Cross-diffusion in concentrated reactive systems revealed by perturbation of FKPP wave front.

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Fisher-KPP equation:

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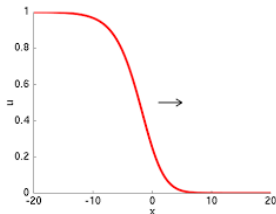Admits two equilibrium states $u = 0$ and $u = 1$

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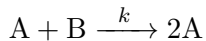Belongs to the class of reaction-diffusion equations
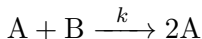Admits two equilibrium states $u = 0$ and $u = 1$
Existence of a travelling wave between the two states

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$$\partial_t B = D_B \partial_x^2 B - kAB$$

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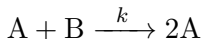$$A + B \xrightarrow{\ k\ } 2A$$

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When $D_A = D_B$, the RD equation of $A(x,t)$ is a Fisher-KPP equation.

In a concentrated system, diffusion is perturbed:

$$\partial_t A = D_A \partial_x \left[\left(1 - \frac{A}{C} \right) \partial_x A \right] - D_B \partial_x \left(\frac{A}{C} \partial_x B \right) + kAB$$

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Questions

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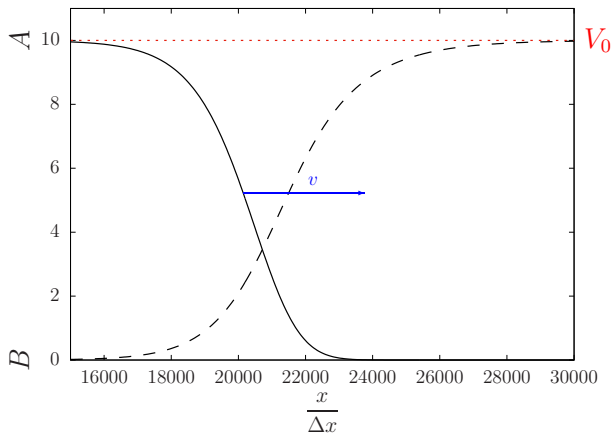
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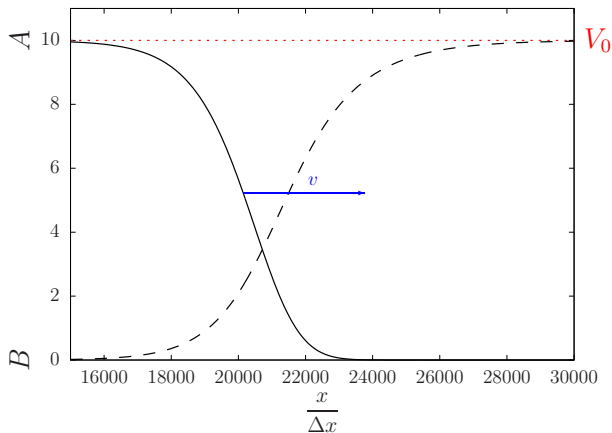
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- **How does $D_A \neq D_B$ affect the velocity and shape of the wave front ?**
- **How does confinement (i.e. $S \to 0$) affect the velocity and shape of the wave front ?**
- **Can we use these effects to detect perturbed diffusion in a concentrated Fisher-KPP front ?**

Velocity v of a Fisher front

$$v = 2\sqrt{kV_0 D_A}$$

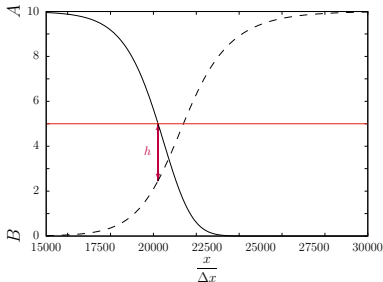## Velocity v of a Fisher front Independent of D_B and S

$$v = 2\sqrt{kV_0 D_A}$$

Shape of the front, 2 parameters:

- **Height** defined as the difference of concentration between

  $A(x_0)$ **and** $B(x_0)$ **where** $A(x_0) = \dfrac{V_0}{2}$

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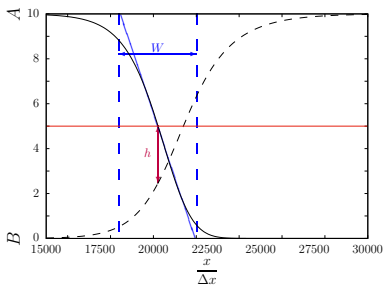- **Width** of the front defined as the inverse of the slope of the A profile where $A(x_0) = \dfrac{V_0}{2}$

