Mixing and reaction efficiency in closed domains

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Outline

1. Advection - Reaction - Diffusion
2. Inert transport
   - Mixing efficiency
   - Flow models
   - Numerical results
3. Reactive case
   - Numerical results
4. Conclusions
Assumptions

- **Reaction term**: \( f(\theta) = \theta(1 - \theta) \) (FKPP-like \( \Rightarrow \) pulled fronts);

- **Incompressibility condition**: 
  \[ \nabla \cdot \mathbf{u} = 0 \Rightarrow \mathbf{u} = (\partial_y \psi, -\partial_x \psi), \]  
  being \( \psi = \psi(x, t) \) the stream function;

- **Steep initial condition**: 
  \( \theta(x, 0) \to 1 \) for \( x \to -\infty \), 
  \( \theta(x, 0) \to 0 \) for \( x \to +\infty \) (exp. fast);
Advection - Reaction - Diffusion
Inert transport
Reactive case
Conclusions

Asymptotic situation (ARD2)

$L$ linear domain size

$\ell_0$ typical length of the flow

**front speed:** $V(t) = \frac{1}{L_y \Delta t} \int dx dy [\theta(x, y, t + \Delta t) - \theta(x, y, t)]$

**effective diffusion coeff.:** $D_{ij}^E = \lim_{t \to \infty} \frac{1}{2t} \langle (x_i - <x_i>)(x_j - <x_j>) \rangle$

- $u = 0 \Rightarrow V_0 = 2 \sqrt{\frac{D}{\tau_r}} f'(0) = 2 \sqrt{\frac{D}{\tau_r}}$
- $u \neq 0 \Rightarrow V_f \leq 2 \sqrt{\frac{D_E}{\tau_r}}$ ($D^E \equiv D_{11}^E$)

- $D^E$ depends on the velocity field
- **Typically:** $D^E \gg D \Rightarrow V_f > V_0$
Inert tracers

\[ \begin{align*}
\text{u} &= 0 \\
\frac{\partial t}{\partial t} \theta &= D \nabla^2 \theta \\
\text{u} &\neq 0 \\
\frac{\partial t}{\partial t} \theta + \text{u} \cdot \nabla \theta &= D \nabla^2 \theta
\end{align*} \]
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Inert tracers
\[ u = 0 \]
\[ \partial_t \theta = D \nabla^2 \theta \]
\[ u \neq 0 \]
\[ \partial_t \theta + u \cdot \nabla \theta = D \nabla^2 \theta \]

Reactive particles
\[ u = 0 \]
\[ \partial_t \theta = D \nabla^2 \theta + \frac{1}{\tau_r} f(\theta) \]
\[ u \neq 0 \]
\[ \partial_t \theta + u \cdot \nabla \theta = D \nabla^2 \theta + \frac{1}{\tau_r} f(\theta) \]
Inert transport

\[ \partial_t \theta + \mathbf{u} \cdot \nabla \theta = D \nabla^2 \theta \]
Inert transport

\[ \partial_t \theta + \mathbf{u} \cdot \nabla \theta = D \nabla^2 \theta \]

\[ \dot{x} = \mathbf{u}(\mathbf{x}, t) + \sqrt{2D} \eta(t) \]

\[ \langle \eta \rangle = 0 \]

\[ \langle \eta_i(t) \eta_j(t') \rangle = \delta_{ij} \delta(t - t') \]
Inert transport

\[ \partial_t \theta + u \cdot \nabla \theta = D \nabla^2 \theta \quad \leftrightarrow \quad \dot{x} = u(x, t) + \sqrt{2D} \eta(t) \]

\[ < \eta > = 0 \]

\[ \langle (\eta_i(t)\eta_j(t')) \rangle = \delta_{ij} \delta(t - t') \]

\[ u = (\partial_y \psi, -\partial_x \psi) \quad \text{(incompressibility)} \]

