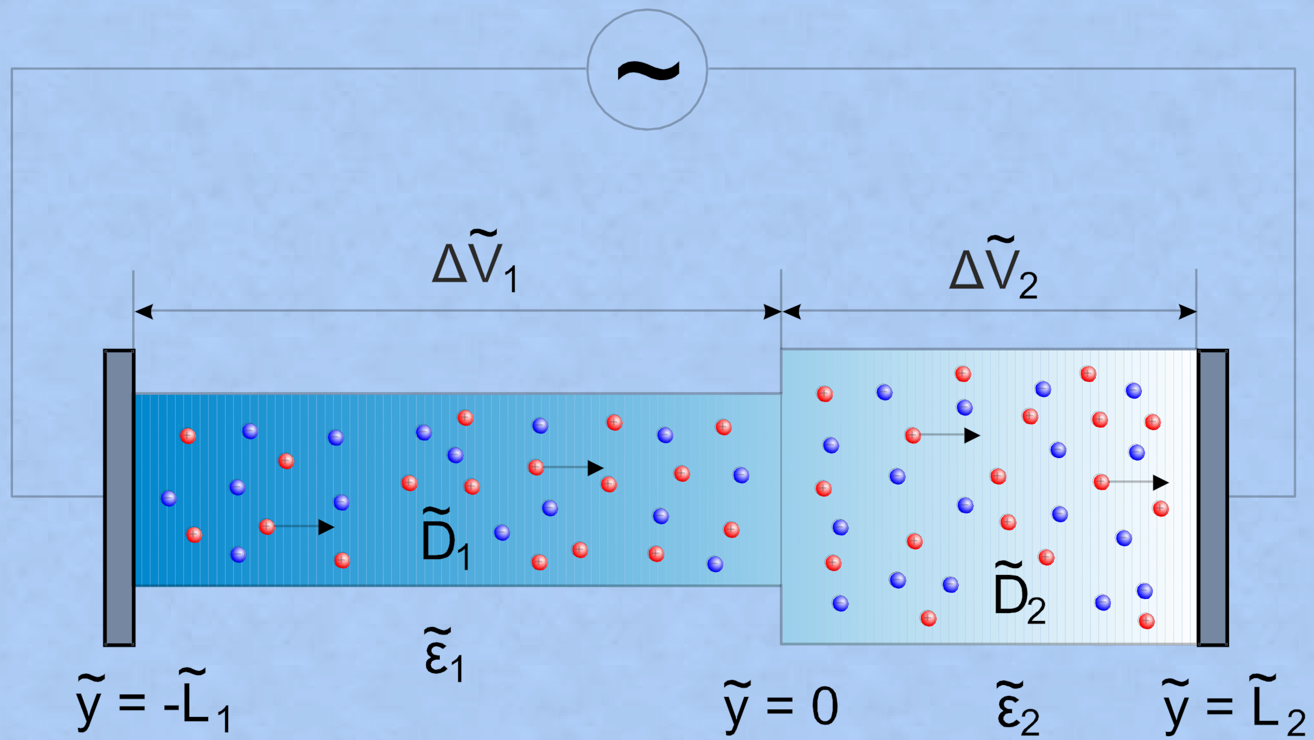
Доклад по теме: «Математическое моделирование явления ассиметричной концентрационной поляризации в растворе электролита»

Авторы: Е.В. Горбачева, Е.А. Франц, Г.С. Ганченко

Постановка



Процесс описывается системой Нерста-Планка-Пуассона

$$-\tilde{L}_1 < \tilde{y} < 0$$

$$\frac{\partial \tilde{c}^+}{\partial \tilde{t}} = \frac{\tilde{D}_1 \tilde{F}}{\tilde{R}\tilde{T}} \frac{\partial}{\partial \tilde{y}}\left(\tilde{c}^+ \frac{\partial \tilde{\Phi}}{\partial \tilde{y}}\right) + \tilde{D}_1 \frac{\partial^2 \tilde{c}^+}{\partial \tilde{y}^2},$$