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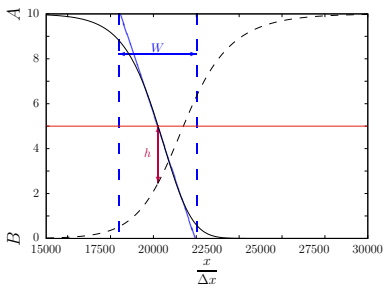- **Width** of the front defined as the inverse of the slope of the A **profile where** $A(x_0) = \dfrac{V_0}{2}$ $\boxed{\Rightarrow W = \dfrac{V_0}{A'(x_0)}}$

To study the RD equations, we define the moving frame:

$$(x, t) \rightarrow (\zeta)$$

$$\zeta = \frac{x}{v} - t$$

$$\zeta_0 = \frac{x_0}{v} - t_0 \equiv 0$$

$$A(x, t) \rightarrow f(\zeta)$$

$$B(x, t) \rightarrow g(\zeta)$$

$$\epsilon = 1/v^2$$

$$d = \textbf{dilute} \text{ (regular diffusion)}$$

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Examples:

$$f_d = \textbf{A concentration in the dilute case}$$
$$g_c = \textbf{B concentration in the concentrated case}$$

Dilute case RD equations in the moving frame:

$$0 = kf_d g_d + f'_d + \epsilon D_A f''_d$$
$$0 = -kf_d g_d + g'_d + \epsilon D_B g''_d$$

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Concentrated case RD equations in the moving frame:

$$0 = kf_c g_c + f'_c + \epsilon \left(D_A \left[\left(1 - \frac{f'_c}{C} \right) f''_c - \frac{(f'_c)^2}{C} \right] - D_B \left[\frac{f_c g''_c}{C} + \frac{f'_c g'_c}{C} \right] \right)$$
$$0 = -kf_c g_c + g'_c + \epsilon \left(D_B \left[\left(1 - \frac{g'_c}{C} \right) g''_c - \frac{(g'_c)^2}{C} \right] - D_A \left[\frac{g_c f''_c}{C} + \frac{f'_c g'_c}{C} \right] \right)$$

We consider k**,** V_0 **and** D_A **such as:**

$$\epsilon \ll 1$$

Diffusion can be considered as a perturbation of reaction (do not mix up with perturbed diffusion !).

We write f **and** g **as a perturbation series:**

$$f = f_0 + \epsilon f_1 + \epsilon^2 f_2 + ...$$
$$g = g_0 + \epsilon g_1 + \epsilon^2 g_2 + ...$$

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Zero-th order solutions (no diffusion) are straightforwardly obtained:

$$f_{d,0} = f_{c,0} = \frac{V_0}{1 + e^{kV_0\zeta}}$$
$$g_{d,0} = g_{c,0} = \frac{V_0}{1 + e^{-kV_0\zeta}}$$

Now, instead of deriving the solutions for the higher-order terms $f_{1,2,\ldots}$ and $g_{1,2,\ldots}$, we focus on the point $\zeta_0 = 0$.

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The expressions for the height and the width, up to the second-order, are given by:

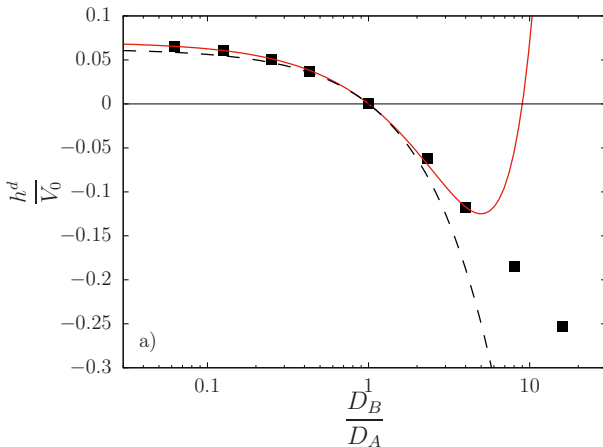$$h_d = \frac{V_0}{16}\left(1 - \frac{D_B}{D_A}\right)\left[1 + \frac{1}{8}\left(1 - \frac{D_B}{D_A}\right)\right]$$

