The domain dependence of reaction processes in chaotic flows

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NSF-DMS-1212144, NSF-DMS-1148771
Introduction

Competitive Advantage of Bacteria Swimming
Competitive Advantage of Bacteria Swimming

Physical Scales
(typical ocean parameters)

Scale (meters)

$\eta = (\frac{\epsilon}{\nu^3})^{-1/4}$

Turbulent eddies

Turbulent nutrient filaments

Batchelor Scale

$\ell_B = \eta / \sqrt{S_c}$

$S_c \equiv \nu / \kappa \sim 10^3$

Zooplankton

Phytoplankton

Bacteria

V iruses

Bacteria Motility range

(Swimming speed x Patch lifetime)
Competitive Advantage of Bacteria Swimming

Taylor & Stocker Science (2012)
Introduction

Competitive Advantage of Bacteria Swimming

Physical Scales
(typical ocean parameters)

Scale (meters)

$\eta = \left( \frac{\epsilon}{\nu^3} \right)^{-1/4}$

Batchelor Scale

$\ell_B = \eta / \sqrt{Sc}$

(Scale $\equiv \nu / \kappa \sim 10^5$)

Kolmogorov Scale

Turbulent eddies

Turbulent nutrient filaments

Biological Scales
(typical cell sizes)

Zooplankton

Phytoplankton

Bacteria

Viruses

Bacteria Motility range

(Swimming speed x Patch lifetime)
Competitive Advantage of Bacteria Swimming

Introduction

Flow topology seems to be relevant, but unable to explain

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Reaction in Coherent Structures
10/16/14
Introduction

Competitive Advantage of Bacteria Swimming

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Introduction

Effects of Chaotic Advection on Reaction Processes


Tzella & Haynes *PRE* (2010)

Neufeld *PRL* (2001)


Mitchell & Mahoney *Chaos* (2012)


Neufeld & Hernández-García (2009)

Finite-time? Bulk behavior (Neufeld et al. 2002)?

Transport barriers?

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Reaction in Coherent Structures
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Károlyi et al. PNAS (2000)
Tzella & Haynes PRE (2010)

Neufeld PRL (2001)
Crimaldi et al. PoF (2008)

Nugent et al. PRL (2004)
Mitchell & Mahoney Chaos (2012)

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Distinct limits of scalar diffusion

- Batchelor regime
  \( \mathcal{L}_B \) : balance - stirring &
  molecular diffusion

Between the two — LONG transient (Bouchaud & Georges 1990)
Welander experiment (Welander 1955), hint of coherent structures
Small-scale sink/source/biology, long-term correlation make
transient-time dynamics important
Distict limits of scalar diffusion

- Batchelor regime
  \( L_B \): balance - stirring & molecular diffusion

- Homogenization regime
  \( L_c \) or \( L_s \gg L_u \): separation of scale, no long-term correlation
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Autocatalytic reaction in chain vortex flow

\[ c_t + \mathbf{u} \cdot \nabla c - \text{Pe}^{-1} \nabla^2 c = Dac(1 - c), \]

\[ \text{Pe} \equiv UL/\kappa_{\text{eddy}} \sim 10 - 10^4, \quad \text{Da} \equiv kC_0L/U \sim 1 \]
Reaction Model 1 — Single Stable State (with C. Luna PoF 2013)

- Autocatalytic reaction in chain vortex flow
  \[ c_t + \mathbf{u} \cdot \nabla c - \text{Pe}^{-1} \nabla^2 c = \text{Da} c (1 - c), \]
  \[ \text{Pe} \equiv \frac{UL}{\kappa_{edd}} \sim 10 - 10^4, \quad \text{Da} \equiv \frac{kC_0 L}{U} \sim 1 \]
- Spatially periodic flow \( \rightarrow \) homogenization, what about transient?
Comparisons

- Initial stretching dictates reaction variability

![Image showing initial stretching]

\[
\langle c \rangle \text{ at } T=7.5
\]

Forward-FTLE

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Comparisons

- Initial stretching dictates reaction variability

\[ \langle c \rangle \text{ at } T=7.5 \]

