Appendix: A Deterministic Mathematical Model for Bidirectional Excluded Flow with Langmuir Kinetics

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A. Proofs

We begin by discussing some symmetry properties of the MFALK.

A. *Symmetry*

The MFALK enjoys two symmetries that will be useful later on. First, let $z_i(t) := 1-x_i(t)$, $i = 1, \dots, n$. In other words, $z_i(t)$ is the amount of "free space" at site i at time t. Then using (1) yields

$$\begin{aligned}
\dot z_1 &= \gamma_0(1-z_1) + \lambda_1 z_2(1-z_1) + \alpha_1(1-z_1) - \gamma_1 z_1(1-z_2) - \lambda_0 z_1 - \beta_1 z_1,\\
\dot z_2 &= \gamma_1 z_1(1-z_2) + \lambda_2 z_3(1-z_2) + \alpha_2(1-z_2) - \gamma_2 z_2(1-z_3) - \lambda_1 z_2(1-z_1) - \beta_2 z_2,\\
&\vdots\\
\dot z_n &= \gamma_{n-1} z_{n-1}(1-z_n) + \lambda_n(1-z_n) + \alpha_n(1-z_n) - \gamma_n z_n - \lambda_{n-1} z_n(1-z_{n-1}) - \beta_n z_n.
\end{aligned} \tag{A.1}$$

This is just the MFALK (1), but with the parameters permuted as follows: $\lambda_k \to \gamma_k$, $\gamma_k \to \lambda_k$, $\beta_k \to \alpha_k$, and $\alpha_k \to \beta_k$ for all k. The symmetry here follows from the fact that we can replace the roles of the forward and backward flows in the MFALK.

Next, let $y_i(t) := 1 - x_{n+1-i}(t)$, $i = 1, \dots, n$. In other words, $y_i(t)$ is the amount of "free space" at site $n+1-i$ at time t. Then using (1) yields

$$\begin{aligned}
\dot y_1 &= \lambda_n(1-y_1) + \gamma_{n-1} y_2(1-y_1) + \alpha_n(1-y_1) - \lambda_{n-1} y_1(1-y_2) - \gamma_n y_1 - \beta_n y_1,\\
\dot y_2 &= \lambda_{n-1} y_1(1-y_2) + \gamma_{n-2} y_3(1-y_2) + \alpha_{n-1}(1-y_2) - \lambda_{n-2} y_2(1-y_3) - \gamma_{n-1} y_2(1-y_1) - \beta_{n-1} y_2,\\
&\vdots\\
\dot y_n &= \lambda_1 y_{n-1}(1-y_n) + \gamma_0(1-y_n) + \alpha_1(1-y_n) - \lambda_0 y_n - \gamma_1 y_n(1-y_{n-1}) - \beta_1 y_n.
\end{aligned} \tag{A.2}$$

This is just the MFALK (1), but with the parameters permuted as follows: $\lambda_k \to \lambda_{n-k}$, $\gamma_k \to \gamma_{n-k}$, $\beta_k \to \alpha_{n+1-k}$, and $\alpha_k \to \beta_{n+1-k}$ for all k. Note that (A.1) is simply (A.2) with the variable renaming $z_i \to y_{n+1-i}$, $i = 1, \dots, n$.

Both symmetries are reminiscent of the *particle-hole symmetry* in ASEP [2], [3]: the basic idea is that the progression of a particle from left to right is also the progression of a "hole" from right to left.