$$\frac{\partial \tilde{c}^-}{\partial \tilde{t}} = -\frac{\tilde{D}_1 \tilde{F}}{\tilde{R}\tilde{T}} \frac{\partial}{\partial \tilde{y}}\left(\tilde{c}^- \frac{\partial \tilde{\Phi}}{\partial \tilde{y}}\right) + \tilde{D}_1 \frac{\partial^2 \tilde{c}^-}{\partial \tilde{y}^2},$$

$$\frac{\partial^2 \tilde{\Phi}}{\partial \tilde{y}^2} = \frac{\tilde{F}}{\tilde{\varepsilon}_1}\left(\tilde{c}^- - \tilde{c}^+\right).$$

$$0 < \tilde{y} < \tilde{L}_2$$

$$\frac{\partial \tilde{s}^+}{\partial \tilde{t}} = \frac{\tilde{D}_2 \tilde{F}}{\tilde{R}\tilde{T}} \frac{\partial}{\partial \tilde{y}}\left(\tilde{s}^+ \frac{\partial \tilde{\varphi}}{\partial \tilde{y}}\right) + \tilde{D}_2 \frac{\partial^2 \tilde{s}^+}{\partial \tilde{y}^2},$$

$$\frac{\partial \tilde{s}^-}{\partial \tilde{t}} = -\frac{\tilde{D}_2 \tilde{F}}{\tilde{R}\tilde{T}} \frac{\partial}{\partial \tilde{y}}\left(\tilde{s}^- \frac{\partial \tilde{\varphi}}{\partial \tilde{y}}\right) + \tilde{D}_2 \frac{\partial^2 \tilde{s}^-}{\partial \tilde{y}^2},$$

$$\frac{\partial^2 \tilde{\varphi}}{\partial \tilde{y}^2} = \frac{\tilde{F}}{\tilde{\varepsilon}_2}\left(\tilde{c}^- - \tilde{c}^+\right).$$

Краевые условия

$$\tilde{y}=0: \qquad \tilde{c}^{+}=\tilde{s}^{+}, \quad \tilde{c}^{-}=\tilde{s}^{-},$$

$$\frac{\tilde{D}_1\tilde{A}_1\tilde{F}}{\tilde{R}\tilde{T}}\tilde{c}^{+}\frac{\partial\tilde{\Phi}}{\partial\tilde{y}}+\tilde{D}_1\tilde{A}_1\frac{\partial\tilde{c}^{+}}{\partial\tilde{y}}=\frac{\tilde{D}_2\tilde{A}_2\tilde{F}}{\tilde{R}\tilde{T}}\tilde{s}^{+}\frac{\partial\tilde{\varphi}}{\partial\tilde{y}}+\tilde{A}_2\tilde{D}_2\frac{\partial\tilde{s}^{+}}{\partial\tilde{y}},$$

$$-\frac{\tilde{D}_1\tilde{A}_1\tilde{F}}{\tilde{R}\tilde{T}}\tilde{c}^{-}\frac{\partial\tilde{\Phi}}{\partial\tilde{y}}+\tilde{D}_1\tilde{A}_1\frac{\partial\tilde{c}^{-}}{\partial\tilde{y}}=-\frac{\tilde{D}_2\tilde{A}_2\tilde{F}}{\tilde{R}\tilde{T}}\tilde{s}^{-}\frac{\partial\tilde{\varphi}}{\partial\tilde{y}}+\tilde{A}_2\tilde{D}_2\frac{\partial\tilde{s}^{-}}{\partial\tilde{y}},$$

$$\tilde{\Phi}=\tilde{\varphi}, \quad \tilde{\varepsilon}_1\frac{\partial\tilde{\Phi}}{\partial\tilde{y}}=\tilde{\varepsilon}_2\frac{\partial\tilde{\varphi}}{\partial\tilde{y}}+\tilde{\sigma},$$

$$\tilde{y}=-\tilde{L}_1: \qquad \frac{\tilde{F}\tilde{D}_1}{\tilde{R}\tilde{T}}\tilde{c}^{+}\frac{\partial\tilde{\Phi}}{\partial\tilde{y}}+\tilde{D}_1\frac{\partial\tilde{c}^{+}}{\partial\tilde{y}}=\tilde{Q}\left(\tilde{c}^{+},\Delta\tilde{\Phi}\right),$$

$$\tilde{\Phi}=-\frac{\Delta\tilde{V}}{2}\cos\tilde{\Omega}\tilde{t}-\Delta\tilde{\Phi}, \quad \frac{\tilde{F}\tilde{c}^{-}}{\tilde{R}\tilde{T}}\frac{\partial\tilde{\Phi}}{\partial\tilde{y}}+\frac{\partial\tilde{c}^{-}}{\partial\tilde{y}}=0,$$

