υ_k, for the co-immobilization spatial immobilization distribution can then be calculated by applying Fick's law at the start ($x = 0$) of the corresponding pore. Since the concentration profiles were calculated analytically, we can also derive analytical expressions for the concentration gradient at the beginning of the pores and use this to get an analytical expression of the apparent reaction rates. For the co-immobilization case, these are presented below.

$$\upsilon_{\mathrm{I}} = p_{1,\beta} \cdot S_{1,0} \tag{64}$$

$$\upsilon_{\mathrm{II}} = p_{2,\beta} \cdot S_{1,0} + p_{3,\beta} \cdot S_{2,0} \tag{65}$$

with

$$p_{1,\beta} = N_\beta \cdot A \cdot D_1 \cdot m_{1,\beta} \cdot \tanh(m_{1,\beta} \cdot L) \tag{66}$$

$$p_{2,\beta} = N_\beta \cdot A \cdot D_2 \cdot m_{2,\beta} \cdot \tanh(m_{2,\beta} \cdot L) \tag{67}$$

$$p_{3,\beta} = \frac{N_\beta \cdot A \cdot D_1 \cdot m_{1,\beta}^2 \cdot m_{2,\beta}^2}{m_{1,\beta}^2 - m_{2,\beta}^2} \cdot [\frac{\tanh(m_{2,\beta} \cdot L)}{m_{2,\beta}} + \\ - \frac{\tanh(m_{1,\beta} \cdot L)}{m_{1,\beta}}] \tag{68}$$

6 Analytical solution of the time profiles in a batch reactor for the single immobilization case

The following system of first order differential equations represents the dynamic material balances for the batch reactor when single immobilization is used as a spatial immobilization strategy (α):

$$\frac{dS_{1,0}}{dt} = -p_{1,\alpha-\mathrm{A}} \cdot S_{1,0} \tag{69}$$

$$\frac{dS_{2,0}}{dt} = +p_{1,\alpha-\mathrm{A}} \cdot S_{1,0} - p_{2,\alpha-\mathrm{B}} \cdot S_{2,0} \tag{70}$$

$$\frac{dS_{3,0}}{dt} = -p_{2,\alpha-\mathrm{B}} \cdot S_{2,0} \tag{71}$$

with the following initial conditions:

$$S_{1,0}|_{t=0} = S_{1,0}^0 \tag{72}$$

$$S_{2,0}|_{t=0} = 0 \tag{73}$$

$$S_{3,0}|_{t=0} = 0 \tag{74}$$

This is a system of first order, linear differential equations. The solution is:

$$S_{1,0} = S_{1,0}^0 \cdot e^{-p_{1,\alpha-\mathrm{A}} \cdot t} \tag{75}$$

$$S_{2,0} = S_{1,0}^0 \cdot \frac{p_{1,\alpha-\mathrm{A}}}{p_{2,\alpha-\mathrm{B}} - p_{1,\alpha-\mathrm{A}}} \cdot (e^{-p_{1,\alpha-\mathrm{A}} \cdot t} - e^{-p_{2,\alpha-\mathrm{B}} \cdot t}) \tag{76}$$

$$S_{3,0} = S_{1,0}^0 - S_{1,0} - S_{2,0} \tag{77}$$

7 Analytical solution of the time profiles in a batch reactor for the co-immobilization case

The following system of first order differential equations represents the dynamic material balances for the batch reactor when co-immobilization is used as a spatial immobilization strategy (β):

$$\frac{dS_{1,0}}{dt} = -p_{1,\beta} \cdot S_{1,0} \tag{78}$$

$$\frac{dS_{2,0}}{dt} = +p_{1,\beta} \cdot S_{1,0} - p_{2,CI} \cdot S_{1,0} - p_{3,CI} \cdot S_{2,0} \tag{79}$$

$$\frac{dS_{3,0}}{dt} = p_{2,CI} \cdot S_{1,0} + p_{3,CI} \cdot S_{2,0} \tag{80}$$

with initial conditions:

$$S_{1,0}|_{t=0} = S^0_{1,0} \tag{81}$$

$$S_{2,0}|_{t=0} = 0 \tag{82}$$

$$S_{3,0}|_{t=0} = 0 \tag{83}$$

This is a system of first order, linear differential equations. The solution is:

$$S_{1,0} = S^0_{1,0} \cdot e^{-p_{1,\beta} \cdot t} \tag{84}$$

$$S_{2,0} = S^0_{1,0} \cdot \frac{p_{1,\beta} - p_{3,\beta}}{p_{2,\beta} - p_{1,\beta}} \cdot (e^{-p_{1,\beta} \cdot t} - e^{-p_{2,\beta} \cdot t}) \tag{85}$$

