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On energy estimates for electro-reaction-diffusion systems involving fast reactions

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Electro-reaction-diffusion system

X_i	species, $i = 1, \ldots, m$	q_i	charge numbers
v_i	chem. pot.	$u_i = \widehat{u}_i g_i(v_i - \widehat{v}_i)$	part. densities
v_0	electrostat. pot.	$u_0 = \sum_{i=1}^m q_i u_i$	charge density
		$\zeta_i = v_i + q_i v_0$	electrochem. pot.

mass fluxes:

$$j_i = -d_i(\cdot, v_i, \nabla\zeta_i)$$

reactions:

$$\alpha_1 X_1 + \cdots + \alpha_m X_m \rightleftharpoons \beta_1 X_1 + \cdots + \beta_m X_m$$

reaction rates:

$$R_i = \sum_{(\alpha,\,\beta)\in\mathcal{R}} k_{\alpha\beta}\Big(\prod_{k=1}^m e^{\alpha_k\zeta_k} - \prod_{k=1}^m e^{\beta_k\zeta_k}\Big)(\alpha_i - \beta_i)$$

differential equations:

$$\boxed{\begin{aligned}
\frac{\partial u_i}{\partial t} + \nabla\cdot j_i + R_i &= 0 \quad \text{on } \mathbb{R}_+ \times \Omega \\
\nu\cdot j_i &= 0 \quad \text{on } \mathbb{R}_+ \times \Gamma \\
u_i(0) &= U_i \ \text{ on } \Omega, \quad i = 1, \ldots, m, \\
-\nabla\cdot(\varepsilon\nabla v_0) &= f^\Omega + u_0 \quad \text{on } \mathbb{R}_+ \times \Omega \\
\nu\cdot(\varepsilon\nabla v_0) + \tau v_0 &= 0 \ \text{ on } \mathbb{R}_+ \times \Gamma_N \\
v_0 &= 0 \ \text{ on } \mathbb{R}_+ \times \Gamma_D
\end{aligned}}$$

Weak formulation

variables:

$$\boldsymbol{v} = (v_0, v_1, \ldots, v_m) \in \boldsymbol{X} = H_0^1(\Omega \cup \Gamma_N) \times H^1(\Omega, \mathbb{R}^m)$$

$$\boldsymbol{u} = (u_0, u_1, \ldots, u_m) \in \boldsymbol{X}^*, \quad \boldsymbol{U} = \Big(\sum_{i=1}^{m} q_i U_i, U_1, \ldots, U_m\Big)$$

operators:

$$A\colon \boldsymbol{X} \cap L^\infty(\Omega, \mathbb{R}^{m+1}) \to \boldsymbol{X}^*, \;\; E = (E_0, \ldots, E_m)\colon \boldsymbol{X} \to \boldsymbol{X}^*$$

$$\langle A\,v, \overline{v}\rangle_X := \int_\Omega \Big\{ \sum_{i=1}^{m} d_i(\cdot, v_i, \nabla\zeta_i) \cdot \nabla\overline{\zeta}_i + \sum_{(\alpha,\,\beta)\in\mathcal{R}} k_{\alpha\beta}\Big(\prod_{k=1}^{m} e^{\alpha_k\zeta_k} - \prod_{k=1}^{m} e^{\beta_k\zeta_k}\Big)(\alpha - \beta)\cdot\overline{\zeta}\Big\}\,\mathrm{d}x$$

$$\langle Ev, \overline{v}\rangle_X := \langle E_0 v_0, \overline{v}_0\rangle + \int_\Omega \sum_{i=1}^{m} \widehat{u}_i g_i(v_i - \widehat{v}_i)\overline{v}_i\,\mathrm{d}x, \quad \overline{v} \in X,$$

$$\langle E_0 v_0, \overline{v}_0\rangle_{H_0^1(\Omega\cup\Gamma_N)} := \int_\Omega (\varepsilon\nabla v_0 \cdot \nabla\overline{v}_0 - f v_0)\,\mathrm{d}x + \int_{\Gamma_N} \tau v_0 \overline{v}_0\,\mathrm{d}\Gamma$$

