

WORKING PAPER

Axial Dispersion as Elastic Diffusion: Micromixing in Tubular Reactors

Danckwerts Boundary Conditions, Zwietering's Bounds and the Method of Lines

Supervised by Dr. T. Zamrik

29-JAN-2023

Matérn RBF interpolant: $s(\mathbf{x}) = \sum_{i=1}^n \lambda_i \varphi(\|\mathbf{x} - \mathbf{x}_i\|)$, $A\lambda = f$, $\varphi(r) = (1 + \sqrt{5}\varepsilon r + \frac{5}{3}\varepsilon^2 r^2) e^{-\sqrt{5}\varepsilon r}$, $n = 37$



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WORKING PAPER



Axial Dispersion as Elastic Diffusion: Micromixing in Tubular Reactors

Danckwerts Boundary Conditions, Zwietering's Bounds and the Method of Lines

Supervised by Dr. T. Zamrik¹

29-JAN-2023

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Abstract. The axial dispersion model of a tubular reactor is closed by Danckwerts' boundary conditions, argued over as physics since 1953. Read probabilistically they are a boundary behaviour: the closed vessel is the exit law of a drifted Brownian particle reflected at the inlet and removed at the outlet at rate Pe per unit of its local time there, Feller's elastic boundary. First-order conversion is then a Feynman–Kac expectation, Wehner–Wilhelm's formula follows, and an absorbing outlet is another vessel, off by up to 0.64 in outlet concentration. For a second-order reaction, the dispersion model lies between Zwietering's complete segregation and maximum mixedness for the same residence-time distribution. The three agree through Da^2 ; at Da^3 they differ in one integral, the mean square of the age averaged over nothing, over position or over life expectancy. Near plug flow the dispersion model's position in the band tends to $\xi_\infty(Da) = (1 + Da)(Da - \ln(1 + Da))/Da^2$, from one half toward one (0.58 at $Pe = 1000$, $Da = 1$, against 0.61); at low conversion it rises from 0 near the stirred tank to 0.23 at $Pe = 10$ and 0.46 at $Pe = 300$. The method of lines, collocation, Laplace inversion and a Monte Carlo compute every number at least twice. Above $Pe \approx 20$ the average of the two limits gives the dispersion model's conversion to within 0.1 percentage points for $Da \leq 10$.

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1. Introduction

A tubular reactor in which the fluid moves nearly as a plug is described by the axial dispersion model, a convection–diffusion–reaction equation in which one coefficient stands for the mixing that a plug lacks. Danckwerts [1] closed it with continuity of the total flux at the inlet, so that the concentration jumps there, and a vanishing gradient at the outlet: the closed vessel. Wehner and Wilhelm [2] solved the first-order case in closed form, examining the conditions with dispersive sections before and after the reactor. The outlet condition was re-examined by Pearson [5] and Van Cauwenberghe [6], and the conditions are still taught as mass balances at the two planes, beside separate accounts of residence

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times and micromixing [11]. Numerically the model is a standard case for the method of lines, developed by Schiesser [12], applied to transport and reaction models by Silebi and Schiesser [13], and carried through many partial differential equation models by Schiesser and Griffiths [14].

This paper asks two questions. What random motion of a fluid particle do Danckwerts' conditions describe? And, for a second-order reaction, where does the dispersion model's conversion fall between the two micromixing limits that hold for the same residence-time distribution?

Danckwerts [3] showed that the residence-time distribution does not fix the conversion of a reaction that is not of first order: it also depends on the state of mixing, which he measured by a degree of segregation. Zwietering [4] defined maximum mixedness, the earliest mixing compatible with a given distribution, gave the equation for its conversion, and showed that complete segregation and maximum mixedness bound the conversion for orders above one. Nauman [10] reviews the theory that grew from these papers.

The comparison this paper revisits has been computed before. Lindfors [20] computed outlet concentrations for second-order reactions under the axial dispersion model and under its segregated and maximum-mixed versions, in a 1974 report; Sawinsky and Deák [21] gave an analytical solution for the completely segregated case that agreed with Lindfors's numbers. Missing, as far as the author knows, is a reason for where the dispersion model sits in the band, and what its position tends to near plug flow.

On the probabilistic side, Feller [7] classified the boundary behaviours of one-dimensional diffusions, among them the elastic boundary, partly reflecting and partly absorbing; Erban and Chapman [9] used Robin conditions as reactive boundaries in stochastic simulations of reaction–diffusion processes.

This paper adds four things. First, Theorem 1: the closed vessel is the exit law of a drifted Brownian particle reflected at the inlet and removed at the outlet at rate Pe per unit of its local time there; to the author's knowledge this reading has not been stated before. Wehner–Wilhelm becomes a Feynman–Kac expectation (Corollary 1), and an absorbing outlet another vessel (Remark 1). Second, the exact Da^2 and Da^3 coefficients of segregation, maximum mixedness and the dispersion model for a second-order reaction, and their one-integral structure (Propositions 1 and 2). Third, the limits: near plug flow the excesses over plug flow have closed forms (Lemmas 2 and 3, formal) and the position tends to $\xi_\infty(Da)$ (Theorem 3); near the stirred tank the dispersion model becomes maximum mixedness (Proposition 3). Fourth, the map of that position over the (Pe, Da) plane, computed independently four ways, and the rule it supports (Corollary 2). The method of lines in Schiesser's form is the workhorse throughout.

2. Setting

Definition 1 (The closed Danckwerts vessel). A tube of length L carries fluid at velocity v with axial dispersion coefficient D ; the feed holds a reactant at concentration c_{in} , consumed by one irreversible reaction of order n with rate constant k . In the position $z = x/L \in [0, 1]$



and the time $\theta = tv/L$, with $\text{Pe} = vL/D$, $\text{Da} = k c_{\text{in}}^{n-1} L/v$ and concentrations scaled by c_{in} , the concentration $c(z, \theta)$ solves

$$\partial_{\theta} c = \text{Pe}^{-1} \partial_{zz} c - \partial_z c - \text{Da} c^n,$$

with $c - \text{Pe}^{-1} \partial_z c = c_{\text{in}}(\theta)$ at $z = 0$, $\partial_z c = 0$ at $z = 1$ and $c(z, 0) = 0$ [1], [2], where $c_{\text{in}}(\theta)$ is the scaled feed, 1 under a steady feed. The conversion is $X = 1 - c(1)$ at steady state, and $\mathcal{L}c = \text{Pe}^{-1} c'' - c'$ is the steady forward operator.

The inlet condition equates the total flux inside the vessel with the feed, so the concentration drops across the inlet plane (Figure 3). The steady outlet with $n = 2$ is c_{disp} .

Definition 2 (Residence-time distribution and its moments). For the vessel of Definition 1 with $\text{Da} = 0$, $E(\theta)$ is the outlet concentration after a unit pulse of tracer, $F(\theta) = \int_0^{\theta} E$, $S = 1 - F$ and $R(\theta) = \int_{\theta}^{\infty} S$; the moments are $m_k = \int_0^{\infty} \theta^k E d\theta$ and the variance is $\sigma^2 = m_2 - m_1^2$. The life expectancy at age λ is $\ell(\lambda) = R(\lambda)/S(\lambda)$, the mean remaining life of fluid that has stayed λ [1], [10].

Under a steady feed, $S(a)$ is also the density of the ages of the fluid in the vessel, the occupation measure of Proposition 2.

Definition 3 (A diffusion reflected at the inlet and elastic at the outlet). Let W be a standard Brownian motion and ε an independent exponential variable of mean one. The particle Z solves

$$dZ_{\theta} = d\theta + \sqrt{2/\text{Pe}} dW_{\theta} + dL_{\theta}^0 - dL_{\theta}^1, \quad Z_0 = z,$$

in $[0, 1]$, where the regulators L^0 and L^1 are continuous, non-decreasing, start at 0 and increase only when $Z = 0$ and $Z = 1$ (the Skorokhod problem on $[0, 1]$). It is removed at $\tau = \inf\{\theta : \text{Pe} L_{\theta}^1 > \varepsilon\}$, so $\mathbb{P}(\tau > \theta \mid Z) = e^{-\text{Pe} L_{\theta}^1}$. $\mathbb{P}_z$ and $\mathbb{E}_z$ refer to the start z , and $\mathcal{L}^* u = \text{Pe}^{-1} u'' + u'$, the formal adjoint of $\mathcal{L}$, is the generator of Z away from the ends [7], [8].

In Feller's classification [7] the inlet is reflecting and the outlet elastic: every unit of push back from the outlet plane carries a chance of removal, at rate Pe , as in Itô and McKean's elastic Brownian motion [8].

Definition 4 (Zwietering's two limits). For a residence-time distribution E of mean 1 and a reaction of order n , let $c'_b = -\text{Da} c_b^n$, $c_b(0) = 1$, be the batch solution, $1/(1 + \text{Da} \theta)$ for $n = 2$. Complete segregation gives $c_{\text{seg}} = \int_0^{\infty} E(\theta) c_b(\theta) d\theta$. Maximum mixedness gives $c_{\text{mm}} = c(0)$, where c is the solution, bounded and positive as $\lambda \rightarrow \infty$, of

$$c'(\lambda) = \text{Da} c^n + h(\lambda) (c - 1), \quad h = E/S,$$

$\lambda \geq 0$ being the life expectancy of a fluid element, the time it has still to spend in the vessel, and h the hazard of E [4], [3].

In segregation each element mixes only at the outlet; in maximum mixedness it mixes on entry with all the fluid of the same life expectancy. For $n > 1$ they give the lowest and



highest outlet concentration with distribution E [4]. Positivity matters: other bounded solutions cross zero.

Definition 5 (The position inside the band). For $n = 2$, with c_{disp} from Definition 1 and $c_{\text{seg}}, c_{\text{mm}}$ from Definition 4 for the vessel's own distribution,

$$\xi = \frac{c_{\text{mm}} - c_{\text{disp}}}{c_{\text{mm}} - c_{\text{seg}}} = \frac{X_{\text{disp}} - X_{\text{mm}}}{X_{\text{seg}} - X_{\text{mm}}},$$

0 at maximum mixedness and 1 at segregation, and $\xi_0(\text{Pe}) = \lim_{\text{Da} \rightarrow 0} \xi$.

As $\text{Da} \rightarrow 0$ both differences vanish like Da^3 (Proposition 1), so ξ_0 is a ratio of third-order coefficients (Proposition 2).

Assumption 1 (Standing assumptions). (i) One irreversible reaction of order $n = 2$ in an isothermal fluid of constant density, with constants $\text{Pe} > 0$ and $\text{Da} > 0$. (ii) The vessel is closed, with Definition 1's conditions at both ends, and Definition 4 uses its own distribution E , except in Lemma 2. (iii) Steady quantities are the limits $\theta \rightarrow \infty$ of Definition 1 under a steady feed; Theorem 1 and Corollary 1 concern tracer and a first-order reaction.

