

Effect of non-uniform passive advection on $A + B \rightarrow C$ radial reaction-diffusion fronts



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Introduction

The interplay between chemical and transport processes can give rise to complex reaction front dynamics, whose understanding is crucial in a wide variety of environmental, hydrological and biological processes, among others. An important class of reactions is $A + B \rightarrow C$ processes, where A and B are two initially segregated miscible reactants that produce C upon contact. Depending on the nature of the reactants and on the transport processes that they undergo, this class of reaction describes a broad set of phenomena, including combustion, atmospheric reactions, calcium carbonate precipitation and more. Due to the complexity of the coupled chemical-hydrodynamic systems, theoretical studies generally deal with the particular case of reactants undergoing passive advection and molecular diffusion. A restricted number of different geometries have been studied, including uniform rectilinear^[1], 1D radial^[2] and 1D spherical^[3] fronts. Here we study the effect of non-uniform advection in a 2D confined axisymmetric system where A is injected radially into B at constant flow rate \bar{Q} .

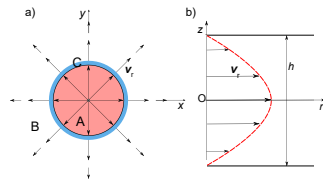
Model

The dynamics of the system is described by the following equations for the concentrations $a(r, z, t)$, $b(r, z, t)$ and $c(r, z, t)$.

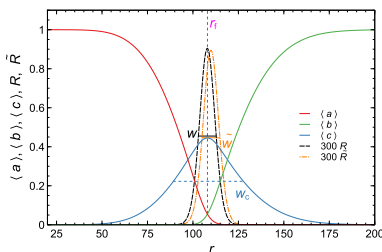
$$\begin{aligned} \partial_t a + (v_r - 1/r)\partial_r a &= \partial_r^2 a + \partial_z^2 a - ab \\ \partial_t b + (v_r - 1/r)\partial_r b &= \partial_r^2 b + \partial_z^2 b - ab \\ \partial_t c + (v_r - 1/r)\partial_r c &= \partial_r^2 c + \partial_z^2 c + ab \end{aligned}$$

Time is rescaled by $\tau = 1/kA_0$ and lengths by $\ell = \sqrt{D\tau}$. k is the kinetic constant of reaction, A_0 and B_0 are the initial concentrations of A and B, D is the diffusion coefficients, which we assume equal for all species and v_r is the radial Poiseuille flow

$$v_r(r, z) = \frac{3Q}{2r} \left(1 - \frac{4z^2}{h^2}\right) \quad Q = \frac{\bar{Q}}{2\pi h D}$$

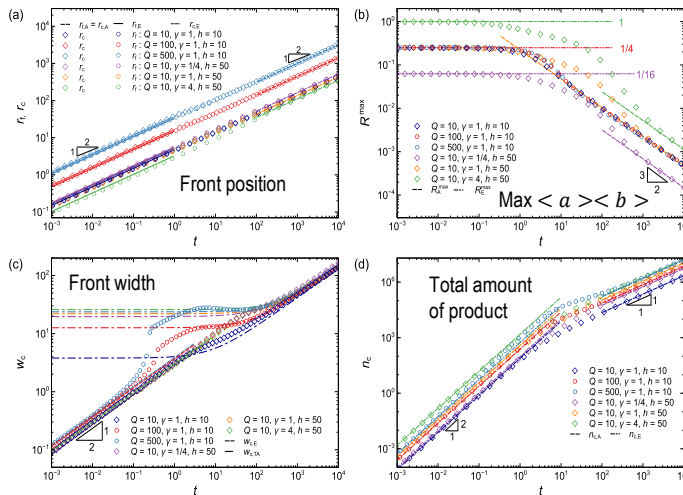
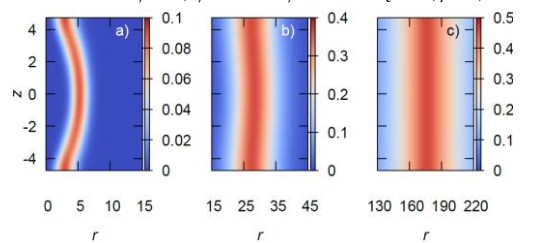


The initial conditions are given as $a(r > 0, z, 0) = c(r, z, 0) = 0$, and $a(0, z, 0) = 1$ and $b(r > 0, z, 0) = B_0/A_0 = \gamma$ and the boundary conditions are $a(0, z, t) = 1$, $a(r \rightarrow \infty, z, t) = b(0, z, t) = c(0, z, t) = c(r \rightarrow \infty, z, t) = \partial_z a(r, \pm h/2, t) = \partial_z b(r, \pm h/2, t) = \partial_z c(r, h/2, t) = 0$ and $b(r \rightarrow \infty, z, t) = \gamma$.



Results

Concentration of C at a) $t = 1$, b) $t = 40$ and c) $t = 1600$ for $Q = 10$, $\gamma = 1$, $h = 10$



Discussion

We have performed theoretical and numerical analysis of the front position, the maximum and the width of the production rate, the position and the width of the radial concentration profile of the product, as well as its total amount. These analyses reveal the occurrence of three distinct temporal regimes. These are (1) the **early-time regime**, where the amount of mixing of the reactants is still small and the front dynamics is well approximated by the equivalent non-reactive system; (2) the **transient regime**, characterized by the interplay between diffusion, dispersion and reaction, where the Poiseuille flow bends the concentration profiles of the reactants and product. While diffusion tends to increase the spreading of the species, dispersion stretches the front. As a result, the front width exhibits a plateau in this regime, which is in agreement with the experimental observations^[4]; finally, (3) the **asymptotic regime** where the z profiles of A, B and C lose their curvature due to Taylor dispersion. In this regime, the system becomes independent on z and its dynamics is conveniently described by the 1D theory for radial fronts^[1].

Acknowledgements

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References

- [1] L. Gálfi, Z. Rácz, Phys. Rev. A 38, 3151 (1988); [2] F. Brau, G. Schuszter, A. De Wit, Phys. Rev. Lett. 118, 134101 (2017); [3] A. Comolli, A. De Wit, F. Brau, Phys. Rev. E 100 (5), 052213 (2019); [4] Á. Tóth, G. Schuszter, N. P. Das, E. Lantos, D. Horváth, A. De Wit, F. Brau, Phys. Chem. Chem. Phys. 22, 10278 (2020).