Problem (P):

$$\boxed{\begin{array}{l} u'(t) + A\,v(t) = 0,\;\; u(t) = Ev(t) \text{ f.a.a. } t \in \mathbb{R}_+\,; \quad u(0) = U \\ u \in H^1_{\mathrm{loc}}(\mathbb{R}_+, X^*),\;\; v \in L^2_{\mathrm{loc}}(\mathbb{R}_+, X) \cap L^\infty_{\mathrm{loc}}(\mathbb{R}_+, L^\infty(\Omega, \mathbb{R}^{m+1})) \end{array}}$$

stochiometric subspace:

$$\mathcal{S} := \operatorname{span}\{\alpha - \beta : (\alpha, \beta) \in \mathcal{R}\}$$

$$\mathcal{U} := \Big\{ u \in X^* \colon u_0 = \sum_{i=1}^{m} q_i u_i, \ (\langle u_1, 1 \rangle_{H^1}, \ldots, \langle u_m, 1 \rangle_{H^1}) \in \mathcal{S} \Big\}$$

$$\mathcal{U}^\perp := \Big\{ v \in X \colon \langle u, v \rangle_X = 0 \quad \forall u \in \mathcal{U} \Big\}$$

Invariants:

If (u, v) is a solution of (P) then

$$u(t) \in \mathcal{U} + U \quad \forall t \in \mathbb{R}_+$$

Stationary problem (S):

$$\boxed{\begin{aligned} &(u^*, v^*) \colon \ Av^* = 0, \ u^* = Ev^*, \\ &u^* \in \mathcal{U} + U, \ v^* \in X \cap L^\infty(\Omega, \mathbb{R}^{m+1}) \end{aligned}}$$

Energy estimates for (P)

E strictly monotone potential operator

$$E(v) = \partial\Phi(v), \quad \Phi\colon X \to \mathbb{R},$$

$$\Phi(v) = \int_\Omega \Big\{ \frac{\varepsilon}{2}|\nabla v_0|^2 - f v_0 + \sum_{i=1}^m \int_0^{v_i} \widehat{u}_i g_i(y - \widehat{v}_i)\,\mathrm{d}y \Big\}\,\mathrm{d}x + \int_{\Gamma_N} \frac{\tau}{2} v_0^2\,\mathrm{d}\Gamma$$

free energy $\quad F\colon X^* \to \overline{\mathbb{R}}, \quad F(u) := \Phi^*(u)$

Φ, F proper, convex, semi-continuous

$$F(u) = \int_\Omega \Big\{ \frac{\varepsilon}{2}|\nabla v_0|^2 + \sum_{i=1}^m \widehat{u}_i \int_0^{v_i} (g_i(v_i - \widehat{v}_i) - g_i(y - \widehat{v}_i))\,\mathrm{d}y \Big\}\,\mathrm{d}x$$
$$+ \int_{\Gamma_N} \frac{\tau}{2} v_0^2\,\mathrm{d}\Gamma \qquad \text{where } u = Ev$$

Theorem 1 (Steady states)

There are unique minimizers

$$u^* \in X^* \text{ of } F \text{ on } \mathcal{U} + U,$$

$$v^* \in X \text{ of } \Phi + \langle U, \cdot \rangle \text{ on } \mathcal{U}^\perp.$$

(u^*, v^*) is the unique solution of (S).