Part (ii) is where the particle's boundary behaviour comes from.

3. The Particle Behind the Danckwerts Conditions

Theorem 1 (The closed vessel is the exit law of the elastic diffusion). Under Assumption 1(ii), let $S(z, \theta) = \mathbb{P}_z(\tau > \theta)$ for the particle of Definition 3. Then S solves $\partial_\theta S = \mathcal{L}^* S$, $S(z, 0) = 1$, $\partial_z S(0, \theta) = 0$, $\partial_z S(1, \theta) = -\text{Pe} S(1, \theta)$, and: (i) the tracer of Definition 1 is the density of the particles fed in and not yet removed, and the pulse response of Definition 2 is the exit law, $E(\theta) d\theta = \mathbb{P}_0(\tau \in d\theta)$, $E = -\partial_\theta S(0, \cdot)$; (ii) with a first-order reaction of rate Da the pulse response is $E(\theta)e^{-\text{Da}\theta}$, the exit law of a particle also removed in the interior at rate Da .

Proof. Let v solve the backward problem with a continuous initial value u ; v is smooth for $\theta > 0$ and continuous at $\theta = 0$. For fixed θ let $N_s = v(Z_s, \theta - s)e^{-\text{Pe}L_s^1}$. Itô's formula with the two regulators gives, with v taken at $(Z_s, \theta - s)$,

$$dN_s = e^{-\text{Pe}L_s^1} [\sqrt{2/\text{Pe}} \partial_z v dW_s + \partial_z v dL_s^0 - (\partial_z v + \text{Pe} v) dL_s^1],$$

the ds terms cancelling as $\partial_\theta v = \mathcal{L}^* v$. L^0 grows only where $\partial_z v = 0$ and L^1 only where $\partial_z v = -\text{Pe} v$, so N is a bounded martingale on $[0, \theta - \delta]$; letting $\delta \rightarrow 0$, $v(z, \theta) = \mathbb{E}_z[u(Z_\theta)e^{-\text{Pe}L_\theta^1}] = \mathbb{E}_z[u(Z_\theta); \tau > \theta]$ [7], [8], and $u = 1$ gives S . For (i), let c solve Definition 1 with $\text{Da} = 0$ and feed c_{in} . Green's identity gives

$$\int_0^1 [(\mathcal{L}c)v - c\mathcal{L}^*v] dz = \left[v(\text{Pe}^{-1}\partial_z c - c) - \text{Pe}^{-1}c\partial_z v \right]_0^1,$$



which is $c_{\text{in}}v(0)$: the outlet term vanishes by $\partial_z c = 0$ and $\partial_z v = -\text{Pe} v$, and the inlet term reduces by $\partial_z v = 0$ and the inlet condition. So $\frac{d}{ds} \int_0^1 c(z, s)v(z, \theta - s) dz = c_{\text{in}}(s)v(0, \theta - s)$, and with $c(\cdot, 0) = 0$, $\int_0^1 c(z, \theta)u dz = \int_0^\theta c_{\text{in}}(s) \mathbb{E}_0[u(Z_{\theta-s}); \tau > \theta - s] ds$: the tracer is the density of surviving particles. With $u = 1$ the holdup is $M = \int_0^\theta c_{\text{in}}(s)S(0, \theta - s) ds$, and integrating Definition 1 over z , $M' = c_{\text{in}} - c(1, \cdot)$; with $S(0, 0) = 1$, $c(1, \theta) = \int_0^\theta c_{\text{in}}(s)(-\partial_\theta S(0, \theta - s)) ds$. The outlet flux is the removal rate. For (ii), after a pulse the boundary conditions are homogeneous, so $e^{-\text{Da}\theta}c$ solves the first-order problem; for the particle, removal at constant rate Da is the Feynman–Kac factor $e^{-\text{Da}\theta}$. Nothing is formal beyond the classical regularity of the two linear problems; stopping at $\theta - \delta$ avoids the corner where the initial value and the outlet condition disagree. $\square$

The zero gradient at the outlet makes the outlet flux equal to the removal rate: the elastic condition seen from the forward side.

Corollary 1 (Wehner–Wilhelm as a Feynman–Kac expectation). With a first-order reaction and a steady feed, the closed vessel’s outlet concentration is $c(1) = \int_0^\infty E(\theta)e^{-\text{Da}\theta} d\theta = \mathbb{E}_0[e^{-\text{Da}\tau}] = u(0)$, where $u(z) = \mathbb{E}_z[e^{-\text{Da}\tau}]$ solves $\text{Pe}^{-1}u'' + u' - \text{Da}u = 0$, $u'(0) = 0$, $u'(1) = \text{Pe}(1 - u(1))$. With $a = \sqrt{1 + 4\text{Da}/\text{Pe}}$ this is the formula of Wehner and Wilhelm [2],

$$c(1) = \frac{4a e^{\text{Pe}/2}}{(1+a)^2 e^{a\text{Pe}/2} - (1-a)^2 e^{-a\text{Pe}/2}}.$$

Proof. The step response $\int_0^\theta E(s)e^{-\text{Da}s} ds$ of Theorem 1(ii) tends to the first expression, and Theorem 1(i) gives the second. Transforming the backward problem of Theorem 1, $\hat{S}(z) = \int_0^\infty e^{-\text{Da}\theta} S d\theta$ solves $\mathcal{L}^* \hat{S} = \text{Da} \hat{S} - 1$, $\hat{S}'(0) = 0$, $\hat{S}'(1) = -\text{Pe} \hat{S}(1)$, and by parts $u = 1 - \text{Da} \hat{S}$, which satisfies the stated problem. With $r_{1,2} = \frac{1}{2}\text{Pe}(-1 \pm a)$, $u = \alpha e^{r_1 z} + \beta e^{r_2 z}$; the inlet condition gives $\beta = \alpha(a - 1)/(a + 1)$ and $u(0) = 2a\alpha/(1 + a)$, and the outlet condition gives $\alpha[(1 + a)^2 e^{r_1} - (1 - a)^2 e^{r_2}] = 2(1 + a)$. Multiplying by $e^{\text{Pe}/2}$ gives the formula. $\square$

Replacing the elastic condition $u'(1) = \text{Pe}(1 - u(1))$ by $u(1) = 1$ is Remark 1.

Lemma 1 (Mean one, and the variance of the closed vessel). Under Assumption 1(ii), $m_1 = 1$, $\sigma^2 = 2/\text{Pe} - 2(1 - e^{-\text{Pe}})/\text{Pe}^2$ and $m_2 = 2 \int_0^1 A dz$, where $A(z) = z + (1 - e^{-\text{Pe}(1-z)})/\text{Pe}$ is the mean age of the fluid at position z under a steady feed; the same chain one step further gives

$$m_3 = 1 + \frac{6}{\text{Pe}} + \frac{6}{\text{Pe}^2} + \frac{18e^{-\text{Pe}}}{\text{Pe}^2} - \frac{24(1 - e^{-\text{Pe}})}{\text{Pe}^3}.$$

Proof. Mass balance: if $\mathcal{L}y = f$ with the homogeneous conditions $y - \text{Pe}^{-1}y' = 0$ at $z = 0$ and $y' = 0$ at $z = 1$, then integrating, $y(1) = -\int_0^1 f dz$. By Corollary 1 with $\text{Da} = k$ the first-order steady outlet is $\mathbb{E}_0[e^{-k\tau}]$; the formula is even in a , hence analytic in k at 0, so all moments are finite and it equals $\sum_j (-k)^j m_j/j!$. Writing the steady solution as $1 + \sum_{j \geq 1} k^j u_j$, the constant takes the inlet condition and $\mathcal{L}u_1 = 1$, $\mathcal{L}u_{j+1} = u_j$ with homogeneous conditions, so $u_j(1) = (-1)^j m_j/j!$. The mass balance gives $u_1(1) = -1$,



so $m_1 = 1$, and $m_2/2 = u_2(1) = -\int_0^1 u_1 dz$; solving, $u_1 = -A$, which gives m_2 and $\sigma^2 = m_2 - 1$ [11]. A is the mean age: under a steady feed the tracer is 1 everywhere and the age it carries obeys $\mathcal{L}A = -1$, fresh fluid entering at age 0. One step more, $m_3/6 = \int_0^1 u_2 dz$ with $\mathcal{L}u_2 = -A$. $\square$

The variance tends to $2/\text{Pe}$ near plug flow and to 1, the stirred tank's, as $\text{Pe} \rightarrow 0$.

Theorem 2 (The spectrum of the closed vessel and the tail of its distribution). Under Assumption 1(ii), for $\theta > 0$, $S(0, \theta) = \sum_{k \geq 1} A_k e^{-\lambda_k \theta}$ with $\lambda_k = \mu_k^2/\text{Pe} + \text{Pe}/4$, where $0 < \mu_1 < \mu_2 < \dots$ are the positive roots of

$$\tan \mu = \frac{4\text{Pe} \mu}{4\mu^2 - \text{Pe}^2},$$

and, with $\varphi_k(z) = \cos \mu_k z + (\text{Pe}/2\mu_k) \sin \mu_k z$ and $\|\varphi_k\|^2 = \int_0^1 \varphi_k^2 dz$,

$$A_k = \frac{\text{Pe} e^{\text{Pe}/2} \varphi_k(1)}{(\text{Pe}^2/4 + \mu_k^2) \|\varphi_k\|^2} \neq 0.$$

Hence $E(\theta) = \sum_k A_k \lambda_k e^{-\lambda_k \theta}$, and the hazard $E(\theta)/S(0, \theta)$ tends to λ_1 .

Proof. With $S = e^{-\text{Pe}z/2} w$ the backward problem of Theorem 1 becomes $\partial_\theta w = \text{Pe}^{-1} \partial_{zz} w - \frac{1}{4} \text{Pe} w$, with $\partial_z w = \frac{1}{2} \text{Pe} w$ at $z = 0$, $\partial_z w = -\frac{1}{2} \text{Pe} w$ at $z = 1$ and $w(z, 0) = e^{\text{Pe}z/2}$: self-adjoint. The eigenproblem $w'' = -\mu^2 w$ with these Robin conditions is a regular Sturm–Liouville problem, and $\mu^2 \|w\|^2 = \int_0^1 (w')^2 dz + \frac{1}{2} \text{Pe} (w(0)^2 + w(1)^2) > 0$, so its eigenvalues are positive and simple and its eigenfunctions complete [7]. The inlet condition gives φ_k with $\varphi_k(0) = 1$, and the outlet condition reduces to the stated equation. Expanding $e^{\text{Pe}z/2}$ and setting $z = 0$ gives $A_k = \langle e^{\text{Pe}z/2}, \varphi_k \rangle / \|\varphi_k\|^2$, and two integrations by parts give $(\text{Pe}^2/4 + \mu_k^2) \langle e^{\text{Pe}z/2}, \varphi_k \rangle = [e^{\text{Pe}z/2} (\frac{1}{2} \text{Pe} \varphi_k - \varphi_k')]_0^1 = \text{Pe} e^{\text{Pe}/2} \varphi_k(1)$, the inlet term vanishing and the outlet term doubling by the two conditions. If $\varphi_k(1) = 0$, the outlet condition would give $\varphi_k'(1) = 0$ and $\varphi_k \equiv 0$. For $\theta > 0$ the series differentiates term by term. $\square$

λ_1 is 1.0167 at $\text{Pe} = 0.1$, near the stirred tank's 1, and 250.0098 at $\text{Pe} = 1000$, barely above $\text{Pe}/4$. The series is Algorithm 2's source.

