Problems in mixing additives

Schumacher & KRS (2010)


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Operations per second

Year

$R_\lambda$
Advection diffusion equation

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

\(\theta(x;t)\), the tracer; \(\kappa\), its diffusivity (usually small);
\(u(x;t)\), the advection velocity

Quite often \(u(x;t)\) does not depend on the additive: this is the case of the “passive scalar”.

\(u(x;t)\) then obeys the same field equations as those without the additive: e.g., \(\text{NS} = 0\).

Equation is then linear with respect to \(\theta\).

As a rule, BCs are also linear (perhaps mixed)

Linearity holds for each realization but the equation is statistically nonlinear because of \(<u \cdot \nabla \theta>\), etc.
Langevin equation

\[ \frac{dx}{dt} = u(x(t); t) \, dt + (2\kappa)^{1/2} \, d\chi(t) \]

\[ \chi(t) = \text{vectorial Brownian motion,} \]
\[ \text{statistically independent in its three components} \]
For smooth velocity fields, single-particle diffusion as well as two-particle dispersion are well understood.

The turbulent velocity field is analytic only in the range \( r < \eta \), and Hölder continuous, or “rough,” in the scaling range \( \Delta_r u \sim r^h \), \( h < 1 \), which introduces various subtleties.
\[ h = 1/3 \text{ for Kolmogorov turbulence.} \]
In practice, it has a distribution:
“multiscaling”

If $\Delta_r u \sim r^h$, $h < 1$

$\Delta_r u (t) \sim t^{1/(1-h)}$, and

memory is lost rapidly.

Lagrangian trajectories are “not unique”
For short times, diffusion effects are additive. The finite time behavior is different.
Model studies

- Assume some artificial velocity field satisfying $\text{div } \mathbf{u} = 0$

Broad-brush summary of results

1. For smooth velocity fields (e.g., periodic and deterministic), homogenization is possible. That is,
   \[ \langle \mathbf{u}(\mathbf{x};t) \nabla(\theta) \rangle = -(\kappa_T \cdot \nabla(\theta(\mathbf{x};t))) \]
   where $\kappa_T$ is an effective diffusivity (Varadhan, Papanicolaou, Majda, and others)

2. Velocity is a homogeneous random field, but a scale separation exists: $L_u/L_\theta \ll 1$. Homogenization is possible here as well.

3. Velocity is a homogeneous random field but delta correlated in time, $L_u/L_\theta = O(1)$; eddy diffusivity can be computed.

II. Kraichnan model


Surrogate Gaussian velocity field

\[ \langle v_i(x,t)v_j(y,t') \rangle = D_{ij}(x-y)\delta(t-t') \]

\[ D_{ij} \sim |x-y|^{2-\gamma}, \; \gamma = 2/3 \] recovers Richardson’s law of diffusion

Forcing for stationarity:

\[ \langle f_\theta(x,t)f_\theta(y,t') \rangle = C(r/L)\delta(t-t') \]

C(r/L) is non-zero only on the large scale, decays rapidly to zero for smaller scale.
• $L_u$ is set by the mesh size
• $L_\theta$ can be set independently and $L_u/L_\theta$ can be varied
• Diffusivity of the scalar can be varied: i.e., Pr or Sc is variable

$\langle \theta^2 \rangle \sim t^{-m}$ (variable $m$)

$m - m_0 = f(Re; Sc; L_u/L_\theta)$?

$m_0$: asymptotic $m$ for large values of the arguments
A proper theory is needed!

Data: Warhaft & Lumley; KRS et al. (both from wind tunnels, heated grid)

PDF of $\theta$ is Gaussian

Initial $L_u/L_\theta$

$m$

Effect of length-scale ratio (stationary turbulence)

Both PDFs are for stationary velocity and scalar fields, under comparable Reynolds and Schmidt numbers.

Passive scalars in homogeneous flows most often have Gaussian tails, but long tails are observed also for column-integrated tracer distributions in horizontally homogeneous atmospheres.


**Probability density function of the passive scalar**
Top: Ferchichi & Tavoularis (2002)
Bottom: Warhaft (2000)
Large-scale features depend on details of forcing, initial conditions and perhaps geometry. Only a few of these features are understood precisely, and our qualitative understanding rests on the models of the sort mentioned.
\[ \langle \Delta_r \theta^2 \rangle \sim r^{\zeta_2} \]
\[ \langle \Delta_r \theta^4 \rangle \sim r^{\zeta_4} \]

Dimensional analysis: \( \zeta_4 = 2 \zeta_2 \)

Flatness, \( \langle \Delta_r \theta^4 \rangle / \langle \Delta_r \theta^2 \rangle^2 \sim r^0 \), a constant

Measurements show that the flatness \( \rightarrow \infty \)

as \( r \rightarrow 0 \)

(because \( \zeta_4 = 2 \zeta_2 \) (or generally \( \zeta_{2n} < n \zeta_2 \))

“Anomalous exponents”
A measure of anomalous scaling, $2\zeta_2 - \zeta_4$, versus the index $\gamma$, for the Kraichnan model. The circles are obtained from Lagrangian Monte Carlo simulations. The results are compared with analytic perturbation theories (blue, green) and an ansatz due to Kraichnan (red).