Brézis formula

(u, v) solution of (P) $\Longrightarrow$

$$v(t) \in \partial F(u(t)), \quad \frac{\mathrm{d}}{\mathrm{d}t} F(u(t)) = \langle u'(t), v(t) \rangle_X \text{ f.a.a. } t \in \mathbb{R}_+$$

$$\begin{aligned} &\mathrm{e}^{\lambda t_2}(F(u(t_2)) - F(u^*)) - \mathrm{e}^{\lambda t_1}(F(u(t_1)) - F(u^*)) \\ &\quad = \int_{t_1}^{t_2} \mathrm{e}^{\lambda s} \Big\{ \lambda (F(u(s)) - F(u^*)) - \langle Av(s), v(s) \rangle_X \Big\} \, \mathrm{d}s \end{aligned}$$

$0 \leq t_1 \leq t_2, \ \lambda \in \mathbb{R}_+$

dissipation rate $\quad \langle Av, v \rangle_X \geq 0 \quad \forall v \in X \cap L^\infty(\Omega, \mathbb{R}^{m+1})$

Theorem 2 (Boundedness of the free energy)

If (u, v) is a solution of (P) then

$F(u(t))$ decays monotonously,

$F(u(t)) \leq F(U) \quad \forall t \geq 0.$

nonlinear Poincaré like inequality

For every $R > 0$ there is a $c_R > 0$ such that

$$F(Ev) - F(u^*) \le c_R \langle Av, v \rangle_X \; \forall v \in M_R$$

where

$$M_R = \Big\{ v: \; F(Ev) - F(u^*) \le R, \; Ev \in \mathcal{U} + U \Big\}$$

Theorem 3 (Exponential decay of the free energy)

There exist c, $\lambda > 0$ such that for any solution (u, v) of (P)

$$F(u(t)) - F(u^*) \le e^{-\lambda t}(F(U) - F(u^*))$$

$$\|v_0(t) - v_0^*\|_{H^1} \le c e^{-\lambda t/2}$$

$$\|u_i(t) - u_i^*\|_{L^1} \le c e^{-\lambda t/2} \quad \forall t \ge 0.$$

A. Glitzky, K. Gröger, and R. Hünlich, *Free energy and dissipation rate for reaction diffusion processes of electrically charged species*, Applicable Analysis 60 (1996), 201–217.

Problems with some fast reactions

$\mathcal{R}_0 \subset \mathcal{R}$, let for $(\alpha, \beta) \in \mathcal{R}_0$

$$k_{\alpha\beta} \to \infty \quad \Longrightarrow \quad \prod_{i=1}^{m} e^{\alpha_i \zeta_i} - \prod_{i=1}^{m} e^{\beta_i \zeta_i} = \prod_{i=1}^{m} e^{\alpha_i v_i} - \prod_{i=1}^{m} e^{\beta_i v_i} = 0$$

occur only states (u, v) with

$$\boxed{(\alpha - \beta) \cdot (v_1, \ldots, v_m) = 0 \ \forall (\alpha, \beta) \in \mathcal{R}_0 \ ; \quad (v_1, \ldots, v_m) \in \mathcal{S}_0^{\perp}}$$

$\mathcal{S}_0 := \mathrm{span}\{\alpha - \beta : \ (\alpha, \beta) \in \mathcal{R}_0\}, \quad l := \dim \mathcal{S}_0^{\perp}$

ex. linear, injective mappings $\widetilde{L} \colon \mathbb{R}^l \to \mathbb{R}^m$, $L \colon \mathbb{R}^{l+1} \to \mathbb{R}^{m+1}$

$$\boxed{\begin{aligned} (v_1, \ldots, v_m) &= \widetilde{L}(\widetilde{v}_1, \ldots, \widetilde{v}_l) \quad \text{with } \mathrm{Im}\, \widetilde{L} = \mathcal{S}_0^{\perp} \\ v = L\widetilde{v} &= \big(v_0, \widetilde{L}(\widetilde{v}_1, \ldots, \widetilde{v}_l)\big) \\ \widetilde{v} &= (v_0, \widetilde{v}_1, \ldots, \widetilde{v}_l) \end{aligned}}$$