$$h_c = \frac{V_0}{16}\left(1 - \frac{D_B}{D_A}\right)\left(1 - \frac{V_0}{C}\right)\left[1 + \frac{1}{8}\left(1 - \frac{D_B}{D_A}\right)\left(1 - 2\frac{V_0}{C}\right)\right]$$

$$W_d = 8\sqrt{\frac{D_A}{kV_0}}\left[1 + \frac{1}{8}\left(1 - \frac{D_B}{D_A}\right) - \frac{1}{64}\frac{D_B}{D_A}\left(3 - \frac{D_B}{D_A}\right)\right]^{-1}$$

$$W_c = 8\sqrt{\frac{D_A}{kV_0}}\left[1 + \frac{1}{8}\left(1 - \frac{D_B}{D_A}\right)\left(1 - \frac{3V_0}{2C}\right) - \frac{1}{64}\left[\frac{D_B}{D_A}\left(3 - \frac{D_B}{D_A}\right)\right.\right.$$
$$\left.\left. + \left(\frac{9}{2} - 8\frac{D_B}{D_A} + \frac{7}{2}\frac{D_B^2}{D_A^2}\right)\frac{V_0}{C} - \left(\frac{7}{2} - 7\frac{D_B}{D_A} + \frac{7}{2}\frac{D_B^2}{D_A^2}\right)\frac{V_0^2}{C^2}\right]\right]^{-1}$$
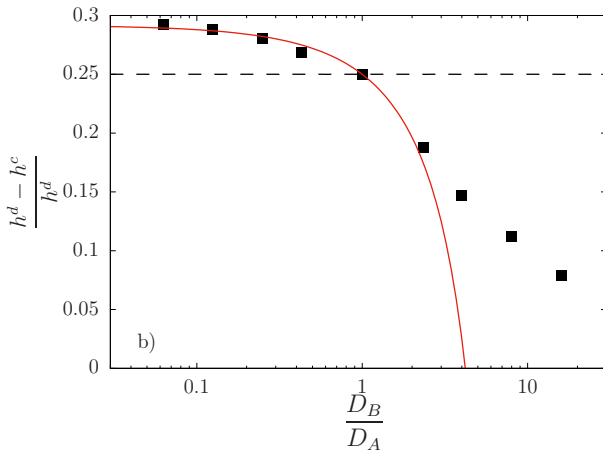
Comparison between analytic and numerical results:

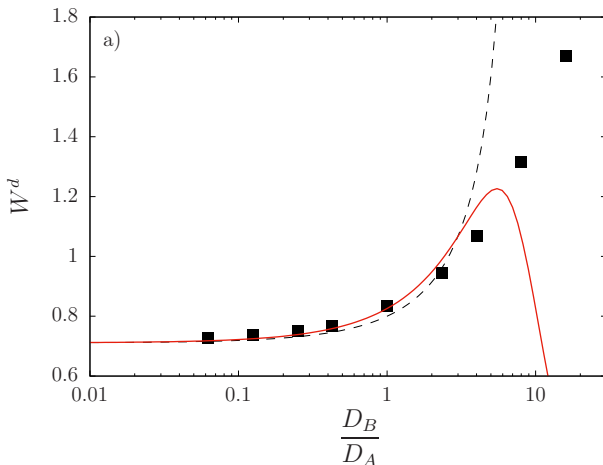**Comparison between analytic and numerical results: Height in the diluted case**

a)

Perturbed diffusion ($V_0/C = 0.25$) vs. regular diffusion ($V_0/C = 0$):
Height
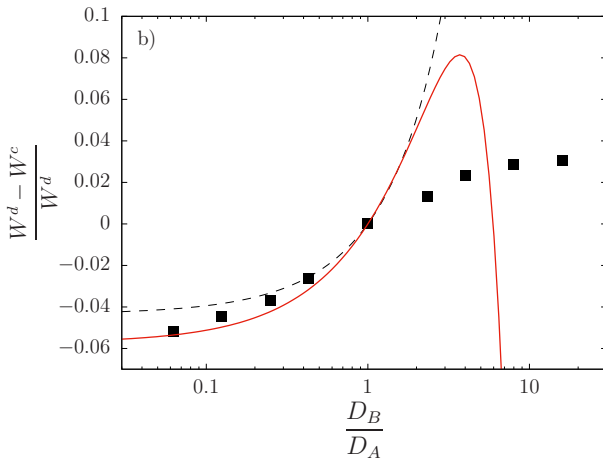