Remark 1 (An absorbing outlet describes another vessel). If the particle leaves at its first contact with the outlet, Corollary 1's condition becomes $u(1) = 1$, giving $2a e^{\text{Pe}/2} / [(1 + a) e^{a\text{Pe}/2} - (1 - a) e^{-a\text{Pe}/2}]$. This is another vessel: its mean residence time, $1 - (1 - e^{-\text{Pe}})/\text{Pe}$, falls short of the space time, and its first-order outlet differs from Wehner–Wilhelm's by up to 0.644, at $\text{Pe} = 0.1$, $\text{Da} \approx 4.4$ (0.819 against 0.174), by 0.382 at $\text{Pe} = 0.5$, $\text{Da} = 2$, and by at most 0.0037 for $\text{Pe} \geq 100$. The outlet condition examined by Pearson [5] and Van Cauwenberghe [6] thereby acquires a meaning: particles reach the outlet plane and come back, and leaving is gradual, on the clock of the local time spent there. Erban and Chapman [9] use Robin conditions in the same way, as partially reactive boundaries in stochastic simulation.



4. Second-Order Kinetics

Zwietering's equation can be expanded in Da without being solved, through one identity.

Start. Definition 4 with $n = 2$: $c' = \text{Da } c^2 + h(c - 1)$, c bounded and positive [4], with $S' = -E$ and $Sh = E$.

Steps. (1) As $S'(c - 1) + Sc' = \text{Da } Sc^2$, integrating $(S(c - 1))' = \text{Da } Sc^2$ over $(0, \infty)$ gives

$$c(0) = 1 - \text{Da} \int_0^\infty S c^2 d\lambda. \quad (4.1)$$

Over (λ, ∞) instead, $S(\lambda)(1 - c(\lambda)) = \text{Da} \int_\lambda^\infty S c^2$, a contraction in the supremum norm on $[0, 1]$ -valued functions when $2\text{Da} \sup \ell < 1$; ℓ is bounded, tending to $1/\lambda_1$ (Theorem 2). So $c = 1 + \text{Da } a + \text{Da}^2 b + \dots$ uniformly in λ . (2) At order Da , $a' = 1 + ha$, with bounded solution $a = -\ell$, since $\ell' = -1 + h\ell$. (3) At order Da^2 , $b' = 2a + hb$, with bounded solution $b(\lambda) = \mathbb{E}[(\theta - \lambda)^2 \mid \theta > \lambda] = (2/S) \int_\lambda^\infty (w - \lambda) S(w) dw$. (4) Put $c^2 = 1 + 2\text{Da } a + \text{Da}^2(a^2 + 2b) + O(\text{Da}^3)$ into the identity: $\int S = m_1 = 1$, $-2 \int Sa = 2 \int R = m_2$, $\int Sb = \int w^2 S(w) dw = m_3/3$, and $\int Sa^2 = \int S\ell^2 = \int R^2/S$.

End. With $K = \int_0^\infty R^2/S d\lambda$,

$$c_{\text{mm}} = 1 - \text{Da} + m_2 \text{Da}^2 - \left(\frac{2}{3}m_3 + K\right) \text{Da}^3 + O(\text{Da}^4). \quad (4.2)$$

The dispersion model expands through the mass balance of Lemma 1's proof, applied to a chain of linear problems.

Start. $\mathcal{L}c = \text{Da } c^2$ with Definition 1's conditions. At $\text{Da} = 0$, $c = 1$, and $\mathcal{L}$ with homogeneous conditions is invertible (its null solutions $\alpha + \beta e^{\text{Pe}z}$ must vanish), so by the implicit function theorem c is analytic in Da near 0.

Steps. (1) With $c = 1 + \text{Da } c_1 + \text{Da}^2 c_2 + \text{Da}^3 c_3 + \dots$,

$$\mathcal{L}c_1 = 1, \quad \mathcal{L}c_2 = 2c_1, \quad \mathcal{L}c_3 = c_1^2 + 2c_2, \quad (4.3)$$

with homogeneous Danckwerts conditions. (2) Lemma 1's chain gives $c_1 = u_1 = -A$ and $c_2 = 2u_2$. (3) The mass balance gives $c_1(1) = -1$, $c_2(1) = 2 \int_0^1 A dz = m_2$ and $c_3(1) = -\int_0^1 A^2 dz - 2 \int_0^1 c_2 dz$. (4) $\int_0^1 c_2 dz = 2 \int_0^1 u_2 dz = -2u_3(1) = m_3/3$.

End.

$$c_{\text{disp}} = 1 - \text{Da} + m_2 \text{Da}^2 - \left(\frac{2}{3}m_3 + \int_0^1 A^2 dz\right) \text{Da}^3 + O(\text{Da}^4), \quad (4.4)$$

and from the closed form of A , $\int_0^1 A^2 dz = \frac{1}{3} + \text{Pe}^{-1} - \text{Pe}^{-2} + \frac{1}{2}\text{Pe}^{-3}(1 - e^{-2\text{Pe}})$. The chain solved by collocation agrees with this to 4.4×10^{-13} .

Proposition 1 (The three models agree through second order in Da). Under Assumption 1, as $\text{Da} \rightarrow 0$, c_{seg} , c_{disp} and c_{mm} all equal $1 - \text{Da} + m_2 \text{Da}^2 + O(\text{Da}^3)$, with $m_2 = 1 + \sigma^2$ (Lemma 1): to second order the mixing does not matter.



Proof. For $x \geq 0$, $1/(1+x) = 1 - x + x^2 - x^3/(1+x)$, so $c_{\text{seg}} = 1 - m_1 \text{Da} + m_2 \text{Da}^2 - \text{Da}^3 \int_0^\infty \theta^3 E/(1 + \text{Da}\theta) d\theta$, and the integral increases to m_3 by monotone convergence; $m_1 = 1$ by Lemma 1. Maximum mixedness and the dispersion model follow from the two expansions above [4]. $\square$

The band of Definition 5 is therefore $O(\text{Da}^3)$ wide at low conversion.

Proposition 2 (The third-order coefficients). Under Assumption 1 the Da^3 coefficients of c_{seg} , c_{disp} and c_{mm} are $-\frac{2}{3}m_3 - \frac{1}{3}m_3$, $-\frac{2}{3}m_3 - \int_0^1 A^2 dz$ and $-\frac{2}{3}m_3 - K$, with $K = \int_0^\infty R^2/S d\theta$, so

$$\xi_0 = \frac{\int_0^1 A^2 dz - K}{\frac{1}{3}m_3 - K}.$$

In the vessel's occupation measure $\frac{1}{3}m_3$ is the mean squared age, $\int_0^1 A^2 dz$ the mean square of the mean age at each position, and K the mean square of the mean age at each life expectancy; hence $\int_0^1 A^2 dz \leq \frac{1}{3}m_3$ and $K \leq \frac{1}{3}m_3$.

Proof. The coefficients come from Proposition 1's proof and the two expansions, and the lower terms of the two differences cancel; the denominator is positive by the inequality below, strict as age is not a function of life expectancy. Under a steady feed without reaction, fluid of age in $(a, a+da)$ and remaining life in $(r, r+dr)$ has residence time $a+r$, so its mass is $E(a+r) da dr$. The age marginal is $\int_0^\infty E(a+r) dr = S(a)$, giving the mean squared age $\int a^2 S = \frac{1}{3}m_3$. Given age a the mean remaining life is $\int r E(a+r) dr / S(a) = \ell(a)$; by the symmetry of $E(a+r)$, the fluid with life expectancy λ has density $S(\lambda)$ and mean age $\ell(\lambda)$, so $K = \int S \ell^2$ is as stated. The tracer is 1 at every z , so the fluid is uniform in position with mean age $A(z)$ (Lemma 1). The age density is S in every description, and Jensen's inequality for conditional expectations gives both inequalities. $\square$

The three models mix, to third order, nothing, the fluid at the same place, and the fluid with the same life expectancy. The ordering $K \leq \int_0^1 A^2 dz$, which puts ξ_0 in $[0, 1]$, is not proved; it holds at all 39 computed Pe.

Lemma 2 (Maximum mixedness near plug flow). For any residence-time distribution with mean 1, variance $\sigma^2 \rightarrow 0$ and tails decaying faster than any power of $|\theta - 1|/\sigma$, formally, for fixed Da,

$$c_{\text{mm}} = \frac{1}{1 + \text{Da} - \sigma^2 \text{Da}^2} + O(\sigma^3),$$

an excess $\sigma^2 \text{Da}^2 / (1 + \text{Da})^2$ over plug flow, whose Da^3 coefficient $-2\sigma^2$ agrees with Proposition 2 to leading order.

Proof. The argument is formal. With $c = 1 - \varepsilon$, Zwietering's equation reads $\varepsilon' = h\varepsilon - \text{Da} + 2\text{Da}\varepsilon - \text{Da}\varepsilon^2$. In the layer $|\lambda - 1| = O(\sigma)$, where $h = O(1/\sigma)$, the expansion of Zwietering's equation gives $\varepsilon = \text{Da}\ell - \text{Da}^2 b + O(\sigma^3)$, since there $\ell = O(\sigma)$, $b = O(\sigma^2)$ and the Da^k term is $O(\sigma^k)$. Below the layer h is negligible, $c' = \text{Da}c^2$, and $1/c(0) = 1/c(\lambda_b) + \text{Da}\lambda_b$. Match at $\lambda_b = 1 - M\sigma$, M fixed and large, $x = 1 - \lambda_b$: up to the tails $\ell(\lambda_b) = x$ and $b(\lambda_b) = x^2 + \sigma^2$, so $1/c(\lambda_b) = 1 + \text{Da}x - \text{Da}^2 \sigma^2 + O(\sigma^3)$ and $1/c(0) = 1 + \text{Da} - \text{Da}^2 \sigma^2 + O(\sigma^3)$, free of



M. In Proposition 2 the excess coefficient is $-\frac{2}{3}(m_3 - 1) - (K - \frac{1}{3}) = -2\sigma^2 + O(\sigma^3)$, as $\ell(\lambda) = 1 - \lambda$ below the layer. $\square$

With an $O(\sigma^3)$ remainder the error in excess/ σ^2 falls only like σ : the observed exponent is -0.48 in Pe at Da = 1, and 0.49 in σ^2 for a gamma distribution of the same variance. The layer expansion runs in powers of Da σ , so at Da = 10 the error falls only from 0.49 at Pe = 50 to 0.23 at 1000, of a limit $100/121$ (exponent -0.26 ; 0.40 for the gamma distribution).