$L \colon \widetilde{X} := H_0^1(\Omega \cup \Gamma_N) \times (H^1)^l \to H_0^1(\Omega \cup \Gamma_N) \times (H^1)^m$

- L linear, injective, continuous,
- Im L is closed in X
- $\mathcal{U}^{\perp} \subset$ Im L
- $L^* \colon H_0^1(\Omega \cup \Gamma_N)^* \times (H^1)^{*m} \to H_0^1(\Omega \cup \Gamma_N)^* \times (H^1)^{*l}$ surjective

Projection scheme

$$\left.\begin{array}{c} u'(t) + Av(t) = 0, \quad u(t) = Ev(t) \\ u(0) = U \end{array}\right\} \qquad \text{(P)}$$

set $v = L\widetilde{v}$ and apply L^* to all equations

define $\widetilde{u} = L^*u$ mass lumping

define $\widetilde{A} = L^*AL$, $\widetilde{E} = L^*EL$, $\widetilde{U} = L^*U$

Problem $(\widetilde{\mathrm{P}})$:

$$\boxed{\begin{array}{c} \widetilde{u}'(t) + \widetilde{A}\,\widetilde{v}(t) = 0, \;\; \widetilde{u}(t) = \widetilde{E}\,\widetilde{v}(t) \text{ f.a.a. } t \in \mathbb{R}_+, \\ \widetilde{u}(0) = \widetilde{U}, \\ \widetilde{u} \in H^1_{\mathrm{loc}}(\mathbb{R}_+, \widetilde{X}^*), \;\; \widetilde{v} \in L^2_{\mathrm{loc}}(\mathbb{R}_+, \widetilde{X}) \cap L^\infty_{\mathrm{loc}}(\mathbb{R}_+, L^\infty(\Omega, \mathbb{R}^{l+1})) \end{array}}$$

$\widetilde{E}(\widetilde{v}) = \partial\widetilde{\Phi}(v)$, $\quad \widetilde{\Phi}(\widetilde{v}) = \Phi(L\widetilde{v})$

free energy $\quad \widetilde{F}(\widetilde{u}) = \widetilde{\Phi}^*(\widetilde{u})$, $\quad \widetilde{F}(\widetilde{u}) = \inf\{F(u) \colon\; L^*u = \widetilde{u}\}$

if $\widetilde{F}$ is subdiff. in $\widetilde{u}$ $\Longrightarrow \widetilde{F}(\widetilde{u}) = F(u)$ with $u = \partial\Phi(L\widetilde{v}) = EL\widetilde{v}$

dissipation rate

$$\langle \widetilde{A}\widetilde{v}, \widetilde{v}\rangle_{\widetilde{X}} = \langle AL\widetilde{v}, L\widetilde{v}\rangle_X \geq 0 \quad \forall \widetilde{v} \in \widetilde{X}$$

Energy estimates and their consequences which are based on the convex structure of (P) can be carried over to $(\widetilde{\mathrm{P}})$

Stationary reduced problem $(\widetilde{\mathrm{S}})$:

$$
\begin{aligned}
&(\widetilde{\boldsymbol{u}}^*, \widetilde{\boldsymbol{v}}^*): \ \widetilde{\boldsymbol{A}}\widetilde{\boldsymbol{v}}^* = 0, \ \widetilde{\boldsymbol{u}}^* = \widetilde{\boldsymbol{E}}\widetilde{\boldsymbol{v}}^*, \\
&\widetilde{\boldsymbol{u}}^* \in \boldsymbol{L}^*[\boldsymbol{\mathcal{U}}] + \widetilde{\boldsymbol{U}}, \ \widetilde{\boldsymbol{v}}^* \in \widetilde{\boldsymbol{X}} \cap \boldsymbol{L}^\infty(\boldsymbol{\Omega}, \mathbb{R}^{l+1})
\end{aligned}
$$

Theorem 4 (Steady states)