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Proof of Proposition 1. If (4) holds then the MFALK satisfies property (**BR**) in [4], and [4, Lemma 1] implies (6). If (5) holds then (A.1) satisfies property (**BR**) in [4], and this implies (6). □

Proof of Proposition (2). Write the MFALK as $\dot{x} = f(x)$. A calculation shows that the Jacobian matrix $J(x) := \frac{\partial f}{\partial x}(x)$ satisfies $J(x) = L(x) + P$, where $L(x)$ is the matrix

$$\begin{bmatrix} -\lambda_1(1-x_2)-\gamma_1 x_2 & \lambda_1 x_1+\gamma_1(1-x_1) & \dots & 0 \\ \lambda_1(1-x_2)+\gamma_1 x_2 & -\lambda_1 x_1-\gamma_1(1-x_1)-\lambda_2(1-x_3)-\gamma_2 x_3 & \dots & 0 \\ 0 & \lambda_2(1-x_3)+\gamma_2 x_3 & \dots & 0 \\ & & \vdots & \\ 0 & 0 & \dots & 0 \\ 0 & 0 & \dots & \lambda_{n-1}x_{n-1}+\gamma_{n-1}(1-x_{n-1}) \\ 0 & 0 & \dots & -\lambda_{n-1}x_{n-1}-\gamma_{n-1}(1-x_{n-1}) \end{bmatrix}, \tag{A.3}$$

and P is the diagonal matrix

$$P = \operatorname{diag}(-\lambda_0-\gamma_0-\alpha_1-\beta_1, -\alpha_2-\beta_2, \dots, -\alpha_{n-1}-\beta_{n-1}, \lambda_n-\gamma_n-\alpha_n-\beta_n). \tag{A.4}$$

Note that $L(x)$ is tridiagonal and Metzler (i.e, every off-diagonal entry is non-negative) for any $x \in C^n$.

Recall that the matrix measure $\mu_1 : \mathbb{R}^{n\times n} \to \mathbb{R}$ induced by the L_1 norm is $\mu_1(A) = \max\{c_1(A), \dots, c_n(A)\}$, where $c_i(A)$ is the sum of the elements in column i of A with off-diagonal elements taken with absolute value [10]. For the Jacobian J of the MFALK, $\mu_1(J(x)) = \eta$ for all $x \in C^n$. It is well-known (see, e.g., [1]) that this implies (7). □

Proof of Proposition (3). For $\zeta \in [0, 1/2]$, let

$$C^n_\zeta := \{x \in C^n : \ \zeta \le x_i \le 1-\zeta, \ i = 1, \dots, n\}.$$

Note that $C^n_0 = C^n$, and that C^n_ζ is a strict subcube of C^n for all $\zeta \in (0, 1/2]$. By Proposition 1, for any $\tau > 0$ there exists $\zeta = \zeta(\tau) \in (0, 1/2)$, with $\zeta(\tau) \to 0$ as $\tau \to 0$, such that

$$x(t+\tau, a) \in C^n_\zeta, \quad \text{for all } t \ge 0 \text{ and all } a \in C^n. \tag{A.5}$$

For any $x \in C^n_\zeta$ every entry L_{ij} on the sub- and super-diagonal of L in (A.3) satisfies $L_{ij} \ge \zeta s$, where $s := \min_{1\le i\le n-1}\{\lambda_i+\gamma_i\} > 0$. Combining this with [4, Theorem 4] implies that for any $\zeta \in (0, 1/2]$ there exists $\varepsilon = \varepsilon(\zeta) > 0$, and a diagonal matrix $D = \operatorname{diag}(1, q_1, q_1q_2, \dots, q_1q_2\dots q_{n-1})$, with $q_i = q_i(\varepsilon) > 0$, such that the MFALK is contractive on C^n_ζ with respect to (w.r.t.) the scaled L_1 norm defined by $|z|_{1,D} := |Dz|_1$. Furthermore, we can choose ε such that $\varepsilon(\zeta) \to 0$ as $\zeta \to 0$, and $D(\varepsilon) \to I$ as $\varepsilon \to 0$. Now Thm. 1 in [5] implies that the MFALK is contractive after a small overshoot and short transient (SOST). Prop. 4 in [5] implies that for the MFALK SOST is equivalent to SO, and this completes the proof. □

