## uravnenia

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## chemistry

$$A \xrightarrow{k_{cis}} A^*$$

$$A + A^* \xrightarrow{k_f^A} [AA^*] \xrightarrow{k_{cat}^A} 2A^*$$

$$PPase + A^* \xrightarrow{k_f^P} [PPaseA^*] \xrightarrow{k_{cat}^P} PPase + A$$

$$N + A^? \xrightarrow{k_f^N} [NA^?], \quad ? \in \{, *\}$$

$$[AN] + A^* \xrightarrow{k^+} [ANA^*] \xrightarrow{k^-} [A^*N] + A^*$$

$$[A^*N] + A \xrightarrow{k^+} [ANA^*]$$

## model

$$(\partial_{t} - D\Delta) A = -k_{cis}A - k_{f}^{A}A^{*}A - k^{+} [NA^{*}] A$$

$$+ k_{r}^{A} [AA^{*}] + k_{cat}^{P} [PPaseA^{*}] - k_{f}^{N}NA + k_{r}^{N} [NA] + k^{-} [ANA^{*}]$$

$$(\partial_{t} - D\Delta) A^{*} = k_{cis}A - k_{f}^{A}AA^{*} + k_{r}^{A} [AA^{*}] + 2k_{cat}^{A} [AA^{*}] - k_{f}^{P}PPaseA^{*} + k_{r}^{P} [PPaseA^{*}] - k_{f}^{N}NA^{*} + k_{r}^{N} [NA^{*}]$$

$$- k^{+} [NA]A^{*} + (k^{-} + k_{*}^{-})[ANA^{*}]$$

$$(\partial_{t} - D\Delta)[AA^{*}] = k_{f}^{A}AA^{*} - (k_{r}^{A} + k_{cat}^{A})[AA^{*}] \quad ? \approx 0?$$

$$(\partial_{t} - D\Delta)PPase = (k_{r}^{P} + k_{cat}^{P})[PPaseA^{*}] - k_{f}^{P}PPaseA^{*} \approx 0$$

$$(\partial_{t} - D\Delta)[PPaseA^{*}] = k_{f}^{P}PPaseA^{*} - (k_{r}^{P} + k_{cat}^{P})[PPaseA^{*}] \approx 0$$

$$\partial_{t}N = -k_{f}^{N}N(A + A^{*}) + k_{r}^{N}([NA] + [NA^{*}])$$

$$\partial_{t}[NA] = k_{f}^{N}NA - (k_{r}^{N} + k^{+}A^{*})[NA] + k^{-}[ANA^{*}]$$

$$\partial_t[NA^*] = k_f^N NA^* - (k_r^N + k^+ A) [NA^*] + (k^- + k_*^-) [ANA^*]$$

$$\partial_t[ANA^*] = -(2k^- + k_*^-) [ANA^*] + k^+ ([NA]A^* + [NA^*]A)$$

$$N + [NA] + [NA^*] + [ANA^*] = N_0$$
(1)

## preobrazovaniya

 $(??) \Rightarrow$ 

$$(\partial_t - D\Delta)A = -k_{cis}A - k_f^A A A^* - k^+ [NA^*]A + k_r^A [AA^*] + k_{cat}^P [PPaseA^*] - k_f^N A (N_0 - [NA^*] - [ANA^*]) + (k_r^N + k_f^N A)[NA] + k^- [ANA^*]$$

$$\begin{split} (\partial_t - D\Delta)A^* &= k_{cis}A - k_f^A A A^* + k_r^A [AA^*] + 2k_{cat}^A [AA^*] - k_f^P P P ase A^* + k_r^P [P P ase A^*] \\ &- k_f^N N_0 A^* + (k_r^N + k_f^N A^*) [NA^*] + (k_f^N - k^+) [NA] A^* + (k^- + k_r^- + k_f^N A^*) [ANA^*] \\ &\qquad (\partial_t - D\Delta) [AA^*] = k_f^A A A^* - (k_r^A + k_{cat}^A) [AA^*] \\ &\qquad (\partial_t - D\Delta) P P ase = (k_r^P + k_{cat}^P) [P P ase A^*] - k_f^P P P ase A^* \approx 0 \\ &\qquad (\partial_t - D\Delta) [P P ase A^*] = k_f^P P P ase A^* - (k_r^P + k_{cat}^P) [P P ase A^*] \approx 0 \\ &\qquad \partial_t [NA] = k_f^N A (N_0 - [NA^*]) - (k_r^N + k^+ A^* + k_f^N A) [NA] + (k^- - k_f^N A) [ANA^*] \\ &\qquad \partial_t [NA^*] = k_f^N A^* (N_0 - [NA]) - (k_r^N + k_f^N A^* + k^+ A) [NA^*] + (k^- + k_r^- - k_f^N A) [ANA^*] \\ &\qquad \partial_t [ANA^*] = -(2k^- + k^+) [ANA^*] + k^+ ([NA]A^* + [NA^*]A) \end{split}$$