- $(\boldsymbol{u}^*, \boldsymbol{v}^*)$ solution of (S) $\Longrightarrow$ $(\boldsymbol{L}^*\boldsymbol{u}^*, (\boldsymbol{L}|_{(\widetilde{\boldsymbol{X}}\to \mathrm{Im}\,\boldsymbol{L})})^{-1}\boldsymbol{v}^*)$ solution of $(\widetilde{\mathrm{S}})$
- $(\widetilde{\boldsymbol{u}}^*, \widetilde{\boldsymbol{v}}^*)$ solution of $(\widetilde{\mathrm{S}})$ $\Longrightarrow$ $(\boldsymbol{E}\boldsymbol{L}\widetilde{\boldsymbol{v}}^*, \boldsymbol{L}\widetilde{\boldsymbol{v}}^*)$ solution of (S)
- $(\widetilde{\mathrm{S}})$ has a unique solution $(\widetilde{\boldsymbol{u}}^*, \widetilde{\boldsymbol{v}}^*)$.

Brézis formula: $(\widetilde{u},\widetilde{v})$ solution of $(\widetilde{\mathrm{P}}) \implies$

$$\widetilde{v}(t) \in \partial \widetilde{F}(\widetilde{u}(t)), \qquad \frac{\mathrm{d}}{\mathrm{d}t}\widetilde{F}(\widetilde{u}(t)) = \langle \widetilde{u}'(t), \widetilde{v}(t)\rangle_{\widetilde{X}} \text{ f.a.a. } t \in \mathbb{R}_+$$

$$\mathrm{e}^{\lambda t_2}(\widetilde{F}(\widetilde{u}(t_2)) - \widetilde{F}(\widetilde{u}^*)) - \mathrm{e}^{\lambda t_1}(\widetilde{F}(\widetilde{u}(t_1)) - \widetilde{F}(\widetilde{u}^*))$$
$$= \int_{t_1}^{t_2} \mathrm{e}^{\lambda s}\Big\{\lambda(\widetilde{F}(\widetilde{u}(s)) - \widetilde{F}(\widetilde{u}^*)) - \langle \widetilde{A}\widetilde{v}(s), \widetilde{v}(s)\rangle_{\widetilde{X}}\Big\}\,\mathrm{d}s$$
$$0 \le t_1 \le t_2, \ \lambda \in \mathbb{R}_+$$

$(\widetilde{u},\widetilde{v})$ solution of $(\widetilde{\mathrm{P}}) \implies$

$$\widetilde{F}(\widetilde{u}) = F(EL\widetilde{v}) \text{ a.e. on } \mathbb{R}_+, \qquad \widetilde{F}(\widetilde{u}^*) = F(u^*)$$
$$\langle \widetilde{A}\widetilde{v}, \widetilde{v}\rangle_{\widetilde{X}} = \langle AL\widetilde{v}, L\widetilde{v}\rangle_X, \qquad L\widetilde{v} \in M_R,\ R = F(U) - F(u^*)$$

Theorem 5 (Energy estimates)

For any solution $(\widetilde{u},\widetilde{v})$ of $(\widetilde{\mathrm{P}})$

- $\widetilde{F}(\widetilde{u}(t))$ decays monotonously ,
- $\widetilde{F}(\widetilde{u}(t)) \le \widetilde{F}(\widetilde{U}) \le F(U) \quad \forall t \in \mathbb{R}_+$,
- $\widetilde{F}(\widetilde{u}(t)) - \widetilde{F}(\widetilde{u}^*) \le e^{-\lambda t}\big(\widetilde{F}(\widetilde{U}) - \widetilde{F}(\widetilde{u}^*)\big) \quad \forall t \in \mathbb{R}_+$.