Proof of Proposition (4). We begin by recursively defining two sequences. For all integers $i \ge 1$, let

$$\begin{aligned} u_{i+1} &= 1 + \ell_1 + \ell_2 + \dots + \ell_i, \\ \ell_{i+1} &= u_i + \ell_1 + \ell_2 + \dots + \ell_{i-1}. \end{aligned} \tag{A.6}$$

with initial conditions $u_0 = u_1 = 1$, $\ell_0 = 0$, and $\ell_1 = 1$. We claim that for $k = 0, 1, \dots, n-1$, the steady-state density in site $n-k$ is generically the ratio of two polynomials in R:

$$e_{n-k} = \frac{p_k(R)}{q_k(R)}, \quad \text{with } \deg(p_k(R)) = u_k, \ \deg(q_k(R)) = \ell_k. \tag{A.7}$$

We prove this by induction on k. By (16), $e_n = aR+b$, with $a := (\lambda_n+\gamma_n+\beta_n+\alpha_n)^{-1}$ and $b := (\gamma_n+\beta_n)a$, and this proves (A.7) for $k = 0$. Using (16) again yields

$$\begin{aligned} e_{n-1} &= \frac{R + \gamma_{n-1} e_n}{\lambda_{n-1}(1 - e_n) + \gamma_{n-1} e_n} \\ &= \frac{R + \gamma_{n-1}(aR + b)}{\lambda_{n-1} + (\gamma_{n-1} - \lambda_{n-1})(aR + b)}, \end{aligned}$$

and this proves (A.7) for $k = 1$. Now assume that there exists $s \geq 2$ such that (A.7) holds for $k = 0, 1, \dots, s-1$. By (16),

$$e_{n-s} = \frac{R + \gamma_{n-s} e_{n-s+1} - g_{n-s+1}(e_{n-s+1}) - g_{n-s+2}(e_{n-s+2}) - \dots - g_{n-1}(e_{n-1})}{\lambda_{n-s}(1 - e_{n-s+1}) + \gamma_{n-s} e_{n-s+1}},$$

and applying (12) and the induction hypothesis yields

$$e_{n-s} = \frac{R + \gamma_{n-s} \frac{p_{s-1}}{q_{s-1}} + (\beta_{n-s+1} + \alpha_{n-s+1}) \frac{p_{s-1}}{q_{s-1}} + (\beta_{n-s+2} + \alpha_{n-s+2}) \frac{p_{s-2}}{q_{s-2}} + \dots + (\beta_{n-1} + \alpha_{n-1}) \frac{p_1}{q_1} + c}{\lambda_{n-s} + (\gamma_{n-s} - \lambda_{n-s}) \frac{p_{s-1}}{q_{s-1}}},$$

where $c := -\beta_{n-s+1} - \dots - \beta_{n-1}$. Multiplying the numerator and the denominator by $q_1 \dots q_{s-1}$ yields $e_{n-s} = p_s / q_s$, where

$$\begin{aligned} \deg(p_s) &= \max\{1 + \deg(q_1 \dots q_{s-1}), \deg(p_{s-1} q_1 \dots q_{s-2}), \dots, \deg(p_1 q_2 \dots q_{s-1})\}, \\ \deg(q_s) &= \max\{\deg(q_1 \dots q_{s-1}), \deg(p_{s-1} q_1 \dots q_{s-2})\}. \end{aligned}$$

By the induction hypothesis,

$$\begin{aligned} \deg(p_s) &= \max\{1 + \ell_1 + \dots + \ell_{s-1}, u_{s-1} + \ell_1 + \dots + \ell_{s-2}, \dots, u_1 + \ell_2 + \dots + \ell_{s-1}\}, \\ \deg(q_s) &= \max\{\ell_1 + \dots + \ell_{s-1}, u_{s-1} + \ell_1 + \dots + \ell_{s-2}\}. \end{aligned} \tag{A.8}$$