\[ \psi(x, y, t) = \psi_0(x, y) + \epsilon \psi_1(x, y, t) \]
Inert transport

\[
\partial_t \theta + \mathbf{u} \cdot \nabla \theta = D \nabla^2 \theta \quad \leftrightarrow \quad \dot{\mathbf{x}} = \mathbf{u}(\mathbf{x}, t) + \sqrt{2D} \eta(t)
\]

\[
< \eta >= 0 \\
\langle (\eta_i(t)\eta_j(t')) \rangle = \delta_{ij}\delta(t-t')
\]

\[
\mathbf{u} = (\partial_y \psi, -\partial_x \psi) \quad \text{(incompressibility)}
\]

\[
\psi(x, y, t) = \psi_0(x, y) + \epsilon \psi_1(x, y, t)
\]

where \( \psi_1 \) is time-periodic (T) \( \Rightarrow \) Lagrangian Chaos

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4. Conclusions
what is the characteristic time $\tau_m$ of the mixing process?
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<td>$\tau_{m1} \sim \frac{1}{\lambda} \log \frac{L}{\delta_0} \sim \frac{1}{\lambda}$</td>
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...where...

$|\delta x(t)| \sim |\delta x(0)| e^{\lambda t}$

$\partial_t \theta = D^E \nabla^2 \theta$

let us observe that...

- $\lambda = \lambda(x) \rightarrow$ better to use $h_{KS} = \int_{\Omega} \lambda(x) d\mu(x)$;
- $\tau_{m_1}$ ignores the existence of barriers and the effect of noise ($D$);
- $\tau_{m_2}$ is appropriate only if $L \gg \ell_0$ and ignores transient effects.
Introduce a coarse graining of the phase space $\Omega$ into $N^M$ square cells of size $\Delta$. $\Rightarrow P_i(t) = n_i(t) / N = 1 / N M \sum_{i=1}^{N M} \theta(P_i(t) - c N M); c \sim 0.25$.

$t^\alpha$: $A(t^\alpha) \rightarrow \text{mixing time}$
Introduce a coarse graining of the phase space $\Omega$ into $N_M$ square cells of size $\Delta$
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Introduce a coarse graining of the phase space \( \Omega \) into \( N_M \) square cells of size \( \Delta \)

\[
\mathcal{N} \gg 1 \text{ particles} \implies P_i(t) = \frac{n_i(t)}{\mathcal{N}}
\]

\[
A(t) = \frac{1}{N_M} \sum_{i=1}^{N_M} \theta \left( P_i(t) - \frac{c}{N_M} \right) ; \quad c \sim 0.25
\]
Introduce a coarse graining of the phase space $\Omega$ into $N_M$ square cells of size $\Delta$

$N \gg 1$ particles $\Rightarrow P_i(t) = \frac{n_i(t)}{N}$

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$t_\alpha : A(t_\alpha) = \alpha$
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The stream function is:
\[
\psi(x, y, t) = -\tanh \left( \frac{y - B(t) \cos kx}{\sqrt{1 + k^2 B(t)^2 \sin^2 kx}} \right) + cy
\]

\[
B(t) = B_0 + \epsilon \cos(\omega t + \phi)
\]

The spatial structure of the stationary flow is:

\[
B_0 = 1.2 \\
k = 4\pi / 15 \\
c = 0.12
\]
Cross-stream transport can be characterized through the overlap of the resonances criterion:

\[ \epsilon_c = \epsilon_c(\omega) \]

\[ \epsilon < \epsilon_c \Rightarrow \text{local chaos} \]

\[ \epsilon > \epsilon_c \Rightarrow \text{global chaos} \]

\[ \omega_0 = 0.25 \]

\[ \phi = \pi/2 \]

Global chaos allows cross-stream transport.
The stream function is:

\[ \psi(x, y, t) = \frac{1}{2} [(y + 1) \cos \phi(t) + (y - 1) \sin \phi(t)](1 - x^2)(1 - y^2) \]

\[ \phi(t) = \frac{2\pi t}{T} \]