$$S_{3,0} = S^0_{1,0} - S_{1,0} - S_{2,0} \tag{86}$$

8 Simplification of $\mathcal{R}_{\alpha/\beta}$

The ratio $\mathcal{R}_{\alpha/\beta}$ can be calculated by the following expression:

$$\mathcal{R}_{\alpha/\beta} = \frac{S^{\alpha}_{3,0}}{S^{\beta}_{3,0}} = \frac{1 - e^{-p_{1,\alpha-\mathrm{A}} \cdot t} - \frac{p_{1,\alpha-\mathrm{A}}}{p_{2,\alpha-\mathrm{B}} - p_{1,\alpha-\mathrm{A}}} \cdot (e^{-p_{1,\alpha-\mathrm{A}} \cdot t} - e^{-p_{2,\alpha-\mathrm{B}} \cdot t})}{1 - e^{-p_{1,\beta} \cdot t} - \frac{p_{1,\beta} - p_{3,\beta}}{p_{2,\beta} - p_{1,\beta}} \cdot (e^{-p_{1,\beta} \cdot t} - e^{-p_{2,\beta} \cdot t})} \tag{87}$$

When the products $m_{1,\mathrm{n}} \cdot L$ and $m_{2,\mathrm{n}} \cdot L$ are larger than one, all tangent hyperbolicus terms become roughly equal to one. In addition, when considering cases where $D_1 = D_2 = D$, Equation (87) can be simplified. The terms $p_{1,n}$, $p_{2,n}$ and $p_{3,n}$ will now be as follows:

$$p_{1,\alpha-\mathrm{A}} = N_{\alpha-\mathrm{A}} \cdot A \cdot D \cdot m_{1,\alpha-\mathrm{A}} \tag{88}$$

$$p_{2,\alpha-\mathrm{B}} = N_{\alpha-\mathrm{B}} \cdot A \cdot D \cdot m_{2,\alpha-\mathrm{B}} \tag{89}$$

$$p_{1,\beta} = N_{\beta} \cdot A \cdot D \cdot m_{1,\beta} \tag{90}$$

$$p_{2,\beta} = N_{\beta} \cdot A \cdot D \cdot m_{2,\beta} \tag{91}$$

$$p_{3,\beta} = \frac{N_{\beta} \cdot A \cdot D \cdot m^2_{1,\beta} \cdot m^2_{2,\beta}}{m^2_{1,\beta} - m^2_{2,\beta}} \cdot \left[\frac{1}{m_{2,\beta}} - \frac{1}{m_{1,\beta}}\right] \tag{92}$$

They can be expressed in terms of $p_{1,\alpha-\mathrm{A}}$ and $p_{2,\alpha-\mathrm{B}}$ as follows:

$$p_{1,\alpha-\mathrm{B}} = p_{1,\alpha-\mathrm{A}} \tag{93}$$

$$p_{1,\beta} = \sqrt{2} \cdot p_{1,\alpha-\mathrm{A}} \tag{94}$$

$$p_{2,\beta} = \sqrt{2} \cdot p_{2,\alpha-\mathrm{B}} \tag{95}$$

$$p_{3,\beta} = \frac{\sqrt{2} \cdot p_{1,\alpha-\mathrm{A}} \cdot p_{2,\alpha-\mathrm{B}}}{p_{1,\alpha-\mathrm{A}} + p_{2,\alpha-\mathrm{B}}} \tag{96}$$

We define two moduli, μ_1 and μ_2 as follows:

$$\mu_1 = p_{1,\alpha-\mathrm{A}} \cdot t \tag{97}$$

$$\mu_2 = p_{2,\alpha-\mathrm{B}} \cdot t \tag{98}$$

Equation (87) can then be reformulated as follows:

$$\mathcal{R}_{\alpha/\beta} = \frac{1 - e^{-\mu_1} - \frac{\mu_1}{\mu_2 - \mu_1} \cdot (e^{-\mu_1} - e^{-\mu_2})}{1 - e^{-\sqrt{2} \cdot \mu_1} - \frac{\mu_1^2}{\mu_2^2 - \mu_1^2} \cdot (e^{-\sqrt{2} \cdot \mu_1} - e^{-\sqrt{2} \cdot \mu_2})} \tag{99}$$

Notes and references

1 E. W. Thiele, Industrial & Engineering Chemistry, 1939, **31**, 916–920.
2 O. Levenspiel, Chemical Reaction Engineering, Wiley, 1999.
3 G. F. Simmons, Differential Equations With Applications and Historical Notes, Productivity Press, Third Edition edn, 2016.