It is straightforward to prove that (A.6) implies that

$$\ell_i \leq u_i \leq \ell_i + 1, \quad i = 0, 1, 2, \dots. \tag{A.9}$$

Combining this with (A.8) yields $\deg(p_s) = 1 + \ell_1 + \dots + \ell_{s-1}$, and $\deg(q_s) = u_{s-1} + \ell_1 + \dots + \ell_{s-2}$. Thus, $\deg(p_s) = u_s$ and $\deg(q_s) = \ell_s$, and this completes the inductive proof of (A.7). In particular, (A.7) yields

$$e_1 = \frac{p_{n-1}(R)}{q_{n-1}(R)}, \tag{A.10}$$

with $\deg(p_{n-1}(R)) = u_{n-1},\ \deg(q_{n-1}(R)) = \ell_{n-1}$. Substituting this in the last equation of (16) yields

$$v \frac{p_{n-1}}{q_{n-1}} = z - R + \sum_{j=2}^{n-1} g_j(e_j),$$

where $v := \lambda_0 + \gamma_0 + \beta_1 + \alpha_1$, and $z := \lambda_0 + \beta_1$. Arguing as above shows that this is a polynomial equation of the form $w(R) = 0$, with $\deg(w) = 1 + \ell_1 + \dots + \ell_{n-1} = u_n$. It is straightforward to prove by induction that (A.6) implies that

$$u_k = 1 + \left\lfloor \frac{2^k}{3} \right\rfloor, \quad \ell_k = \frac{2^k - (-1)^k}{3},$$

(we note in passing that the latter sequence is known as the Jacobsthal sequence [8]), and this completes the proof of Proposition 4. $\square$

Proof of Proposition 5. We begin by proving that $R > 0$ implies that $\prod_{i=0}^{n} \lambda_i > \prod_{i=0}^{n} \gamma_i$. If $R > 0$

then (18) yields

$$\begin{aligned}\lambda_0(1-e_1) &> \gamma_0 e_1,\\ \lambda_i e_i(1-e_{i+1}) &> \gamma_i e_{i+1}(1-e_i), \quad i=1,\dots,n-1,\\ \lambda_n e_n &> \gamma_n(1-e_n).\end{aligned} \tag{A.11}$$

Multiplying all these inequalities, and using the fact that $e \in \operatorname{Int}(C^n)$ yields

$$\prod_{i=0}^{n} \lambda_i > \prod_{i=0}^{n} \gamma_i. \tag{A.12}$$

To prove the converse implication, assume that (A.12) holds. Multiplying both sides of this inequality by the strictly positive term $\prod_{j=1}^{n} e_j(1-e_j)$ yields

$$\prod_{i=0}^{n} a_i > \prod_{i=0}^{n} b_i,$$

where $a_0 := \lambda_0(1-e_1)$, $a_i := \lambda_i e_i(1-e_{i+1})$, $i=1,\dots,n-1$, $a_n = \lambda_n e_n$, $b_0 := \gamma_0 e_1$, $b_i := \gamma_i e_{i+1}(1-e_i)$, $i=1,\dots,n-1$, and $b_n = \gamma_n(1-e_n)$. This means that $a_\ell > b_\ell$ for some index $\ell \in \{0,\dots,n\}$. Since $R = a_\ell - b_\ell$ (see (18)), it follows that $R > 0$. Summarizing, we showed that $R > 0$ if and only if $\prod_{i=0}^{n} \lambda_i > \prod_{i=0}^{n} \gamma_i$. The proof that $R < 0$ if and only if $\prod_{i=0}^{n} \lambda_i < \prod_{i=0}^{n} \gamma_i$ is similar. This implies that $R = 0$ if and only if $\prod_{i=0}^{n} \lambda_i = \prod_{i=0}^{n} \gamma_i$. This completes the proof of (19).