The spatial structure of the stationary flow is:

\[ V_{top} = \cos(\Phi(t)) \]
\[ V_{bot} = \sin(\Phi(t)) \]
\[ V_{top}^2 + V_{bot}^2 = 1 \]
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Dispersion of tracers \((D = 0)\)

- **local chaos**
- **global chaos**
Dispersion of tracers \((D = 0)\)

**Local chaos**

\[ \omega = 0.625 \]
\[ \epsilon = 0.03 \]

**Global chaos**

\[ \omega = 0.625 \]
\[ \epsilon = 0.24 \]

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Mixing and reaction efficiency in closed domains
Dispersion of tracers \((D = 0)\) (AD7)

**Local chaos**
\[
\begin{align*}
\omega &= 0.625 \\
\epsilon &= 0.03
\end{align*}
\]

**Global chaos**
\[
\begin{align*}
\omega &= 0.625 \\
\epsilon &= 0.24
\end{align*}
\]

\(T = 1\) and \(T = 16\) (Stokes)
Mixing efficiency
Flow models
Numerical results

Mixing (AD8)

Occupied area

$D = 0.001$

$D = 0.004$

$D = 0.001$

$D = 0.004$

$D = \frac{0.001}{0.004}$

Mixing and reaction efficiency in closed domains
Mixing efficiency
Flow models
Numerical results

Mixing (AD8)

Occupied area

Mixing times $t_\alpha$: $A(t_\alpha) = \alpha; \ \alpha = 0.9$

$D = 0.001$

$D = 0.002$

$D = 0.004$

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Mixing and reaction efficiency in closed domains
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Mixing

Occupied area

Mixing times $t_\alpha$: $A(t_\alpha) = \alpha; \alpha = 0.9$

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Mixing and reaction efficiency in closed domains
Reactive case

\[ \partial_t \theta + u \cdot \nabla \theta = D \nabla^2 \theta + \frac{1}{\tau_r} f(\theta) \]
Reactive case

\[ \partial_t \theta + u \cdot \nabla \theta = D \nabla^2 \theta + \frac{1}{\tau_r} f(\theta) \]

Discrete-time approach \(\rightarrow\) numerical integration 3-step process:

1. **backward diffusion**: \(x \rightarrow x - \sqrt{2D\Delta tw}\)
2. **backward advection**: \(x - \sqrt{2D\Delta tw} \rightarrow F_{\Delta t}^{-1}(x - \sqrt{2D\Delta tw})\)
3. **forward reaction**: \(\theta(t + \Delta t) = G_{\Delta t}(\theta(t))\)
Reactive case

$$\partial_t \theta + \mathbf{u} \cdot \nabla \theta = D \nabla^2 \theta + \frac{1}{\tau_r} f(\theta)$$

Discrete-time approach $\rightarrow$ numerical integration 3-step process:

1. **backward diffusion**: $x \rightarrow x - \sqrt{2D\Delta t} w$

2. **backward advection**: $x - \sqrt{2D\Delta t} w \rightarrow F_{\Delta t}^{-1}(x - \sqrt{2D\Delta t} w)$

3. **forward reaction**: $\theta(t + \Delta t) = G_{\Delta t}(\theta(t))$

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# Reactive case

\[
\partial_t \theta + \mathbf{u} \cdot \nabla \theta = D \nabla^2 \theta + \frac{1}{\tau_r} f(\theta)
\]

Discrete-time approach \(\rightarrow\) numerical integration 3-step process:

1. **backward diffusion**: \(x \rightarrow x - \sqrt{2D\Delta t}w\)
2. **backward advection**: \(x - \sqrt{2D\Delta t}w \rightarrow F_{\Delta t}^{-1}(x - \sqrt{2D\Delta t}w)\)
3. **forward reaction**: \(\theta(t + \Delta t) = G_{\Delta t}(\theta(t))\)

\[
x(t + \Delta t) = F_{\Delta t}(x(t)) + \sqrt{2D\Delta t}w(t) \quad \text{(lagrangian map)}
\]

\[
\theta(t + \Delta t) = G_{\Delta t}(\theta(t)) \quad \text{(reaction map)}
\]

\[
F_{\Delta t}(x) \simeq x + \mathbf{u}(x)\Delta t, \quad G_{\Delta t} \simeq \theta + \frac{\Delta t}{\tau_r} f(\theta)
\]

\[
\theta(x, t + \Delta t) = \left\langle G_{\Delta t} \left( \theta(F_{\Delta t}^{-1}(x - \sqrt{2D\Delta t}w(t)), t) \right) \right\rangle
\]