Comparison of the models

$(\widetilde{u}, \widetilde{v})$ solution of $(\widetilde{\mathrm{P}})$, (u, v) solution of (P)

prolongated quantities:

$$\boxed{\breve{v} := L\widetilde{v}, \quad \breve{u} := EL\widetilde{v}}$$

steady states:

$$\boxed{\breve{v}^* := L\widetilde{v}^* = v^*, \quad \breve{u}^* := EL\widetilde{v}^* = u^*}$$

on trajectories of $(\widetilde{\mathrm{P}})$

$$\widetilde{F}(\widetilde{u}(t)) = F(\breve{u}(t)) \quad \text{f.a.a. } t \in \mathbb{R}_+$$

conclusions from energy estimates for (P) and $(\widetilde{\mathrm{P}})$**:**

$$\boxed{\begin{aligned} &|F(\breve{u}(t)) - F(u(t))| \le ce^{-\lambda t}, \\ &\|\breve{v}_0(t) - v_0(t)\|_{H^1} \le ce^{-\lambda t/2}, \\ &\|\breve{u}_i(t) - u_i(t)\|_{L^1} \le ce^{-\lambda t/2} \qquad \text{f.a.a. } t \in \mathbb{R}_+ \end{aligned}}$$

A. Glitzky & R. Hünlich, ***Energy estimates for electro–reaction–diffusion systems with partly fast kinetics*** **(in preparation)**

Assumptions

Ω bounded Lipschitzian domain in $\mathbb{R}^2$, $\Gamma := \partial\Omega$,
Γ_D, Γ_N disjoint open subsets of Γ, $\Gamma = \overline{\Gamma_D} \cup \overline{\Gamma_N}$,
$\overline{\Gamma_D} \cap \overline{\Gamma_N}$ consists of finitely many points;

$q_i \in \mathbb{Z}$, $\overline{v}_i$, $\overline{u}_i$, $U_i \in L^\infty(\Omega)$, $\overline{u}_i$, $U_i \geq c > 0$,
$f \in L^2(\Omega)$, $U_0 := \sum_{i=1}^m q_i U_i$, $q := (q_1, \ldots, q_m)$;
$\varepsilon \in L^\infty(\Omega)$, $\varepsilon \geq c > 0$, $\tau \in L^\infty_+(\Gamma_N)$, $\operatorname{mes}\Gamma_D + \|\tau\|_{L^1(\Gamma_N)} > 0$;

$g_i \in C^1(\mathbb{R})$, $\lim\limits_{y\to\infty} \frac{1}{y} g_i(y) = +\infty$, $\delta \min\{1, \mathrm{e}^y\} \leq g_i(y) \leq \delta^{-1}\,\mathrm{e}^y$,
$0 < \delta \min\{1, g_i(y)\} \leq g_i'(y) \leq \delta^{-1} g_i(y)\ \forall y \in \mathbb{R}$, $i = 1, \ldots, m$;

$d_i \colon \Omega \times \mathbb{R} \times \mathbb{R}^2 \to \mathbb{R}^2$ Carathéodory functions,
$\delta\, g_i(y)|\xi|^2 \leq d_i(x, y, \xi) \cdot \xi$, $|d_i(x, y, \xi)| \leq \delta^{-1} g_i(y)|\xi|$
f.a.a. $x \in \Omega$, $\forall y \in \mathbb{R}$, $\forall \xi \in \mathbb{R}^2$, $i = 1, \ldots, m$;

$\mathcal{R}$ finite subset of $\mathbb{Z}_+^m \times \mathbb{Z}_+^m$, $(\alpha - \beta) \cdot q = 0\ \ \forall(\alpha, \beta) \in \mathcal{R}$;
for $(\alpha, \beta) \in \mathcal{R}$ we define $R_{\alpha\beta} := k_{\alpha\beta}(x, y)\,(e^{\alpha\cdot\zeta} - e^{\beta\cdot\zeta})$,
$x \in \Omega$, $y = (y_0, y_1, \cdots, y_m) \in \mathbb{R}^{m+1}$,
$\zeta_i := y_i + q_i y_0$, $i = 1, \ldots, m$, where
$k_{\alpha\beta} \colon \Sigma \times \mathbb{R}^{m+1} \to \mathbb{R}_+$ Carathéodory functions,
$k_{\alpha\beta}(x, y) \geq c_R > 0$ f.a.a. $x \in \Omega$, $\forall y \in \mathbb{R}^{m+1}$ with $y_0 \in [-R, R]$;

there are no "false" equilibria in the sense of
Prigogine & Defay, *Chemical thermodynamics*, London 1954