- Four stages of the ADR process based on scalar budget \( \langle c \rangle \)

\[ \langle c \rangle = 0.01 \]

\[ \langle c \rangle = 0.1 \]
Scalar budget

- Evolution of scalar density and related quantities

\[
\frac{d\langle c \rangle}{dt} = Da \langle c \rangle - Da \langle c^2 \rangle \equiv Da \langle c \rangle - Da \langle c \rangle^2 - Da \langle c'^2 \rangle, \\
\frac{d\langle c^2 \rangle}{dt} = 2Da \langle c \rangle^2 - 2Da \langle c \rangle^3 - 2Da \langle c \rangle \langle c'^2 \rangle , \\
\frac{d\langle c'^2 \rangle}{dt} = -\frac{2}{Pe} \langle |\nabla c'|^2 \rangle + 2Da \langle c'^2 \rangle - 4Da \langle c \rangle \langle c'^2 \rangle - 2Da \langle c'^3 \rangle.
\]
Behavior at different stages

- Stage 1: decay due to scalar dissipation

\[ c_t - \lambda \hat{x} c_{\hat{x}} + \lambda \hat{y} c_{\hat{y}} = \frac{1}{Pe} (c_{\hat{x}\hat{x}} + c_{\hat{y}\hat{y}}) \]
Behavior at different stages

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- Approximately solution kernel is
  
  \[ G(\hat{x}, \hat{y}, t; x', y') = \frac{Pe}{4\pi t} \exp \left\{ - \frac{Pe[(\hat{x} - x')^2 e^{2\lambda t} + (\hat{y} - y')^2 e^{-2\lambda t}]}{4t} \right\}, \]
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- Based on this approximation dissipation rate is (\(\sigma^2\) : initial variance)

\[ \langle |\nabla c|^2 \rangle = \frac{\pi \sigma^4 e^{\lambda t} (\sigma^2 e^{2\lambda t} + te^{4\lambda t} Pe^{-1} + tPe^{-1})}{(\sigma^2 e^{2\lambda t} + 2tPe^{-1})^{3/2} (\sigma^2 + 2te^{2\lambda t} Pe^{-1})^{3/2}} \]
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- Small \( t \) behavior is \( \pi [1 + 3t\lambda(1 - \sigma^2) + 2t(1/\sigma^2 - 3)/Pe] \)
Behavior at different stages

Stage 2: maintenance of filament width at Batchelor scale

\[ c_t - \lambda \hat{x} c_{\hat{x}} = \frac{1}{Pe} c_{\hat{x}\hat{x}} + Dac. \]
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\[ c_t - \lambda \hat{x} c_{\hat{x}} = \frac{1}{Pe} c_{\hat{x}\hat{x}} + Dac. \]

- Balance of straining-diffusion leads to spatial profile across filament:

\[ X = c_1 \exp(-\lambda Pe \hat{x}^2 / 2) \]

\[ T = e^{Da t} \]
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- The larger the stretching, the smaller the dissipation
Behavior at different stages

- **Stage 2**: maintenance of filament width at Batchelor scale

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- Scalar dissipation scales as \( O(e^{-2\lambda t} e^{\lambda t} e^{Da t}) = O(e^{(Da-\lambda)t}) \)
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- **Stage 3**: homogenization in different zones

**Stage 4**: almost uniform reaction
Behavior at different stages

- **Stage 2**: maintenance of filament width at Batchelor scale

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- **Stage 3**: homogenization in different zones

- **Stage 4**: almost uniform reaction
Modeling based on Lagrangian stretching rate

- Model effective reaction rate \( \langle c^2 \rangle = f(FTLE_w, \langle c \rangle) \)
Parametric dependence

- Quantify variability based on gap at intermediate time to saturation

![Graph showing parametric dependence](image-url)
Parametric dependence

- Quantify variability based on gap at intermediate time to saturation

- Vary Da, Pe independently
Bistable dynamics with single scalar:

\[(c_t + u \cdot \nabla c) - Pe^{-1} \nabla^2 c = Da(c - c)(c - 1),\]

\[Pe = 1000, \quad \alpha = 0.2, \quad Da \text{ varies}\]
- Bistable dynamics with single scalar

\[(c_t + u \cdot \nabla c) - Pe^{-1} \nabla^2 c = Da(c - c^2)(c - 1),\]
\[Pe = 1000, \quad \alpha = 0.2, \quad Da \text{ varies}\]