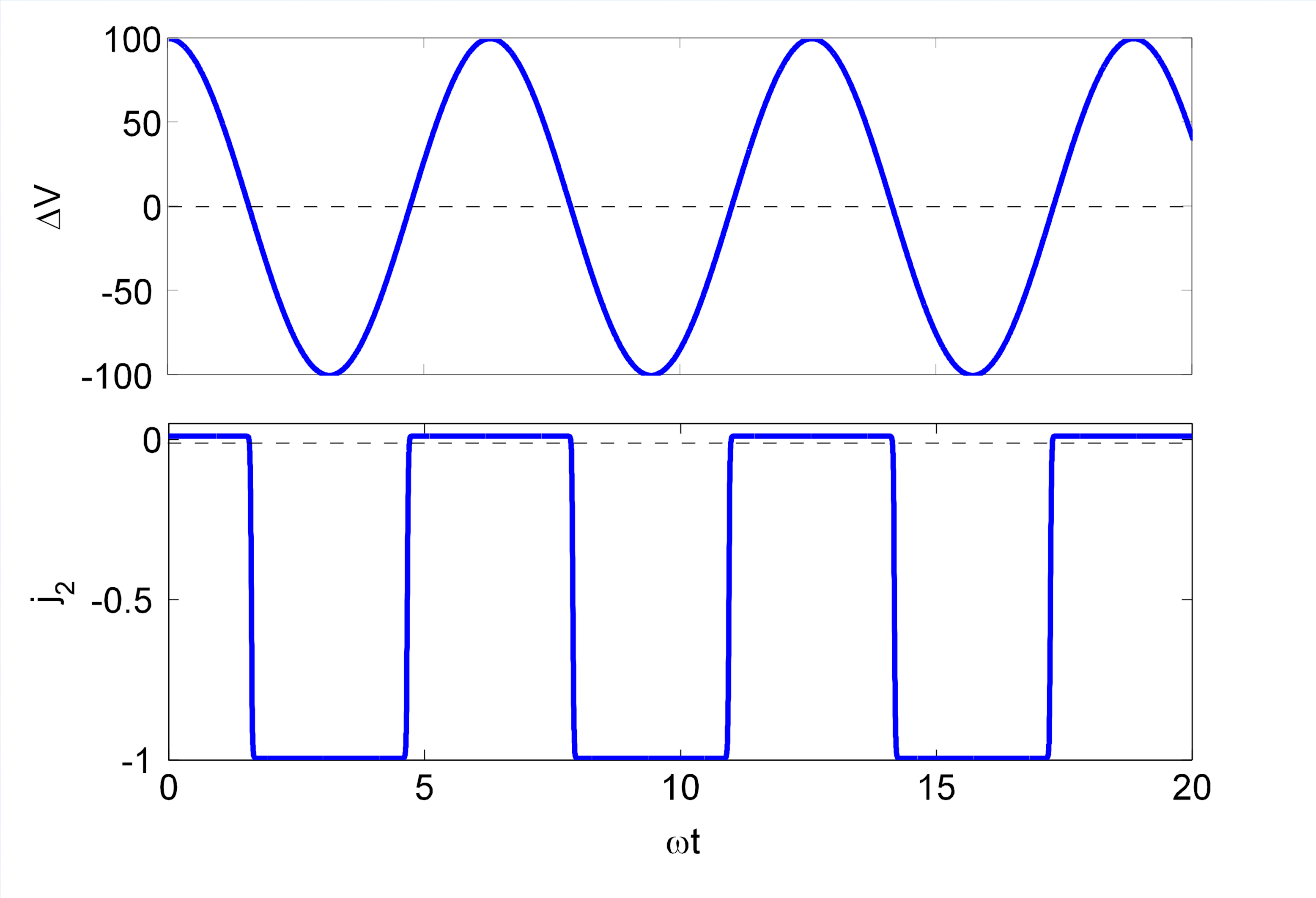
$$\tilde{y}=\tilde{L}_2: \qquad -\frac{\tilde{F}\tilde{D}_2}{\tilde{R}\tilde{T}}\tilde{s}^{+}\frac{\partial\tilde{\varphi}}{\partial\tilde{y}}-\tilde{D}_2\frac{\partial\tilde{s}^{+}}{\partial\tilde{y}}=\tilde{Q}\left(\tilde{s}^{+},\Delta\tilde{\Phi}\right),$$