Lemma 3 (The dispersion model near plug flow). Under Assumption 1, formally, for fixed Da as $\text{Pe} \rightarrow \infty$,

$$c_{\text{disp}} = \frac{1}{1 + \text{Da}} + \frac{2}{\text{Pe}} \frac{\text{Da} \ln(1 + \text{Da})}{(1 + \text{Da})^2} + O(\text{Pe}^{-2}),$$

an excess $\sigma^2 \text{Da} \ln(1 + \text{Da}) / (1 + \text{Da})^2$, as $\sigma^2 = 2/\text{Pe} + O(\text{Pe}^{-2})$; its Da^3 coefficient $-\frac{5}{2}\sigma^2$ agrees with Proposition 2.

Proof. The argument is formal. Away from the outlet put $c = c^{(0)} + \text{Pe}^{-1}c^{(1)}$: then $c^{(0)} = 1/(1 + \text{Da}z)$, and $\partial_z c^{(1)} + 2\text{Da}c^{(0)}c^{(1)} = \partial_{zz}c^{(0)}$ with $c^{(1)}(0) = \partial_z c^{(0)}(0) = -\text{Da}$ from the inlet condition. The integrating factor $(1 + \text{Da}z)^2$ gives

$$(1 + \text{Da}z)^2 c^{(1)} = -\text{Da} + 2\text{Da} \ln(1 + \text{Da}z).$$

A layer $\text{Be}^{\text{Pe}(z-1)}$ of width $1/\text{Pe}$, where reaction is negligible, restores $\partial_z c(1) = 0$ with $B = -\text{Pe}^{-1}\partial_z c^{(0)}(1) = \text{Pe}^{-1}\text{Da}/(1 + \text{Da})^2$. The sum at $z = 1$ is the stated term. Since $\text{Da} \ln(1 + \text{Da}) / (1 + \text{Da})^2 = \text{Da}^2 - \frac{5}{2}\text{Da}^3 + \dots$, and in Proposition 2 $-\frac{2}{3}(m_3 - 1) - (\int_0^1 A^2 dz - \frac{1}{3}) = -5/\text{Pe} + O(\text{Pe}^{-2})$, the coefficients agree. $\square$

The outlet layer contributes at the same order as the interior. The error in excess/ σ^2 falls as $\text{Pe}^{-0.99}$ at Da = 1 ($\text{Pe}^{-0.92}$ at the worst Da).

Theorem 3 (The limit curve near plug flow). Under Assumption 1 and Lemmas 2 and 3, for each fixed Da > 0, as $\text{Pe} \rightarrow \infty$,

$$\xi \rightarrow \xi_\infty(\text{Da}) = \frac{(1 + \text{Da})(\text{Da} - \ln(1 + \text{Da}))}{\text{Da}^2},$$

which increases strictly from $\xi_\infty(0^+) = \frac{1}{2}$ toward 1 as $\text{Da} \rightarrow \infty$. At Da^3 the excesses over plug flow have coefficients $-3\sigma^2$, $-\frac{5}{2}\sigma^2$ and $-2\sigma^2$ for segregation, the dispersion model and maximum mixedness. The limit is as formal as Lemmas 2 and 3, and its rate is not proved.

Proof. Taylor's theorem about $\theta = 1$, with $|c_b''| \leq 6\text{Da}^3$ on $\theta \geq 0$, gives $c_{\text{seg}} = 1/(1 + \text{Da}) + \sigma^2 \text{Da}^2 / (1 + \text{Da})^3 + \rho$ with $|\rho| \leq \text{Da}^3 \mathbb{E}|\theta - 1|^3 = O(\sigma^3)$. With Lemmas 2 and 3 the three excesses over $1/(1 + \text{Da})$ are σ^2 times

$$\frac{\text{Da}^2}{(1 + \text{Da})^3}, \quad \frac{\text{Da} \ln(1 + \text{Da})}{(1 + \text{Da})^2}, \quad \frac{\text{Da}^2}{(1 + \text{Da})^2},$$



up to $o(\sigma^2)$, and in the ratio ξ the factor σ^2 cancels, leaving ξ_∞ . As $\text{Da} - \ln(1 + \text{Da}) = \frac{1}{2}\text{Da}^2 - \frac{1}{3}\text{Da}^3 + \dots$, $\xi_\infty(0^+) = \frac{1}{2}$; as $\ln(1 + \text{Da}) > \text{Da}/(1 + \text{Da})$, $\xi_\infty < 1$, and $\xi_\infty \rightarrow 1$ since $\ln(1 + \text{Da})/\text{Da} \rightarrow 0$. Differentiating, $\text{Da}^3 \xi'_\infty = \phi(\text{Da})$ with $\phi(x) = (2 + x) \ln(1 + x) - 2x$, and $\phi(0) = \phi'(0) = 0$, $\phi''(x) = x/(1 + x)^2 > 0$, so $\xi'_\infty > 0$. The three excesses expand as $\sigma^2 \text{Da}^2$ times $1 - 3\text{Da}$, $1 - \frac{5}{2}\text{Da}$ and $1 - 2\text{Da}$, plus $O(\text{Da}^2)$. $\square$

At low conversion the dispersion model sits midway between Zwietering's limits; as the reaction quickens it moves toward segregation, $\xi_\infty(1) = 0.6137$, $\xi_\infty(10) = 0.8362$. For the closed vessel the third central moment $m_3 - 1 - 3\sigma^2$ is $12/\text{Pe}^2 + O(\text{Pe}^{-3})$ (Lemma 1), so the segregation remainder is smaller still. The observed rate is $\text{Pe}^{-1/2}$, with $(\frac{1}{2} - \xi_0)\sqrt{\text{Pe}} \rightarrow 0.640$, and slower at large Da : at $\text{Pe} = 1000$, $\xi = 0.582$ against 0.6137 at $\text{Da} = 1$ but 0.768 against 0.8362 at $\text{Da} = 10$.

Proposition 3 (Near the stirred tank the dispersion model is maximum mixedness). Under Assumption 1, as $\text{Pe} \rightarrow 0$ with Da fixed, $E(\theta) \rightarrow e^{-\theta}$; c_{disp} and c_{mm} tend to the stirred tank's $c_{\text{cstr}} = (\sqrt{1 + 4\text{Da}} - 1)/(2\text{Da})$ and c_{seg} to the segregated stirred tank, so $\xi \rightarrow 0$. In the coefficients $A \rightarrow 1$, $\int_0^1 A^2 dz \rightarrow 1$, $K \rightarrow 1$ and $\frac{1}{3}m_3 \rightarrow 2$, so $\xi_0 \rightarrow 0$. The coefficient limits are exact; those of the full models are formal.

Proof. As $\text{Pe} \rightarrow 0$, $a \rightarrow \infty$ but $a\text{Pe} \rightarrow 0$, and expanding the exponentials the transform of Corollary 1 tends to $1/(1 + s)$, that of $e^{-\theta}$. With $h \equiv 1$, Zwietering's equation $c' = \text{Da}c^2 + c - 1$ has the constant solution c_{cstr} , and every other solution grows without bound or crosses zero. The dispersion model times Pe , $c'' - \text{Pe}c' = \text{PeDa}c^2$ with $c'(0) = \text{Pe}(c(0) - 1)$ and $c'(1) = 0$, has a constant solution at $\text{Pe} = 0$, fixed at the next order by $1 - c = \text{Da}c^2$. The segregated stirred tank lies below c_{cstr} for $\text{Da} > 0$ [4], so the denominator of ξ stays positive while its numerator vanishes. Finally $e^{-\text{Pe}(1-z)} = 1 - \text{Pe}(1 - z) + O(\text{Pe}^2)$ gives $A \rightarrow 1$; for $e^{-\theta}$, $R = S$, so $K \rightarrow 1$; and $m_3 \rightarrow 6$. $\square$

At $\text{Pe} = 0.1$, c_{mm} and c_{disp} lie within 9.6×10^{-3} and 9.7×10^{-3} of the stirred tank, and $\xi \leq 0.0022$.

Corollary 2 (The midpoint rule). At every (Pe, Da) ,

$$X_{\text{disp}} = \frac{1}{2}(X_{\text{seg}} + X_{\text{mm}}) + (\xi - \frac{1}{2})(X_{\text{seg}} - X_{\text{mm}}),$$

so the midpoint of Zwietering's band (Definition 4) errs by $|\xi - \frac{1}{2}|$ times its width. Near plug flow the width is $O(\sigma^2)$ and $\xi \rightarrow \xi_\infty$ (Theorem 3). On the computed grid with $\text{Pe} \geq 20$ and $\text{Da} \leq 10$ the error is at most 0.098 percentage points.

Proof. With $X = 1 - c$, Definition 5 is $X_{\text{disp}} = X_{\text{mm}} + \xi(X_{\text{seg}} - X_{\text{mm}})$; rearrange. The width is the difference of the excesses in Theorem 3's proof, formally $O(\sigma^2)$. The bound is measured, not proved. Both limits need only the residence-time distribution, so the rule needs no solution of the dispersion model. $\square$

Remark 2 (Three, five halves, two). Near plug flow the Da^3 coefficients exceed plug flow's -1 by $-3\sigma^2$, $-\frac{5}{2}\sigma^2$ and $-2\sigma^2$ (Theorem 3). The common part is $-\frac{2}{3}(m_3 - 1) = -2\sigma^2 +$



$O(\sigma^4)$; the rest is the mean square of the averaged age less the plug's $\frac{1}{3}$, which is σ^2 when nothing is averaged, $\frac{1}{2}\sigma^2$ over position and $o(\sigma^2)$ over life expectancy, up to $O(\sigma^4)$. Hence $\xi_0 \rightarrow \frac{1}{2}$. The averaged ages share the mean $m_2/2$, so with V_{age} , V_{pos} , V_{life} the variances of the age and of its means at a position and at a life expectancy,

$$\xi_0 = \frac{V_{\text{pos}} - V_{\text{life}}}{V_{\text{age}} - V_{\text{life}}} = \frac{J - J_{\text{mm}}}{1 - J_{\text{mm}}},$$

where $J = V_{\text{pos}}/V_{\text{age}}$ is Danckwerts' degree of segregation [3], the variance of the mean age at a point over that of the age, and $J_{\text{mm}} = V_{\text{life}}/V_{\text{age}}$: Danckwerts' measure made exact at third order, with its zero moved from complete mixing to maximum mixedness.