To prove (20), note that (18) yields

$$\begin{aligned}e_n &= \frac{R+\gamma_n}{\lambda_n+\gamma_n},\\ e_i &= \frac{R+\gamma_i e_{i+1}}{\lambda_i(1-e_{i+1})+\gamma_i e_{i+1}}, \quad i=n-1,\dots,1,\\ e_1 &= \frac{\lambda_0 - R}{\lambda_0+\gamma_0}.\end{aligned} \tag{A.13}$$

Substituting $R = 0$ completes the proof of Prop. 5. □

Proof of Theorem 1. The Jacobian of the PMFALK is $J(t, x(t)) = L(t, x(t)) + P(t)$, with L given in (A.3), and P in (A.4) (but now with time-varying rates). Pick an initial time $t_0 \ge 0$, and $\tau_0 > 0$. The stated conditions guarantee the existence of $\zeta \in (0, 1/2)$ such that $x(t, t_0, a) \in C^n_\zeta$ for all $t \ge t_0 + \tau$ and all $a \in C^n$. Also, [4, Thm. 4] implies that there exists a diagonally-scaled L_1 norm such that the PMFALK is contractive on C^n_ζ w.r.t. this norm. Now entrainment follows from known results on contractive systems with a periodic excitation (see, e.g. [7]). □

Proof of Proposition 6. Since the Jacobian $J(x)$ of the MFALK is Metzler (i.e. every off-diagonal entry is non-negative) for any $x \in C^n$, the MFALK is a cooperative system [9], and this yields (24).

When $\lambda_i + \gamma_i > 0$, $i = 1,\dots,n-1$, the matrix $L(x)$ and, therefore, $J(x)$, is irreducible for every $x \in \operatorname{Int}(C^n)$, and combining this with Prop. 1 implies (25) (see, e.g., [9, Ch. 4]). □

Proof of Proposition 7. First, using Remark 1 and the argument used in the proof of [6, Prop. 4] shows that all the derivatives in the statement of of Prop. 7 exist.

Given a MFALK, pick $j \in \{1,\dots,n\}$ and consider the new MFALK obtained by changing α_j to $\tilde{\alpha}_j$, with $\tilde{\alpha}_j > \alpha_j$, and all other rates unchanged. Let $\tilde{e}$, $\tilde{R}$ denote the steady-state density and production rate in the modified MFALK, respectively. Seeking a contradiction, assume that

$$\tilde{e}_n \ge e_n. \tag{A.14}$$

Then (14) implies that

$$\tilde{R} \ge R, \tag{A.15}$$

and if $j = n$ then $\tilde{R} > R$. By (15) with $i = n-1$, $R = \lambda_{n-1}e_{n-1}(1-e_n) - \gamma_{n-1}e_n(1-e_{n-1})$ and $\tilde{R} = \lambda_{n-1}\tilde{e}_{n-1}(1-\tilde{e}_n) - \gamma_{n-1}\tilde{e}_n(1-\tilde{e}_{n-1})$, and combining this with (A.14) and (A.15) yields

$$\tilde{e}_{n-1} \geq e_{n-1}. \tag{A.16}$$

Now using (15) with $i = n-2$ yields $\tilde{e}_{n-2} \geq e_{n-2}$, and $\tilde{e}_{n-2} > e_{n-2}$ if $j = n-1$. Proceeding in this way shows that

$$\tilde{e}_k \geq e_k, \quad k = n, n-1, \dots, j, \tag{A.17}$$

$$\tilde{e}_k > e_k, \quad k = j-1, j-2, \dots, 1. \tag{A.18}$$

Combining this with (15) with $i = 0$ yields $\tilde{R} < R$. This contradicts (A.15), so

$$\tilde{e}_n > e_n. \tag{A.19}$$

Proceeding as above yields $\tilde{e}_i > e_i$ for all i, so $\frac{\partial e_i}{\partial \alpha_j} < 0$ for all i, j. The proofs of all the other equations in Prop. 7 are very similar and therefore omitted. □

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