$$\tilde{\Phi}=\frac{\Delta\tilde{V}}{2}\cos\tilde{\Omega}\tilde{t}-\Delta\tilde{\Phi}, \quad -\frac{\tilde{F}\tilde{s}^{-}}{\tilde{R}\tilde{T}}\frac{\partial\tilde{\varphi}}{\partial\tilde{y}}+\frac{\partial\tilde{s}^{-}}{\partial\tilde{y}}=0.$$

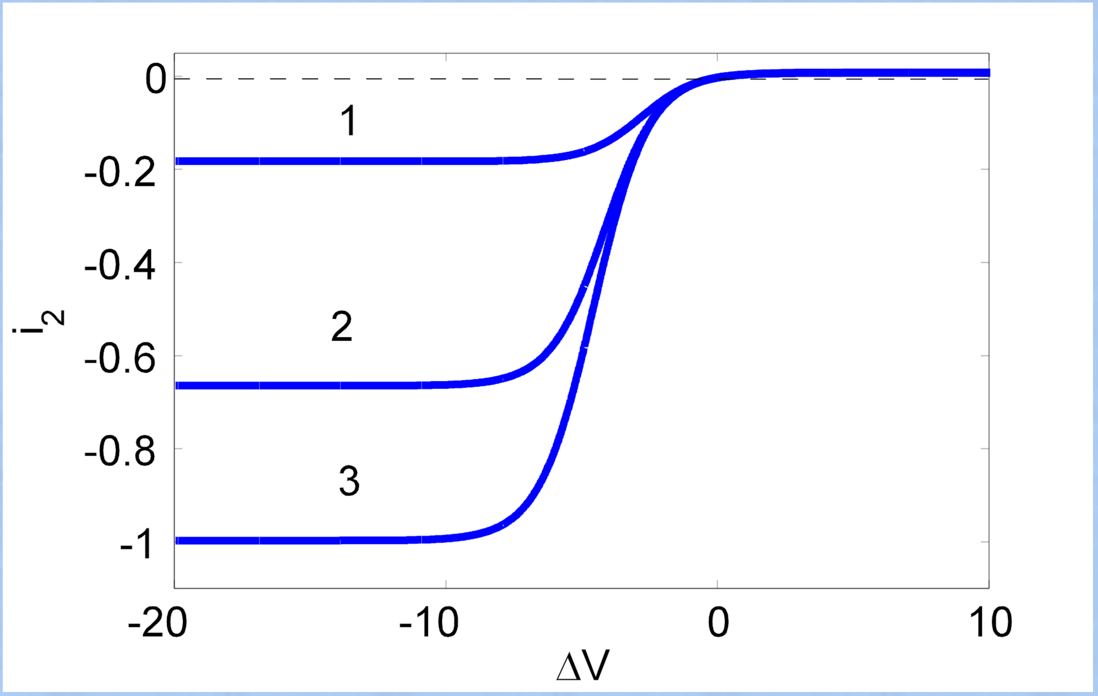
Наиболее важные параметры

$$\alpha = \frac{\tilde{D}_2}{\tilde{D}_1}\frac{\tilde{L}_1}{\tilde{L}_2}, \quad \gamma = \frac{\tilde{L}_1}{\tilde{L}_1 + \tilde{L}_2}.$$