Example 1 (A worked example). A closed vessel with $Pe = 10$, below the range of the midpoint rule, so that $\sigma^2 = 0.180$, carries a second-order reaction with $Da = 2$.

Parameters. $n = 2$; Algorithm 1 with $N = 1601$, checked by collocation; Algorithm 2 for the limits.

Computation. Plug flow gives $X = 0.6667$ and the stirred tank $X = 0.5$. Segregation gives $X_{\text{seg}} = 0.6426$, maximum mixedness $X_{\text{mm}} = 0.6232$, and the dispersion model $X_{\text{disp}} = 0.6295$ (collocation agrees to 6×10^{-13}). The band is 1.95 points wide and $\xi = 0.325$; the midpoint, 0.6329, lies 0.34 points above X_{disp} , as Corollary 2 requires with $\xi < \frac{1}{2}$.

Shows. The dispersion model sits a third of the way up a band under two points wide; at this Pe the midpoint misses by more than three times the rule's bound.

5. Computing the Three Answers


Algorithm 1 — The method of lines for the Danckwerts vessel

Inputs: Pe , Da , n , the feed $c_{in}(\theta)$, N nodes and an end time. *Output:* c at the nodes over time; at steady state, $c(1)$ and its change over the last stretch.

1. Nodes $z_i = ih$, $h = 1/(N - 1)$.
2. First-derivative matrix D : five-point fourth-order stencils with Fornberg's weights [15], centred inside and one-sided near the ends; where $Pe h > 2$, Schiesser's biased upwind stencil for convection [12].
3. Stagewise boundary conditions [12], [14]: $\partial_z c = Dc$; overwrite its end values by $Pe(c_0 - c_{in}(\theta))$ at $z = 0$ and 0 at $z = 1$; then $\partial_{zz} c = D(\partial_z c)$.
4. $dc_i/d\theta = Pe^{-1}(\partial_{zz} c)_i - (\partial_z c)_i - Da c_i^n$ at all nodes, both stages in extended precision.
5. Integrate from $c = 0$ by variable-order BDF formulas [16]; for the steady state, to $\theta = 34/r$ and $6/r$ more, with $r = \min(\lambda_1, 2Da/(1 + Da))$.

Cost. $O(N)$ per step; the round-off of the double differentiation, about machine precision times N^2/Pe , is why step 4 uses extended precision. For the map, $N - 1 = 800 \cdot 2^j \geq 100 Pe$, up to 51 201 nodes, resolves the layer $e^{Pe(z-1)}$, so convection is centred throughout. With $Da = 0$ the stagewise operator has one spurious stationary mode, zero at both end nodes; it leaves $c(1)$ and $S(0, \theta)$ alone but is damped only by the reaction, hence the second rate in r . All computations use Python with NumPy, SciPy and mpmath.

Algorithm 2 — The RTD two ways, and Zwietering's limits from it

Inputs: Pe , the values of Da , the far level 10^{-24} . *Output:* S , E , R , h on Chebyshev panels; m_1 , m_2 , m_3 , K ; c_{seg} and c_{mm} .

1. Spectral source (Theorem 2): bracket the k -th root in $((k - 1)\pi, k\pi)$, polish it in high precision, form λ_k , A_k ; use enough terms and digits for the sums at the smallest node θ_{lo} : 64 terms at 52 digits for $Pe = 0.1$, 1940 terms at 1331 digits for $Pe = 10^4$.
2. Find λ_{max} with $S(0, \lambda_{max}) = 10^{-24}$; cover $[\theta_{lo}, \lambda_{max}]$ with 59 to 128 Chebyshev panels.
3. At every node sum S , E and $R = \sum_k A_k e^{-\lambda_k \theta} / \lambda_k$; form $h = E/S$ and R^2/S .
4. Moments and K by Clenshaw-Curtis quadrature, the two ends in closed form.
5. Segregation: $c_{seg} = \int_0^\infty e^{-x} \hat{E}(Da x) dx$, $\hat{E}$ the Wehner-Wilhelm transform; checked by quadrature of $E/(1 + Da \theta)$.
6. Maximum mixedness: from the root of $Da c^2 + \lambda_1(c - 1) = 0$ at λ_{max} , integrate Zwietering's equation [4] backward by Chebyshev collocation and Newton's method on each panel; on $[0, \theta_{lo}]$, where h is negligible, take the exact batch step.
7. Checks: F by Talbot inversion of $\hat{E}(s)/s$ [18] and by the forward and backward problems of Algorithm 1; far point moved to 10^{-16} ; panels halved; the exponential distribution must return the stirred tank.

Cost. The high-precision sums dominate. An error in the start of step 6 is damped by $\exp(-\int (2Da c + h) d\lambda) \leq S(\lambda_{max})/S(\lambda)$.


Algorithm 3 — Simulating the elastic particle

Inputs: Pe , the step $\Delta\theta$, M particles, a seed, and the outlet rule (elastic or absorbing). *Output:* exit times τ_i ; means and standard errors of $e^{-Da\tau}$ and τ .

1. Set $Z = 0$, $\theta = 0$.
2. Draw ζ standard normal; $Z \leftarrow Z + \Delta\theta + \sqrt{2\Delta\theta/Pe}\zeta$, $\theta \leftarrow \theta + \Delta\theta$.
3. If $Z < 0$, set $Z \leftarrow 0$; the undershoot is the increment of L^0 .
4. If $Z > 1$: absorbing, stop; elastic, let $\delta = Z - 1$, the increment of L^1 , set $Z \leftarrow 1$, and stop with probability $1 - e^{-Pe\delta}$.
5. If stopped, record $\tau = \theta$; otherwise go to step 2.
6. Repeat for M particles and several $\Delta\theta$ with independent seeds; fit $V + C\sqrt{\Delta\theta}$ to the means.

Cost. About $M/\Delta\theta$ steps, the mean exit time being 1 (Lemma 1). Seeing the boundary only at step times, the scheme has a bias of order $\Delta\theta^{1/2}$ [19], the order the extrapolation assumes.

6. Verification

Script. Algorithm 3 at $Pe = 3$: seven paths, and 10^5 exit times.

Shows. Theorem 1.

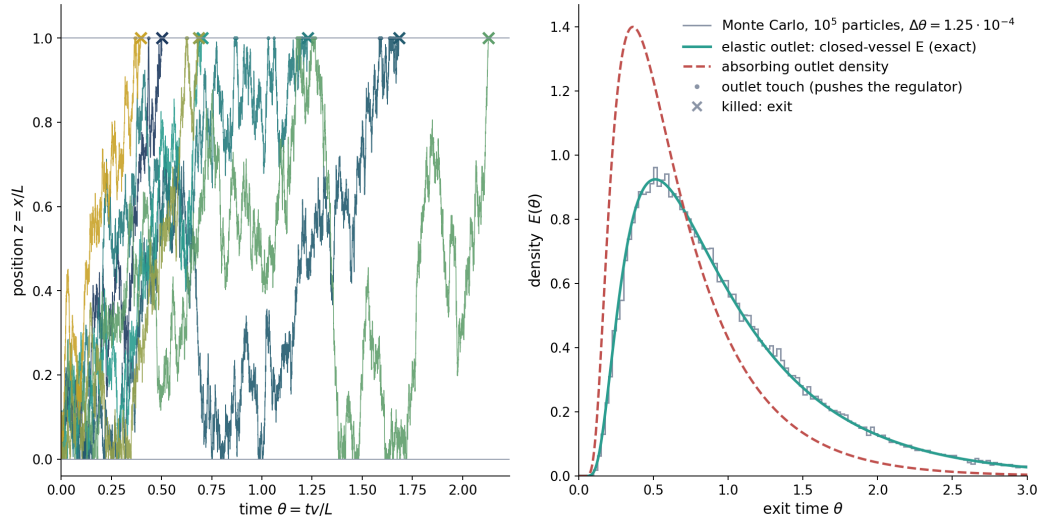


Figure 1: Left: seven paths of the elastic particle at $Pe = 3$, with a dot at each step on which the outlet pushes a particle back and a cross where it is removed. Right: exit times of 10^5 particles against the closed-vessel E and the absorbing outlet's density.

No particle left at its first touch: the seven touched the outlet on 6 to 67 steps and left between $\theta = 0.40$ and 2.13. The histogram follows E , of mean 1; the absorbing density peaks earlier and higher, with mean 0.683.

The Monte Carlo against the closed form. *Method.* Algorithm 3, elastic and absorb-



ing, for $\mathbb{E}_0[e^{-\tau}]$ (the first-order outlet at $\text{Da} = 1$) and $\mathbb{E}_0[\tau]$, extrapolated by $V + C\sqrt{\Delta\theta}$ [19].

Parameters. $\text{Pe} = 3$; 10^5 particles per step; $\Delta\theta$ from 10^{-3} to 1.25×10^{-4} by halving; independent fixed seeds.

Result. Elastic: the bias of $e^{-\tau}$ shrinks from -0.0106 to -0.0032 (order 0.57) and extrapolates to 0.4345 ± 0.0009 against Wehner–Wilhelm’s 0.4337; the mean exit time to 0.9966 ± 0.0030 against 1 (order 0.63). Absorbing: 0.5472 ± 0.0008 against 0.5467 and 0.6822 ± 0.0020 against 0.6833 (orders 0.51, 0.49).

Error. The extrapolations lie $+0.89$, -1.10 , $+0.65$ and -0.51 standard errors from their closed forms; each rule converges to its own. This verifies Theorem 1 at $\text{Pe} = 3$.

Source. Algorithm 1 with $n = 1$ at steady state against Corollary 1, $\text{Da} = 2$, centred convection; orders from successive doublings.

Columns. Grid points N ; relative error of $c(1)$ and observed order at $\text{Pe} = 1, 10$ and 100 .

Table 1: Relative error of the method of lines against Wehner–Wilhelm at $\text{Da} = 2$ as the grid is refined.

N	$\text{Pe} = 1$	order	$\text{Pe} = 10$	order	$\text{Pe} = 100$	order
51	2.9×10^{-8}		9.1×10^{-5}		1.8×10^{-1}	
101	1.2×10^{-9}	4.64	3.6×10^{-6}	4.67	3.3×10^{-2}	2.46
201	5.2×10^{-11}	4.50	1.3×10^{-7}	4.83	2.7×10^{-3}	3.61
401	2.5×10^{-12}	4.35	4.2×10^{-9}	4.91	1.4×10^{-4}	4.30
801	1.2×10^{-13}	4.36	1.3×10^{-10}	4.95	5.5×10^{-6}	4.65
1601	4.1×10^{-14}	1.59	4.3×10^{-12}	4.97	1.9×10^{-7}	4.83
3201	2.9×10^{-13}	-2.81	1.1×10^{-13}	5.33	6.5×10^{-9}	4.91

Once the outlet layer is resolved the order lies between 4.3 and 5, above the nominal four; at $\text{Pe} = 1$ round-off, growing like N^2 , sets a floor near 10^{-13} .