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Comparison between analytic and numerical results:

Perturbed diffusion $(V_0/C = 0.25)$ vs. regular diffusion $(V_0/C \to 0)$:

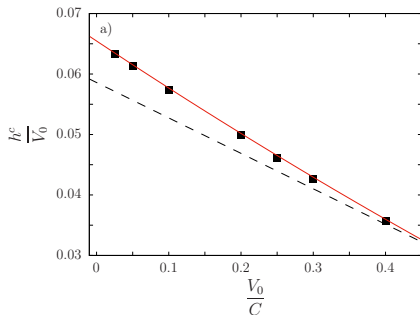**Perturbed diffusion ($V_0/C = 0.25$) vs. regular diffusion ($V_0/C \to 0$): Width**
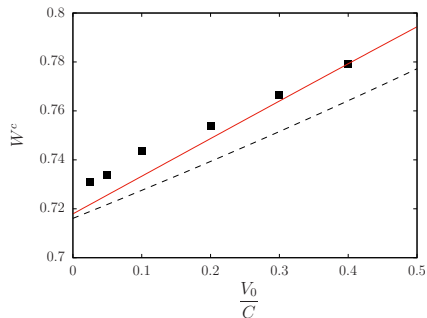
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Height   **Width**

for $D_B/D_A = 1/16$

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- The **width** is also **mainly** affected by the ratio D_B/D_A and V_0/C, working better for large values of D_B/D_A.

Thank You

[1] Morgado, Nowakowski, Lemarchand, Phys. Rev. E **99**, 022205 (2019)

Cross-diffusion terms derivation from linear irreversible thermodynamics

The entropy production per unit mass due to isothermal diffusion is given by:

$$\sigma = \frac{1}{T} \sum_{X=A,B,S} \vec{j}_X \cdot \left(-\vec{\nabla} \mu_X \right)$$

where T is the temperature, $\vec{j}_X$ the flux of species X, and μ_X is the chemical potential of species X.

We consider the framework of the solvent. The flux of species X in this framework is defined by:

$$\vec{j_X^*} = \rho_X \left(\vec{u}_X - \vec{u}_S \right) = \rho_X \left(\vec{u}_X - \vec{u} \right) + \rho_X \left(\vec{u} - \vec{u}_S \right)$$
$$= \vec{j}_X - \frac{\rho_X}{\rho_S} \vec{j}_S$$

where ρ_X is the concentration of X, and $\vec{u}_X$ is the velocity of X.

Prigogine's theorem: Entropy production does not depend on the chosen framework.
Therefore:

$$\sigma = \frac{1}{T} \sum_{X=A,B,S} \vec{\jmath}_X \cdot \left(-\vec{\nabla}\mu_X\right) = \frac{1}{T} \sum_{X=A,B} \vec{\jmath}_X^* \cdot \left(-\vec{\nabla}\mu_X\right)$$

Assuming that the solution is ideal, we can write:

$$\mu_X = \mu_X^0 + RT\ln\frac{\rho_X}{\rho}$$

Using the expression for $\vec{\jmath}_X^*$ **and** μ_X**, we get:**

$$\begin{pmatrix} \vec{\jmath}_A \\ \vec{\jmath}_B \end{pmatrix} = \begin{pmatrix} 1 - \dfrac{\rho_A}{\rho} & -\dfrac{\rho_A}{\rho} \\ -\dfrac{\rho_B}{\rho} & 1 - \dfrac{\rho_B}{\rho} \end{pmatrix} \begin{pmatrix} \vec{\jmath}_A^* \\ \vec{\jmath}_B^* \end{pmatrix}$$

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Hypothesis: $\vec{\jmath}_X^* = -D_X \vec{\nabla}\rho_X$ **(Fick's first law in solvent framework)**
Then:

$$\begin{pmatrix} \vec{\jmath}_A \\ \vec{\jmath}_B \end{pmatrix} = - \begin{pmatrix} 1 - \dfrac{\rho_A}{\rho} & \dfrac{\rho_A}{\rho} \\ \dfrac{\rho_B}{\rho} & 1 - \dfrac{\rho_B}{\rho} \end{pmatrix} \begin{pmatrix} D_A \vec{\nabla}\rho_A \\ D_B \vec{\nabla}\rho_B \end{pmatrix}$$