- Without flow, \(c = 1\) is more stable. With flow (\(Da=53\)): 

![Diagram of a star-shaped structure]
Domain Partition

- Dependence on $Da$

FTLE (with $T=1$) alone insufficient to explain (at least for $Da=38$)

- Reaction in Coherent Structures

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Domain Partition

- Dependence on $Da$

FTLE (with $T=1$) alone insufficient to explain (at least for $Da = 38$)
Closer look for small $Da$

- $Da = 38$, lower stretching $\rightarrow 0$, higher stretching $\rightarrow 1$
Closer look for small $Da$

- $Da = 38$, lower stretching $\rightarrow 0$, higher stretching $\rightarrow 1$

- Bifurcation location (I.C. dependent)
Closer look for small $Da$

- $Da = 38$, lower stretching $\rightarrow 0$, higher stretching $\rightarrow 1$

- $Da = 38$ vs $Da = 43$
Turbulence

- 2D turbulence randomly forced to maintain modal energy at medium wavenumber and low-mode damped to avoid inverse cascade

\[ \omega_t + J[\psi, \omega] = \frac{1}{Re} \nabla^2 \omega + \psi + f, \quad \omega = \nabla^2 \psi \]
Turbulence

- 2D turbulence randomly forced to maintain modal energy at medium wavenumber and low-mode damped to avoid inverse cascade

\[ \omega_t + J[\psi, \omega] = \frac{1}{Re} \nabla^2 \omega + \psi + f, \quad \omega = \nabla^2 \psi \]

- \( Re = 1000, Sch = 1 \), distinct behaviors at \( Da = 8 \)
Domain Partition

- Dependence on $Da$

![Graphs showing domain partition with varying Da values](image)

- Percentage of domain converging to 1
- Cumulative distribution of FTLE
Motile species move via chemotaxis

\[
(C_t + \mathbf{u} \cdot \nabla C) - \text{Pe}^{-1} \nabla^2 C = -\text{Da} C(B + 1),
\]

\[
(B_t + \mathbf{u} \cdot \nabla B) - \text{Pe}^{-1} \nabla^2 B = -\chi \nabla (B \nabla C),
\]

Pe = 1000, Da = 0.001, \( \chi = 0.01 \)
Motile species move via chemotaxis

\[
(C_t + \mathbf{u} \cdot \nabla C) - \text{Pe}^{-1} \nabla^2 C = -\text{Da} C(B + 1),
\]
\[
(B_t + \mathbf{u} \cdot \nabla B) - \text{Pe}^{-1} \nabla^2 B = -\chi \nabla(B \nabla C),
\]
\[
\text{Pe} = 1000, \quad \text{Da} = 0.001, \quad \chi = 0.01
\]

\[
U_M = \frac{\int_D B_M \cdot C \, dD}{\int_D B_M \, dD}, \quad U_{NM} = \frac{\int_D B_{NM} \cdot C \, dD}{\int_D B_{NM} \, dD},
\]
Conclusions

FKPP

- Spread further to react fast
- Chaotic advection affects early reaction, dictates bulk reaction speed
- Lagrangian measures (FTLE) can be used to parameterize this variability, even with transport barriers

Bistable Equilibria

- Flow topology can lead to distinct states
- Similarity and distinction from FKPP
- Distinct fates even when eddies are transient

Current work

- Determination of bifurcation boundary for bistable reaction
- Mixing between fixed point and limit cycle
- Domain dependence for chemotaxis

References

- Tang, W. & Dhumuntarao, C., Bistability in inhomogeneity — effects of flow coherent structures on the fate of a bistable reaction. submitted
- Tang, W. & Jones, K., The domain dependence of chemotactic advantage in two-dimensional flows. in preparation