First-order conversion, and the absorbing outlet’s error. *Method.* The first-order steady outlet by Algorithm 1, by Chebyshev collocation, and by the backward problems of Corollary 1 and Remark 1 solved exactly in 60 digits, each against its closed form; the absorbing error is the difference of the closed forms.

Parameters. Method of lines at $\text{Pe} = 1$ to 1000, $\text{Da} = 0.5$ and 2 (Table 1); collocation on the map’s grid; exact solves at 24 pairs; the absorbing error also on a 401×401 grid.

Result. The exact solves reproduce both formulas to 1.2×10^{-59} , and collocation agrees to 3.0×10^{-11} . At $N = 801$ the method of lines reaches 1.2×10^{-13} at $\text{Pe} = 1$ and 1.4×10^{-10} at $\text{Pe} = 10$, but only 3.0×10^{-6} and 5.5×10^{-6} at $\text{Pe} = 100$ ($\text{Da} = 0.5, 2$). The absorbing outlet is off by up to 0.644 at $\text{Pe} = 0.1$, $\text{Da} = 4.42$, by 0.382 at $\text{Pe} = 0.5$, $\text{Da} = 2$, and by



at most 0.0037 for $Pe \geq 100$.

Error. One check fails: the threshold set in advance, 10^{-8} at $N = 801$ for $Pe \leq 100$, is missed at $Pe = 100$, where $Pe h = 0.125$ under-resolves the outlet layer; it is met only at $N = 3201$, which is why the map's grids are sized to the layer. This verifies Corollary 1 and Remark 1.

Script. The spectral expansion of Theorem 2, and the absorbing outlet's density by Talbot inversion.

Shows. Theorem 1: one family from the stirred tank to plug flow, beside the absorbing outlet's.

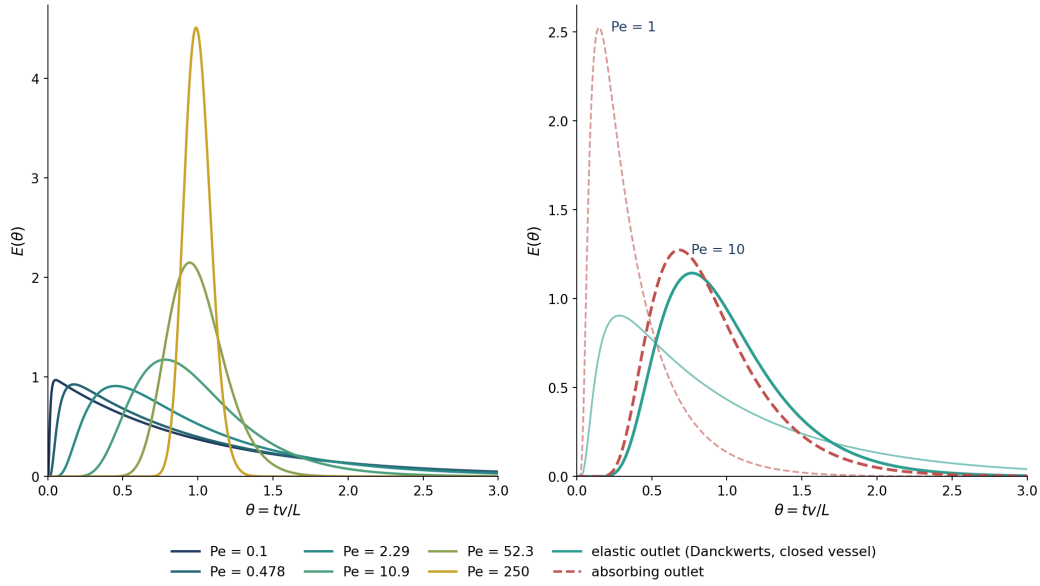


Figure 2: Left: the closed-vessel residence-time distribution $E(\theta)$ at $Pe = 0.1, 0.478, 2.29, 10.9, 52.3$ and 250 . Right: the elastic (Danckwerts) and absorbing exit densities at $Pe = 1$ and 10 , solid and dashed.

At $Pe = 0.1$ the distribution is nearly $e^{-\theta}$; at 250 it is a narrow peak of variance near $2/Pe$. The absorbing densities peak earlier and higher, far more at $Pe = 1$ than at 10 .

One distribution, three computations. *Method.* F from the forward step response and $1 - S(0, \theta)$ from the backward problem, both by Algorithm 1 with $Da = 0$, and by Talbot inversion of $\hat{E}(s)/s$ [18], with the spectral expansion as a fourth; moments from derivatives of the transform in high precision and by quadrature of the spectral E .

Parameters. $Pe = 0.5, 5, 50$; $N = 801$; 150 times each. Moments at eight Pe from 0.1 to 1000 .

Result. The largest difference in F is 6.5×10^{-10} , 9.2×10^{-10} and 1.9×10^{-7} ; forward and backward routes agree with each other to 5.5×10^{-10} , 8.6×10^{-10} and 2.2×10^{-9} , and spectral with Talbot to 1.1×10^{-16} . The derivatives give $m_1 = 1$ exactly and m_2, m_3 within 5.3×10^{-50} and 9.1×10^{-48} of Lemma 1; quadrature within 1.1×10^{-15} and 5.3×10^{-15} .



Error. At $Pe = 50$ the 1.9×10^{-7} is the grid's, nearly the same in both routes. The forward route is the tracer and the backward one the particle's survival, so their agreement is Theorem 1(i) on the grid. This verifies Theorem 1 and Lemma 1.

The decay rate against the computed hazard. *Method.* λ_1 from Theorem 2's equation against the long-time hazard $-\partial_\theta \ln S(0, \theta)$, from Algorithm 1 in the symmetrised variable $w = e^{Pe z/2} S$ run to $\theta = 30/(\lambda_2 - \lambda_1)$; and the A_k against the residues of the transform.

Parameters. 13 values of Pe from 0.1 to 1000; residues at $Pe = 0.5, 5, 50, 500$.

Result. $\lambda_1 = 1.0167, 3.0219, 25.091$ and 250.0098 at $Pe = 0.1, 10, 100$ and 1000 . The largest relative difference from the hazard is 1.5×10^{-9} , and 4.1×10^{-6} for the small $\lambda_1 - Pe/4$. The A_k match the residues to 4.2×10^{-53} or better.

Error. In the variable S the discrete eigenvalues are ill-conditioned by about $e^{Pe/2}$, and a shift-and-invert solve at $Pe = 100$ gave a wrong rate; the symmetrised variable removes the factor. Algorithm 2's far point precedes the exponential tail at large Pe (hazard $0.60 \lambda_1$ at 1000), yet moving it changes c_{mm} by only 2.7×10^{-15} . This verifies Theorem 2.

Script. Algorithm 1 with $N = 801$ after a unit step in feed.

Shows. The inlet jump of Definition 1, and a step passing through the vessel.

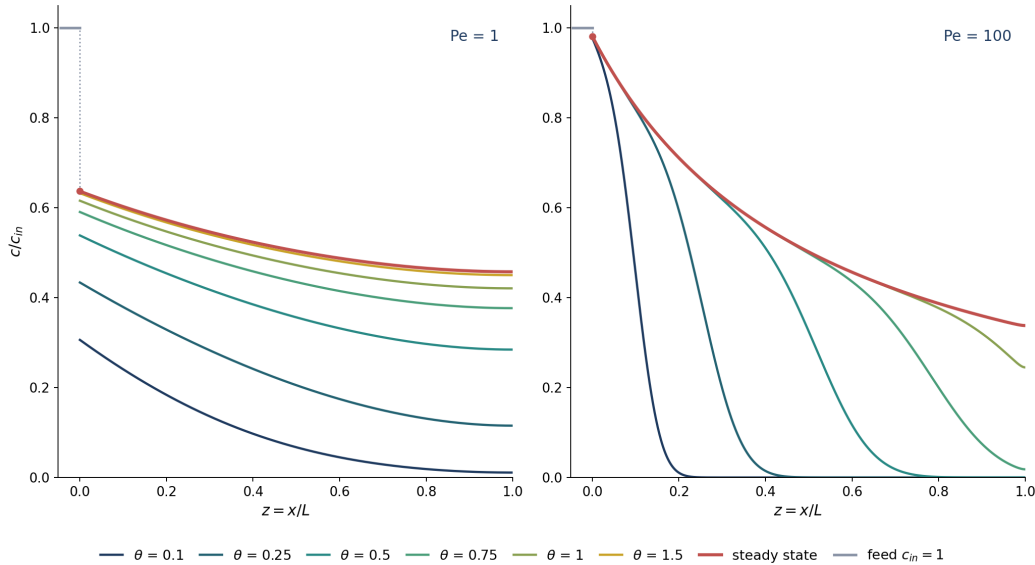


Figure 3: Profiles c/c_{in} after a unit step in feed, second-order reaction with $Da = 2$, at $Pe = 1$ (left) and $Pe = 100$ (right), at $\theta = 0.1, 0.25, 0.5, 0.75, 1$ and 1.5 and at steady state, the feed drawn left of the inlet.

At steady state the concentration drops across the inlet plane to 0.637 at $Pe = 1$ and 0.981 at 100 . At $Pe = 1$ the vessel fills at once; at 100 a front moves at unit speed (outlet 3.3×10^{-7} at $\theta = 0.5, 0.245$ at 1 , the steady 0.338 at 1.5).

The coefficients against their limits. *Method.* Proposition 2's coefficients from Lemma 1's closed forms, K by Algorithm 2 (and by Talbot inversion at $Pe = 1$), and the disper-



sion chain by collocation, against finite differences in Da of the full computations, whose dispersion solutions the collocation solver of [17] confirms on a subgrid.

Parameters. 39 values of Pe from 0.1 to 10^4 ; finite differences at $Pe = 1, 10, 100$, $Da = 0.01$ to 0.06.

Result. The second-order coefficient equals m_2 to 5.9×10^{-13} ; the two values of K at $Pe = 1$ agree to every printed digit, 0.75418561711554. The third-order coefficients agree with the finite differences to 4.0×10^{-6} relative, and ξ at $Da = 0.01$ differs from ξ_0 by at most 1.8×10^{-3} . In units of σ^2 the excess coefficients are 3.0006, 2.5004 and 2.0130 at $Pe = 10^4$; $K - \frac{1}{3}$ falls from 7.8×10^{-5} to 2.5×10^{-6} between $Pe = 1000$ and 10^4 , as $Pe^{-3/2}$. Fitting $(\frac{1}{2} - \xi_0)\sqrt{Pe} = C + D/\sqrt{Pe}$ over $Pe \geq 100$ gives $C = 0.640$.