Example:

basic pairdiffusion model

species:

$I^{(j)}$,	$j \in J_I$	intersitials
$V^{(j)}$,	$j \in J_V$	vacancies
$A^{(s)}$		dopant
$AI^{(s+j)}$,	$j \in J_{AI}$	dopant-interstitial pair
$AV^{(s+j)}$,	$j \in J_{AV}$	dopant-vacancy pair
n		electrons

$j \in J_i$ describes different charge states

reactions:

(a) generation/disintegration of dopant-defect pairs

$$A^{(s)} + I^{(\mu)} \rightleftharpoons AI^{(s+\nu)} + (\nu - \mu)n$$

$$A^{(s)} + V^{(\iota)} \rightleftharpoons AV^{(s+\kappa)} + (\kappa - \iota)n$$

(b) generation/recombination of defects

$$I^{(\mu)} + V^{(\iota)} \rightleftharpoons -(\mu + \iota)n$$

$$AI^{(s+\nu)} + V^{(\iota)} \rightleftharpoons A^{(s)} - (\nu + \iota)n$$

$$AV^{(s+\kappa)} + I^{(\mu)} \rightleftharpoons A^{(s)} - (\kappa + \mu)n$$

$$AI^{(s+\nu)} + AV^{(s+\kappa)} \rightleftharpoons 2\, A^{(s)} - (\nu + \kappa)n$$

(c) ionization of defects

$$I^{(\mu)} \rightleftharpoons I^{(\nu)} + (\nu - \mu)n$$

$$V^{(\iota)} \rightleftharpoons V^{(\kappa)} + (\kappa - \iota)n$$

(d) ionization of pairs

$$AI^{(s+\nu)} \rightleftharpoons AI^{(s+\mu)} + (\mu - \nu)n$$

$$AV^{(s+\kappa)} \rightleftharpoons AV^{(s+\iota)} + (\iota - \kappa)n$$

ionization reactions in (c) and (d) are very fast $\Longrightarrow$

reduced pairdiffusion model

lumping induced by L^* leads to total densities

$$\begin{aligned} u_I^{tot} &= \sum_{j\in J_I} u_{I(j)}, & u_V^{tot} &= \sum_{j\in J_V} u_{V(j)}, \\ u_A &= u_A, & & \\ u_{AI}^{tot} &= \sum_{j\in J_{AI}} u_{AI(s+j)}, & u_{AV}^{tot} &= \sum_{j\in J_{AV}} u_{AV(s+j)} \end{aligned}$$