measureless

$$A^{?} = A_0 a^{?}; \quad PPase = \Pi_0 p; \quad N = \nu_0 n; \quad \tau = 1/k_{cis}$$

$$?[AA^*] = A_0[aa^*]? \quad ?[PPaseA^*] = A_0[pa^*]? \quad ?[NA^?] = A_0[na^?]?$$

$$\Delta \to \frac{\Delta}{L^2}; \quad \partial_t \to \frac{\partial_t}{\tau}$$

$$(\partial_t - \frac{\tau D\Delta}{L^2})a = -a - \tau k_f^A A_0 a a^* - \tau k^+ A_0 [na^*] a + \tau k_r^A [aa^*] + \tau k_{cat}^P [pa^*]$$
$$- \tau k_f^N \nu_0 a (n_0 - \frac{A_0}{\nu_0} [na^*] - \frac{A_0}{\nu_0} [ana^*]) + \tau (k_r^N + k_f^N A_0 a) [na] + \tau k^- [ana^*]$$

$$(\partial_t - \frac{\tau D\Delta}{L^2})a^* = a - \tau k_f^A A_0 a a^* + \tau k_r^A [aa^*] + 2\tau k_{cat}^A [aa^*] - \tau k_f^P \Pi_0 p a^* + \tau k_r^P [pa^*] - \tau k_f^N \nu_0 n_0 a^* + \tau (k_r^N + k_f^N A_0 a^*) [na^*] + \tau (k_f^N - k^+) [na] A_0 a^* + \tau (k^- + k_*^- + k_f^N A_0 a^*) [ana^*]$$

$$(\partial_t - \frac{\tau D\Delta}{L^2})[aa^*] = \tau k_f^A A_0 aa^* - \tau (k_r^A + k_{cat}^A)[aa^*]$$
 
$$(\partial_t - \frac{\tau D\Delta}{L^2})p = \frac{\tau}{\Pi_0} (k_r^P + k_{cat}^P) A_0[pa^*] - \tau k_f^P p A_0 a^* \approx 0$$
 
$$(\partial_t - \frac{\tau D\Delta}{L^2})[pa^*] = \tau k_f^P \Pi_0 p a^* - \tau (k_r^P + k_{cat}^P)[pa^*] \approx 0$$
 
$$\partial_t [na] = \tau k_f^N \nu_0 a (n_0 - \frac{A_0}{\nu_0} [NA^*]) - \tau (k_r^N + k^+ A_0 a^* + k_f^N A_0 a)[na] + \tau (k^- - k_f^N A_0 a)[ana^*]$$
 
$$\partial_t [na^*] = \tau k_f^N \nu_0 a^* (n_0 - \frac{A_0}{\nu_0} [na]) - \tau (k_r^N + k_f^N A_0 a^* + k^+ A_0 a)[na^*] + \tau (k^- + k_*^- - k_f^N A_0 a)[ana^*]$$
 
$$\partial_t [ana^*] = -\tau (2k^- + k^+)[ana^*] + \tau k^+ A_0 ([na]a^* + [na^*]a)$$

further

$$d = \frac{\tau D}{L^2}$$
 
$$\kappa_f^a = \tau k_f^A A_0; \quad \kappa^+ = \tau k^+ A_0$$
 
$$\kappa_f^p = \tau k_f^P \Pi_0 \dots$$
 
$$\kappa_f^n = \tau k_f^N \nu_0 \dots$$
 
$$\kappa_r^? = \tau k_r^?; \quad \kappa^- = \tau k^-; \quad \kappa_{cat}^? = \tau k_{cat}^?$$
 
$$\alpha_0 = \frac{A_0}{\nu_0}; \quad \beta_0 = \frac{A_0}{\Pi_0}$$

$$(\partial_t - d)a = -a - \kappa_f^a a a^* - \kappa^+ [na^*] a + \kappa_r^a [aa^*] + \kappa_{cat}^p [pa^*] - \kappa_f^n a (n_0 - \alpha_0([na] + [na^*] + [ana^*])) + \kappa_r^n [na] + \kappa^- [ana^*]$$