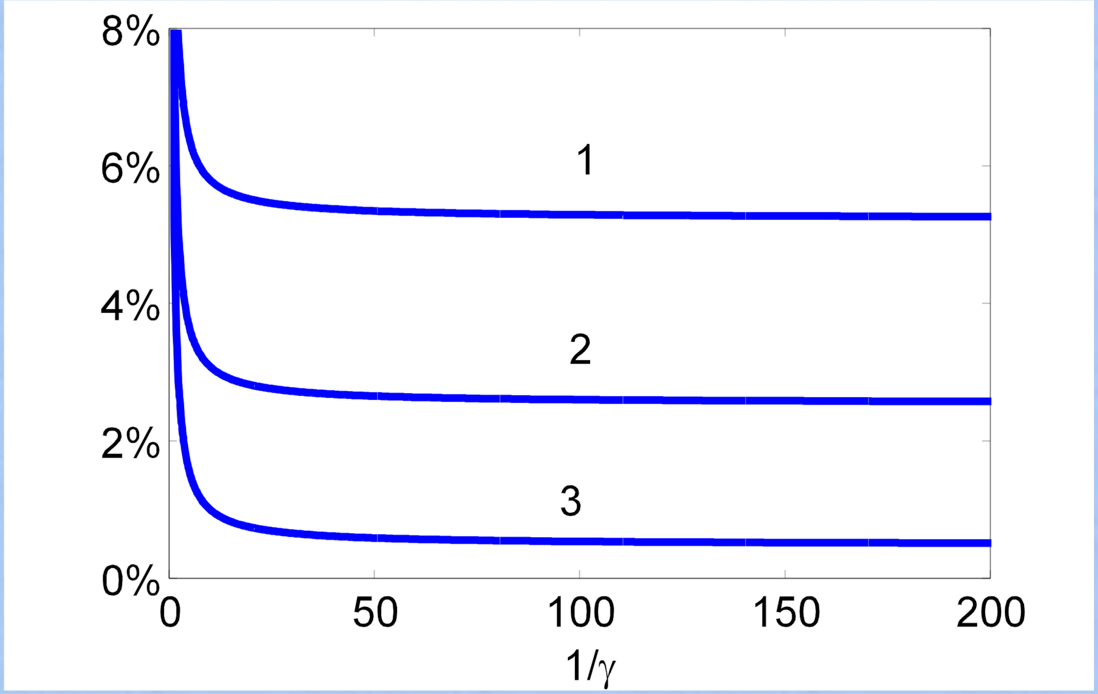
Типичное изменение во времени разности потенциала на клеммах и выпрямленного тока



Вольт-амперные характеристики при разных γ и α=100



Зависимость качества выпрямления от параметра γ



Спасибо за внимание

$$\tilde{Q}(\tilde{c}^{+},\Delta\tilde{\Phi})=\tilde{k}_{c}\cdot\tilde{c}^{+}\exp\left(-\frac{\tilde{\alpha}_{c}\tilde{F}\Delta\tilde{\Phi}}{\tilde{R}\tilde{T}}\right)-\tilde{k}_{a}\cdot\tilde{c}_{M}\exp\left(\frac{\tilde{\alpha}_{a}\tilde{F}\Delta\tilde{\Phi}}{\tilde{R}\tilde{T}}\right),$$

$$t=0,\quad \tilde{c}^{+}=\tilde{c}_{0},\quad \tilde{c}^{-}=\tilde{c}_{0},$$

$$\tilde{A}_{1}\int_{-\tilde{L}_{1}}^{0}\tilde{c}^{-}d\tilde{y}+\tilde{A}_{2}\int_{0}^{\tilde{L}_{2}}\tilde{s}^{-}d\tilde{y}=\tilde{c}_{0}\left(\tilde{A}_{1}\tilde{L}_{1}+\tilde{A}_{2}\tilde{L}_{2}\right).$$

$$\tilde{j}=\frac{\tilde{D}_{2}\tilde{F}^{2}}{\tilde{R}\tilde{T}}\tilde{s}^{+}\frac{\partial\tilde{\varphi}}{\partial\tilde{y}}+\tilde{D}_{2}\tilde{F}\frac{\partial\tilde{s}^{+}}{\partial\tilde{y}}.$$