Fast Chemical Reactions in Chaotic Flows: Reaction Rate and Mixdown Time
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**Fast Chemical Reactions**
We consider infinitely fast bimolecular reactions in fluid flows:

\[ A + B \rightarrow 2P \]

*e.g.* NaOH(aq) + HCl(aq) → NaCl(aq) + H₂O(ℓ)

**Advection-Diffusion-Reaction Equations**

\[
\begin{align*}
\frac{\partial a}{\partial t} + \mathbf{u} \cdot \nabla a &= \kappa \nabla^2 a - \gamma ab \\
\frac{\partial b}{\partial t} + \mathbf{u} \cdot \nabla b &= \kappa \nabla^2 b - \gamma ab \\
\frac{\partial b}{\partial t} + \mathbf{u} \cdot \nabla b &= \kappa \nabla^2 b + 2\gamma ab
\end{align*}
\]

- **Fast reactions:** reaction time \( \ll \) advection time \( \ll \) diffusion time
- **Goal:** time dependence of product concentration \( \langle p \rangle = 1 - 2\langle a \rangle \)

**Progress of Reaction**

- **Initial slow phase** \( t < 10\tau \): very little fine structure in the concentration fields \( a \) and \( b \)
- **Exponential phase** \( 10\tau < t < 40\tau \): filamentary structure developed, \( \langle p \rangle \) reaches 90% of its ultimate value
- **Classical chemical kinetics** \( t > 60\tau \): system is fairly homogeneous, advection and diffusion become unimportant

**Relation to Decaying Passive Scalars**

Consider the quantity:

\[
\phi = a - b
\]

\[
\frac{\partial \phi}{\partial t} + \mathbf{u} \cdot \nabla \phi = \kappa \nabla^2 \phi
\]

\( \Rightarrow \phi \sim \text{decaying passive scalar} \)

For **infinitely fast reactions** the fields \( a(x, t) \) and \( b(x, t) \) never overlap

\[
|\phi| = |a - b| = a + b
\]

\[
\langle a \rangle = \langle b \rangle = \frac{|\phi|}{2}
\]

**Strangeness of Decaying Passive Scalars**

\[
\phi(x, t) = \phi(x, 0) e^{-|\phi|/2} t
\]

where \( \phi(x, t) \) is statistically stationary, hence

\[
\langle |\phi|^n \rangle \sim e^{-n|\phi|/2} t
\]

**Decay of Scalar Variance**

\[
\langle \phi^2 \rangle \sim e^{-\lambda t} \text{ as } \kappa \rightarrow 0
\]

- **With Scale Separation**, \( k_f L \gg 1 \\
\]

- **Without Scale Separation**, \( k_f L \approx 1 \\
\]

**Theory of Decaying Passive Scalar**

**Finite-time Lyapunov Exponent**, \( h \)

\[
h(x, t) = \frac{1}{t} \log \frac{|\delta x(t)|}{|\delta x(0)|}
\]

\[
\hat{h} = \lim_{t \rightarrow \infty} h(x, t)
\]

- **Probability density function of** \( h, \rho(h, t) \) with **large time asymptotic form**

\[
\rho(h, t) \sim e^{-4G(h)}
\]

- **Local stretching theory predicts**

\[
s = \min(h + G(h))
\]

**Predicting \( \lambda \)**

\[
1 - \langle |\phi| \rangle = 2\langle a \rangle \sim e^{-\lambda t}
\]

\[
\langle a \rangle \sim \langle |\phi| \rangle \sim e^{-|\phi|/2} t
\]

\[
\lambda = \frac{\hat{h}}{2}
\]

**Theory vs. Simulations**

For \( k_f L = 5 \), using \( \kappa_{\text{eff}} = U^2\tau/8 \) with \( U = 0.25 \) and \( \tau = 10 \), we get \( \lambda_{\text{theory}} = 0.0031 \). Numerical simulation gives \( \lambda = 0.0033 \).

**Initially Isolated Reactants**

- **Broadcast spanning** (Crandall, Cawdwell and Weiss 2008)
- **Parameterization in atmospheric chemical transport models** (Thuburn and Tan 1997)

Reaction does not start until the separation \( 2\tau \) is reduced to the diffusion length scale \( L \) by the action of the fluid. The time taken to do so is the **mixdown time**, \( \tau_{\text{mix}} \).