$$\begin{split} (\partial_{t}-d)a^{*} &= a - \kappa_{f}^{a}aa^{*} + \kappa_{r}^{a}[aa^{*}] + 2\kappa_{cat}^{a}[aa^{*}] - \kappa_{f}^{p}pa^{*} + \kappa_{r}^{p}[pa^{*}] \\ &- \kappa_{f}^{n}n_{0}a^{*} + (\kappa_{r}^{n} + \kappa_{f}^{n}\alpha_{0}a^{*})[na^{*}] + (\alpha_{0}\kappa_{f}^{n} - \kappa^{+})[na]a^{*} + (\kappa^{-} + \kappa_{*}^{-} + \kappa_{f}^{n}a^{*})[ana^{*}] \\ &(\partial_{t}-d)[aa^{*}] = \kappa_{f}^{a}aa^{*} - (\kappa_{r}^{a} + \kappa_{cat}^{a})[aa^{*}] \\ &(\partial_{t}-d)p = \beta_{0}(\kappa_{r}^{p} + \kappa_{cat}^{p})[pa^{*}] - \beta_{0}\kappa_{f}^{p}pa^{*} \approx 0 \\ &(\partial_{t}-d)[pa^{*}] = \kappa_{f}^{p}pa^{*} - (\kappa_{r}^{p} + \kappa_{cat}^{p})[pa^{*}] \approx 0 \\ &\partial_{t}[na] = \kappa_{f}^{n}a(n_{0} - \alpha_{0}[na^{*}]) - (\kappa_{r}^{n} + \kappa^{+}a^{*} + \kappa_{f}^{n}\alpha_{0}a)[na] + (\kappa^{-} - \kappa_{f}^{n}\alpha_{0}a)[ana^{*}] \\ &\partial_{t}[na^{*}] = \kappa_{f}^{n}a^{*}(n_{0} - \alpha_{0}[na]) - (\kappa_{r}^{n} + \kappa_{f}^{n}\alpha_{0}a^{*} + \kappa^{+}a)[na^{*}] + (\kappa^{-} + \kappa_{*}^{-} - \kappa_{f}^{n}\alpha_{0}a)[ana^{*}] \end{split}$$

$$\partial_t [ana^*] = -(2\kappa^- + \kappa^+)[ana^*] + \kappa^+ ([na]a^* + [na^*]a)$$

finally

$$p \approx 1$$

$$[pa^*] \approx \frac{\kappa_f^p}{\kappa_r^p + \kappa_{cat}^p} a^* = \kappa_M a^*$$

$$(\partial_t - d)a = -a - \kappa_f^a a a^* - \kappa^+ [na^*] a + \kappa_r^a [aa^*] + \kappa_{cat}^p \kappa_M a^* - \kappa_f^a a (n_0 - \alpha_0([na] + [na^*] + [ana^*])) + \kappa_r^n [na] + \kappa^- [ana^*]$$

$$(\partial_{t} - d)a^{*} = a - \kappa_{f}^{a}aa^{*} + \kappa_{r}^{a}[aa^{*}] + 2\kappa_{cat}^{a}[aa^{*}] + (\kappa_{M}\kappa_{r}^{p} - \kappa_{f}^{p})a^{*}$$
$$- \kappa_{f}^{n}n_{0}a^{*} + (\kappa_{r}^{n} + \kappa_{f}^{n}\alpha_{0}a^{*})[na^{*}] + (\alpha_{0}\kappa_{f}^{n} - \kappa^{+})[na]a^{*} + (\kappa^{-} + \kappa_{*}^{-} + \kappa_{f}^{n}\alpha_{0}a^{*})[ana^{*}]$$
$$(\partial_{t} - d)[aa^{*}] = \kappa_{f}^{a}aa^{*} - (\kappa_{r}^{a} + \kappa_{cat}^{a})[aa^{*}]$$

$$\partial_t[na] = \kappa_f^n a(n_0 - \alpha_0[na^*]) - (\kappa_r^n + \kappa^+ a^* + \kappa_f^n \alpha_0 a)[na] + (\kappa^- - \kappa_f^n \alpha_0 a)[ana^*]$$

$$\partial_t[na^*] = \kappa_f^n a^*(n_0 - \alpha_0[na]) - (\kappa_r^n + \kappa_f^n \alpha_0 a^* + \kappa^+ a)[na^*] + (\kappa^- + \kappa_*^- - \kappa_f^n \alpha_0 a)[ana^*]$$

$$\partial_t [ana^*] = -(2\kappa^- + \kappa^+)[ana^*] + \kappa^+ ([na]a^* + [na^*]a)$$

и всё бы ничего, но

$$?[ANA^*] = [A^*NA]?$$

$$[AN] + A^* \rightleftharpoons [ANA^*] \rightarrow [A^*N] + A^*$$

$$[A^*N] + A \rightleftharpoons [A^*NA] \rightarrow [A^*N] + A^*$$