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• **Asymptotic situation** \((L_x = 50 \quad \omega = 0.4 \quad \epsilon = 0.3 \quad \tau_r = 2)\)

Concentration field (MJ) (R2)
Concentration field (MJ) (R2)

- **Asymptotic situation** \( (L_x = 50 \; \omega = 0.4 \; \epsilon = 0.3 \; \tau_r = 2) \)

- In a **non asymptotic situation** the evolution is **not** characterized by **front propagation**

---

**local chaos**
\[
\begin{align*}
L_x &= 15 \\
\omega &= 0.625 \\
\epsilon &= 0.03 \\
\tau_r &= 2
\end{align*}
\]

**global chaos**
\[
\begin{align*}
L_x &= 15 \\
\omega &= 0.625 \\
\epsilon &= 0.24 \\
\tau_r &= 2
\end{align*}
\]
how to measure the characteristic time of the reactive process (complete ARD eq.)?
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"burnt" material $\longrightarrow \theta = 1$
"fresh" material $\longrightarrow \theta = 0$
Reaction efficiency

how to measure the characteristic time of the reactive process (complete ARD eq.)?

"burnt" material $\rightarrow \theta = 1$
"fresh" material $\rightarrow \theta = 0$

$$S(t) = \frac{1}{|\Omega|} \int_{\Omega} dx dy \theta(x, y, t)$$
Reaction efficiency

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"burnt" material $\rightarrow \theta = 1$
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$$t_\alpha : S(t_\alpha) = \alpha$$
Reaction efficiency

how to measure the characteristic time of the reactive process (complete ARD eq.)?

"burnt" material $\rightarrow \theta = 1$
"fresh" material $\rightarrow \theta = 0$

$$S(t) = \frac{1}{|\Omega|} \int_{\Omega} dx dy \theta(x, y, t)$$

$t_{\alpha} : S(t_{\alpha}) = \alpha$ ← burning time
Burnt area

\[ D = 0.001 \]

\[ D = 0.004 \]
Burnt area

Burning times \( t_\alpha \): \( S(t_\alpha) = \alpha; \ \alpha = 0.9 \)

\[
\begin{align*}
D &= 0.001 \\
D &= 0.002 \\
D &= 0.004
\end{align*}
\]
Numerical results

Burnt area

\[ D = 0.001 \]

\[ D = 0.004 \]

**Burning times** \( t_\alpha \): \( S(t_\alpha) = \alpha; \alpha = 0.9 \)

\[ D = 0.001 \]
\[ D = 0.002 \]
\[ D = 0.004 \]

\[ D = 0.0005 \]
\[ D = 0.001 \]
\[ D = 0.004 \]
Non asymptotic situation $L \sim \ell_0$

- In the **inert case** different dynamical regimes (local or global chaos) imply very different mixing properties.

- **The reactive case** is substantially unaffected by the presence of global chaos. The details of the velocity field have weak influence on the “burning” process, so that a more efficient mixing seems not to imply a better reaction efficiency.
M. Cencini, C. López, and D. Vergni

M. Abel, A. Celani, D. Vergni and A. Vulpiani
*Front propagation in laminar flows*

G. Boffetta, A. Celani, M. Cencini, G. Lacorata and A. Vulpiani
*Nonasymptotic properties of transport and mixing*
A. S. Bower
*A simple kinematic mechanism for mixing fluid parcels across a meandering-jet*

A. Vikhansky
*Control of stretching rate in time periodic flows*

C. López, D. Vergni and A. Vulpiani
*Efficiency of a stirred reaction in a closed vessel*