model equations consist of 5 continuity equations for the species

$$I^{tot},\ V^{tot},\ A,\ AI^{tot},\ AV^{tot}$$

containing the 6 reactions

(a) generation/disintegration of dopant-defect pairs

$A + I^{tot} \rightleftharpoons AI^{tot}$

$A + V^{tot} \rightleftharpoons AV^{tot}$

(b) generation/recombination of defects

$I^{tot} + V^{tot} \rightleftharpoons \emptyset$

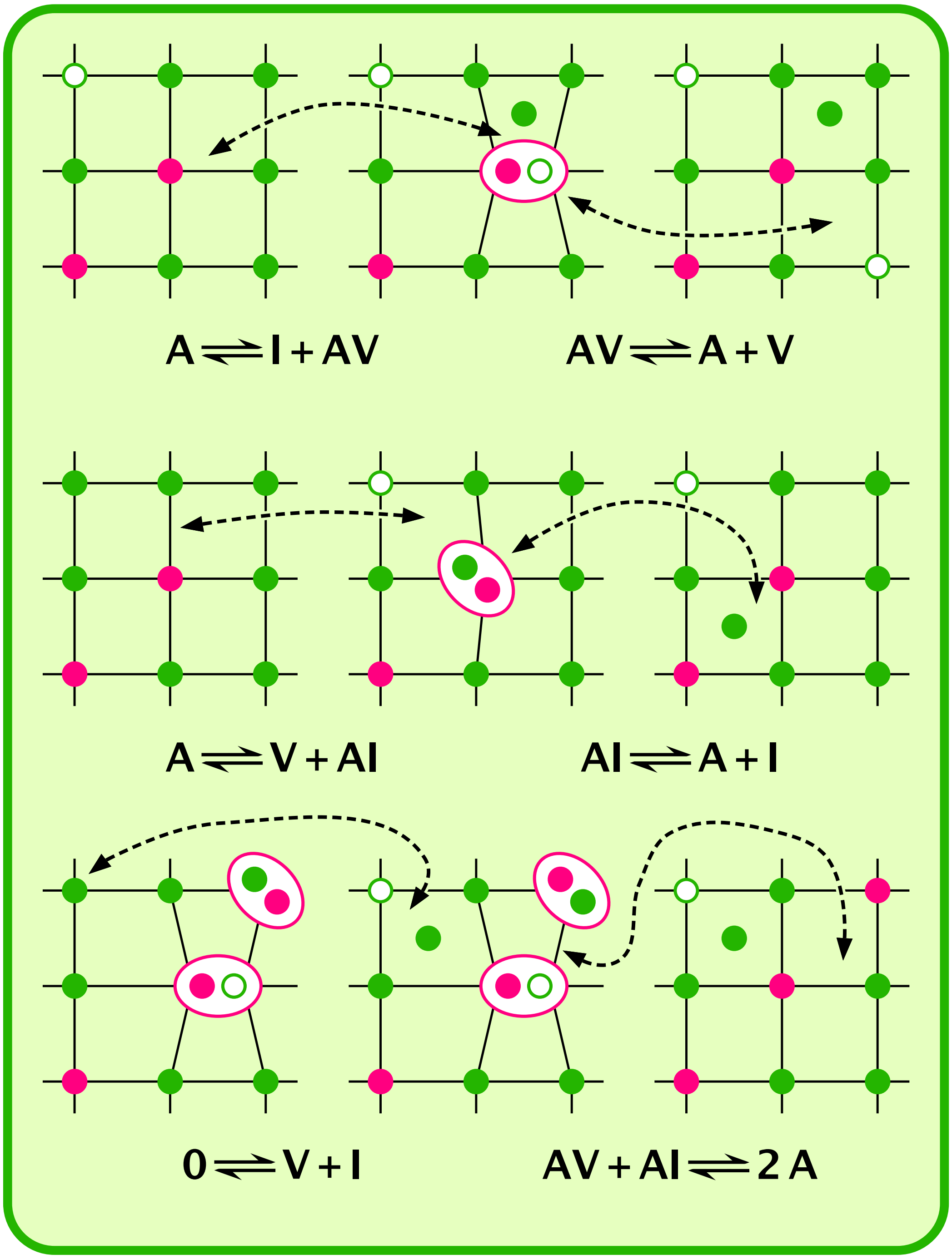
$AI^{tot} + AV^{tot} \rightleftharpoons 2\,A$

$AI^{tot} + V^{tot} \rightleftharpoons A$

$AV^{tot} + I^{tot} \rightleftharpoons A$

and a Poisson equation

A. Glitzky and R. Hünlich, *Global properties of pair diffusion models*, Adv. Math. Sci. Appl. (accepted)



		host atom on lattice site
I		host atom on interstice
V		vacancy
A		dopant atom on lattice site
AI		dopant–interstitial pair
AV		dopant–vacancy pair