Error. The maximum-mixedness coefficient approaches 2 only like σ , Lemma 2's remainder. This verifies Propositions 1 and 2 and the coefficients of Theorem 3.

Source. Lemma 1 for σ^2 and m_3 ; $\int_0^1 A^2 dz = -c_3(1) - \frac{2}{3}m_3$ from the dispersion chain, equal to its closed form to rounding; K by Algorithm 2; coefficients and ξ_0 by Proposition 2.

Columns. Pe ; σ^2 ; the three mean squares of Proposition 2; the Da^3 coefficients of segregation, the dispersion model and maximum mixedness; ξ_0 .

Table 2: Third-order coefficients of the three models and the position at low conversion, from the stirred tank to plug flow.

Pe	σ^2	$m_3/3$	$\int A^2$	K	seg.	disp.	m.m.	ξ_0
0.1	0.9675	1.9351	0.96796	0.96775	-5.8054	-4.8382	-4.8380	0.00021
1	0.7358	1.4836	0.76567	0.75419	-4.4509	-3.7330	-3.7215	0.0157
10	0.1800	0.54534	0.42383	0.38658	-1.6360	-1.5145	-1.4773	0.2347
100	0.01980	0.35353	0.34323	0.33558	-1.0606	-1.0503	-1.0426	0.4266
300	0.006644	0.34002	0.33666	0.33379	-1.0201	-1.0167	-1.0138	0.4598
1000	0.001998	0.33534	0.33433	0.33341	-1.00601	-1.00500	-1.00408	0.4788
10^4	0.0002000	0.33353	0.33343	0.33334	-1.00060	-1.00050	-1.00040	0.4935

In every row $K < \int_0^1 A^2 dz < m_3/3$, so $0 < \xi_0 < 1$; the first inequality is measured, not proved.

Script. ξ_0 from Proposition 2, and ξ from the full computations.

Shows. Proposition 3 at the left, Theorem 3 at the right.

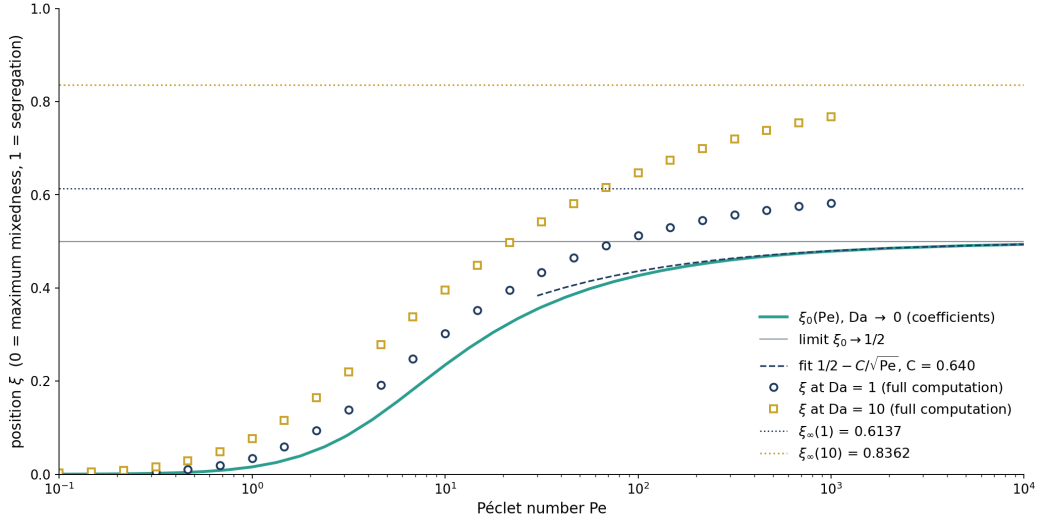


Figure 4: The position $\xi_0(\text{Pe})$ at low conversion between maximum mixedness (0) and segregation (1), second-order reaction, Pe from 0.1 to 10^4 , with the fit $1/2 - C/\sqrt{\text{Pe}}$, $C = 0.640$, and ξ at $\text{Da} = 1$ and 10 against $\xi_\infty(1) = 0.6137$ and $\xi_\infty(10) = 0.8362$.

ξ_0 is 0.0157 at $\text{Pe} = 1$, 0.235 at 10 and 0.494 at 10^4 ; at $\text{Pe} = 1000$, ξ is 0.582 at $\text{Da} = 1$ and 0.768 at $\text{Da} = 10$.

Script. Excesses at $\text{Pe} = 1000$, and ξ over Da , from the full computations.

Shows. Proposition 2 and Theorem 3.

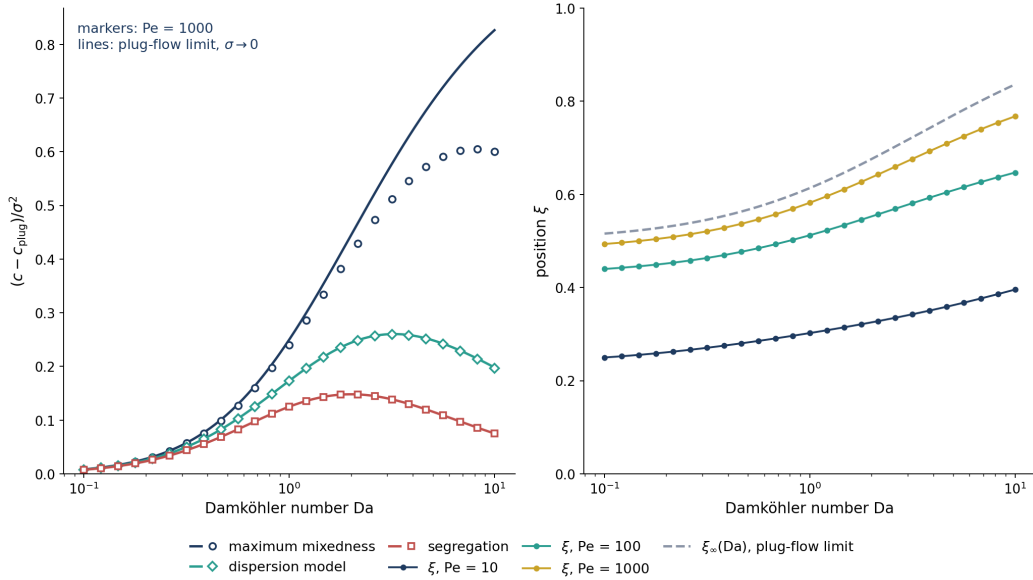


Figure 5: Left: excess over plug flow $(c - c_{\text{plug}})/\sigma^2$ of the three models at $\text{Pe} = 1000$ (markers) against their plug-flow limits (lines), second-order reaction, Da from 0.1 to 10. Right: ξ against Da at $\text{Pe} = 10, 100$ and 1000, with $\xi_\infty(\text{Da})$ dashed.

Segregation and the dispersion model sit on their curves; maximum mixedness falls 0.23 short of 100/121 at $\text{Da} = 10$. At $\text{Pe} = 1000$, ξ runs from 0.494 to 0.768 against 0.516 to



0.836.

Script. ξ from the full computations on the 25×25 grid.

Shows. Theorem 3 and Proposition 3 together.

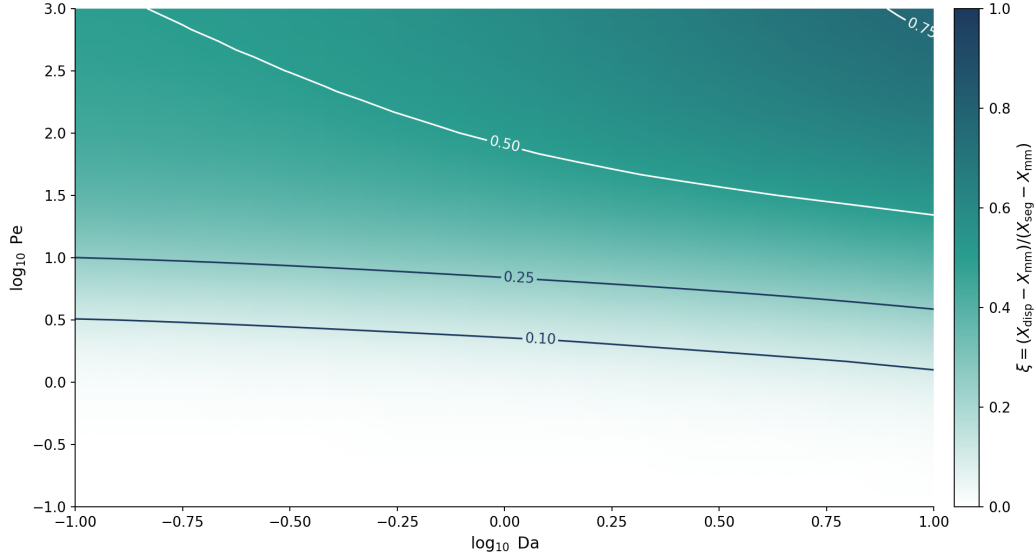


Figure 6: The position ξ of the dispersion model in Zwietering's band for a second-order reaction over Da from 0.1 to 10 and Pe from 0.1 to 1000, logarithmic axes, with contours at 0.10, 0.25, 0.50 and 0.75.

ξ rises with both numbers, from at most 0.0022 at $Pe = 0.1$ to 0.768; above $Pe \approx 20$ it lies between 0.34 and 0.77 while the band narrows, so the midpoint rule works there.

The map, computed independently four ways. *Method.* The dispersion model by Algorithm 1, by Chebyshev collocation, and on a 7×7 subgrid by the residual-controlled solver of [17]; the two limits a fourth way, by Algorithm 2.

Parameters. $n = 2$; 25 values each of Pe from 0.1 to 1000 and Da from 0.1 to 10; 801 to 51 201 nodes.

Result. Method of lines and collocation agree to 1.5×10^{-10} in $c(1)$ and 5.0×10^{-5} in ξ ; the subgrid solver agrees to 1.4×10^{-10} , even at its one unconverged point. Segregation by identity and quadrature agree to 4.4×10^{-16} ; moving Zwietering's far point changes c_{mm} by 2.7×10^{-15} ; the exponential case returns the stirred tank to 1.2×10^{-15} . $X_{mm} \leq X_{disp} \leq X_{seg}$ at all 625 points, with smallest margins 1.2×10^{-7} and 7.3×10^{-7} . The band is 0.044 points wide at $Da = 0.1$, $Pe = 0.1$, and at most 6.9 points. At $Da = 1$, $\xi = 0.302$, 0.512 and 0.582 at $Pe = 10, 100, 1000$.

Error. The agreement lies far below the differences displayed, except in ξ where the band is narrowest. This verifies Proposition 1 and Theorem 3 on the computed plane.

How good the midpoint rule is. *Method.* From the map, $|X_{disp} - \frac{1}{2}(X_{seg} + X_{mm})|$ in percentage points, against the band $X_{seg} - X_{mm}$.

Parameters. The map's grid; $Pe \geq 20$ covers its eleven values from 21.5 to 1000.



Result. For $Pe \geq 20$, $Da \leq 10$ the largest error is 0.098 points, at $Pe = 21.5$, $Da = 2.15$, where $\xi = 0.426$ in a band of 1.33 points; over that range the band is at most 1.8 points. Over all Pe the error reaches 3.43 points, at $Pe = 0.1$. The worst error over Da is 2.52 points at $Pe = 1$, 0.39 at 10, 0.057 at 31.6, 0.097 at 68.1 and 0.028 at 1000.

Error. The error is $|\xi - \frac{1}{2}|$ times the band (Corollary 2): it falls as the band narrows, rises between $Pe \approx 30$ and 70 as ξ passes one half at large Da , then falls like σ^2 . The bound is measured, not proved. This verifies Corollary 2.

7. Discussion

A zero gradient at the outlet is often read as nothing happening there. For the particle the outlet is where leaving is decided: it reaches the plane, is pushed back, returns, and leaves only after enough local time at the plane, at rate Pe per unit; the paths of Figure 1 touch it on 6 to 67 steps first. The zero gradient is the forward face of this behaviour: dispersion carries nothing across the plane, and the outlet flux equals the removal rate (Theorem 1). Leaving at the first contact is another vessel (Remark 1).

The averaging structure says where the dispersion model mixes: to third order in Da , the fluid found at the same place, and only that. Near plug flow the spread of ages that dispersion adds survives in full under segregation, by half under averaging over position and not at all over life expectancy, so the dispersion model sits half-way (Remark 2). Near the stirred tank position says nothing about age, and the dispersion model becomes maximum mixedness.

Remark 3 (Against the earlier tables). Lindfors [20] computed outlet concentrations for second-order reactions under the axial dispersion model and its segregated and maximum-mixed versions; that report was not consulted, and its tables are not compared here. The segregated outlet here comes from a one-line Laplace identity: as $1/(1 + Da\theta) = \int_0^\infty e^{-x(1+Da\theta)} dx$, $c_{\text{seg}} = \int_0^\infty e^{-x} \hat{E}(Da x) dx$ with $\hat{E}$ the transform of Corollary 1; Sawinsky and Deák [21] gave an analytical solution for the same quantity. This paper adds the full plane, 625 points over $0.1 \leq Pe \leq 1000$ and $0.1 \leq Da \leq 10$, its limits at both ends (Theorem 3, Proposition 3), and four independent computations of it.

Remark 4 (What this paper does not cover). The second-order results hold for $n = 2$; for $n < 1$ the reaction can complete inside the reactor and the steady problem becomes a free-boundary problem. The fluid is isothermal and of constant density, with one irreversible reaction. The vessel is closed (Assumption 1(ii)); open vessels change the particle's boundary behaviour and need their own Theorem 1. Lemmas 2 and 3 are formal, and Theorem 3 with them; the ordering $K \leq \int_0^1 A^2 dz$ and the bound of Corollary 2 are measured, not proved. With $Da = 0$ the stagewise operator of Algorithm 1 has one spurious stationary mode, zero to 2.0×10^{-12} at $Pe = 5$ beside an intact $-\lambda_1 = -1.9430465$; it leaves $c(1)$ and $S(0, \theta)$ unchanged but sets the slowest decay at small Da .



8. Conclusion

Danckwerts' boundary conditions describe a particle reflected at the inlet and elastic at the outlet, removed there at rate Pe per unit of local time. The residence-time distribution is its exit law, Wehner–Wilhelm a Feynman–Kac expectation, the moments a mass balance on the backward equation and the tail a Sturm–Liouville spectrum; an absorbing outlet is another vessel.

For a second-order reaction, segregation, the dispersion model and maximum mixedness agree through Da^2 and differ at Da^3 in one integral, the mean square of the age averaged over nothing, over position or over life expectancy. Near plug flow their excesses over plug flow are σ^2 times $Da^2/(1+Da)^3$, $Da \ln(1+Da)/(1+Da)^2$ and $Da^2/(1+Da)^2$, so the dispersion model's position tends to $\xi_\infty(Da)$, from one half toward one; near the stirred tank it becomes maximum mixedness. Every number was computed at least twice. Above $Pe \approx 20$ the average of the two limits, both computable from the residence-time distribution alone, gives the dispersion model's conversion to within 0.1 percentage points for $Da \leq 10$.



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Zamrik Quant Research

The research arm of Zamrik Quant Lab

About the Desk

Applied Mathematics Desk

Zamrik Quant Research

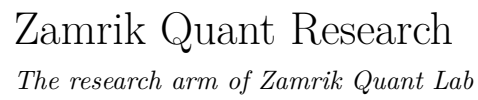
Mathematics in the wild — floods, fires, cellars, patterns and maps — and everything else worth solving.

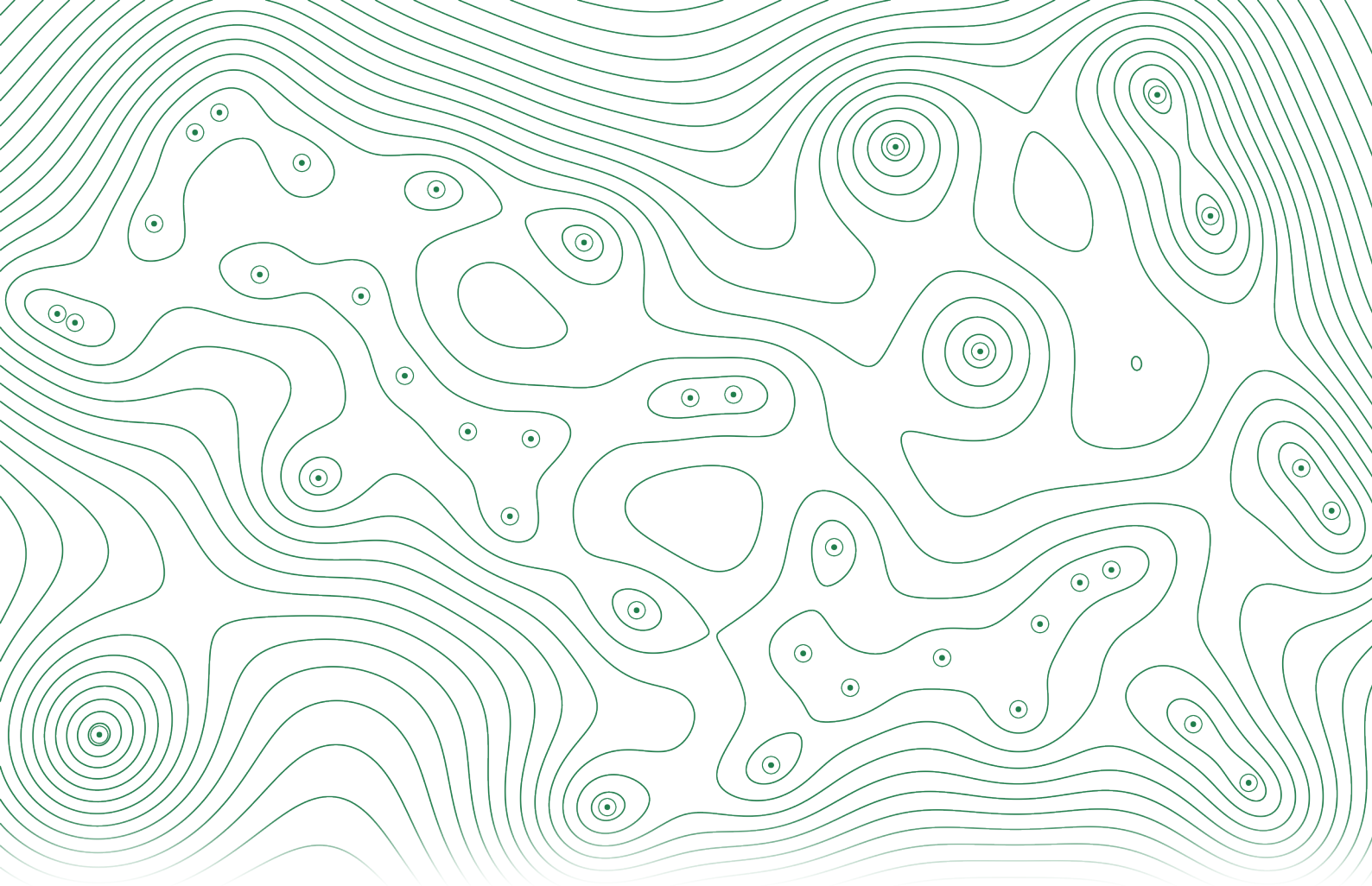
The Applied Mathematics desk solves problems numerically, whatever field they come from. Its subject is the method: how a class of equations is discretised, how fast the approximation converges, and how to know that the number on the screen is the solution and not an artefact of the grid.

Its work spans the main classes of partial differential equations. Parabolic problems — heat in a sphere, the seasonal lag that leaves a cellar warmest in winter, axial dispersion in a tubular reactor — are solved with finite elements and finite differences. Hyperbolic problems cover waves solved by spectral methods, shocks and tidal bores. Reaction–diffusion systems produce the patterns on an animal’s coat, and the induction equation of magnetohydrodynamics carries magnetic diffusion through the Sun.

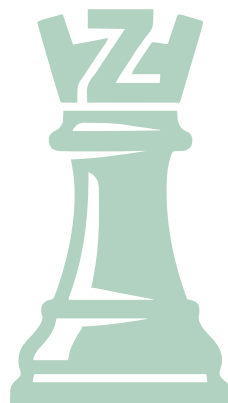
Alongside the equations sit the general tools every modeller depends on: quadrature for rapidly oscillating integrands by the Filon and Levin methods, Monte Carlo and the quasi-Monte Carlo methods that beat its $1/\sqrt{N}$ rate, matrix factorisations for sampling correlated variables, and stochastic simulation of systems of many interacting parts, from flocks of birds to molecular motors. Each method is checked against an exact solution or a second, independent method before its result is published.

The desk is supervised by **Dr. T. Zamrik**, Head of Zamrik Quant Research, PhD, Imperial College London (2011).





Power function of the Matérn interpolant: $P(\mathbf{x})^2 = \varphi(0) - \varphi_X(\mathbf{x})^\top A^{-1} \varphi_X(\mathbf{x})$, zero at every data point $\mathbf{x}_i$



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