$\gamma = 0.5$, $8192^2$

Mixing process itself imprints large-scale features independent of the velocity field!
The case of large Schmidt number

Schmidt number, $\text{Sc} = \nu/\kappa \sim O(1000)$

$\text{Sc} \gg 1$

$N = \text{Re}^3 \text{Sc}^2$

Batchelor regime

$\phi_\theta(k) \sim qk^{-1}$
$q = O(1)$

as for the velocity
The Batchelor regime

Reynolds number: $Re >> 1$

Schmidt number, $Sc = \nu/\kappa >> 1$

In support of the -1 power law

Gibson & Schwarz, JFM 16, 365 (1963)


Expressing doubts

Miller & Dimotakis, JFM 308, 129 (1996)


Simulations in support


Batchelor (1956)

$E_\theta(k) = q\kappa(\nu/\varepsilon)^{1/2}k^{-1}\exp[-q(k\eta_B)^2]$

Kraichnan (1968)

$E_\theta(k) = q\kappa(\nu/\varepsilon)^{1/2}k^{-1} [1+(6q)^{1/2}k\eta_B \times \exp(-(6q)^{1/2}k\eta_B)]$
Effective diffusivity

Best fit: \(-0.144 \times \log(\text{Sc}) + 1.36\)
Intermittency effects
Some consequences of fluctuations

0. Traditional definitions
\[ \langle \eta \rangle = \left( \frac{\nu^3}{\varepsilon} \right)^{1/4}, \quad \langle \eta_B \rangle = \frac{\langle \eta \rangle}{\text{Sc}^{1/2}}, \quad \langle \tau_d \rangle = \frac{\langle \eta_B \rangle^2}{\kappa} \]

1. Local scales
\[ \eta = \left( \frac{\nu^3}{\varepsilon} \right)^{1/4}, \text{ or define } \eta \text{ through } \eta \delta_{\eta u} \nu = 1 \]
\[ \eta_B = \frac{\eta}{\text{Sc}^{1/2}}, \quad \tau_d = \frac{\eta_B^2}{\kappa} \]

2. Distribution of length scales

Schumacher, Yakhot
3. The velocity field is analytic only in the range $r < \eta$ (and the scalar field only for $r < \eta_B$)

4. Minimum length scale $\eta_{\text{min}} = \langle \eta \rangle \, \text{Re}^{-1/4}$
   (Schumacher, KRS and Yakhot 2007)

5. Average diffusion time scale $<\tau_d> = \langle \eta_B^2 \rangle / \kappa$, not $<\tau_d> = \langle \eta_B \rangle^2 / \kappa$

6. From the distribution of length scales, we have $<\tau_d> = \langle \eta_B^2 \rangle / \kappa \approx 10 \, \langle \eta_B \rangle^2 / \kappa$

7. Eddy diffusive time/molecular diffusive time $\approx \text{Re}^{1/2}/100$; exceeds unity only for $\text{Re} \approx 10^4$
   (mixing transition advocated by Dimotakis, short-circuit in cascades of Villermaux, etc)
Classes of mixing problems

- Passive mixing
  - Mixing of fluids of different densities, where the mixing has a large influence on the velocity field (e.g., thermal convection, Rayleigh-Taylor instability)
  - Those accompanied by changes in composition, density, enthalpy, pressure, etc. (e.g., combustion, detonation, supernova)
Active scalars

\[ \partial_t a = \mathbf{v} \cdot \nabla a + \kappa \Delta a + F_a \]

\[ V_i(x,t) = \int d\mathbf{y} \; G_i(x,y) \; a(y,t) \]

Simple case: Boussinesq approximation

\[ \text{NS} = -\beta \mathbf{g} a \]
Earth’s mantle

$10^6 < Ra < 10^{17}$
(for some Pr)

$10^{-3} < Pr < 10^3$
(for some Ra)

atmosphere

Solar convection

oceans

cooling towers
Helium gas convection (with and without rotation)

\[
\Gamma = \frac{1}{2}
\]

\[
\text{Nu}_{\text{corr}} = 0.088 \text{Ra}^{0.32}
\]

Slightly revised:

[Pioneers: Threlfall (Cambridge); Libchaber, Kadanoff and coworkers (Chicago)]

Latest theoretical bound for the exponent (X. Wang, 2007): 1/3 for \( \text{Pr}/\text{Ra} = \mathcal{O}(1) \)
Upperbound results in the limit of $Ra \to \infty$

1. *Arbitrary Prandtl number*
   
   $\text{Nu} < Ra^{1/2}$ for all $Pr$ (Constantin).
   
   Rules out, for example, $Pr^{1/2}$ and $Pr^{-1/4}$.

2. *Large but finite Prandtl numbers*
   
   For $Pr > c Ra$, $\text{Nu} < Ra^{1/3}(\ln Ra)^{2/3}$ (Wang)
   
   For higher Rayleigh numbers, the $1/2$ power holds.

3. *Infinite Prandtl number*
   
   $\text{Nu} < CRa^{1/3}(\ln Ra)^{1/3}$ (Doering et al., exact)
   
   $\text{Nu} < aRa^{1/3}$ (Ierley et al., “almost exact”)

   (Early work by Howard and Malkus gave $1/3$ for all $Pr$.)

2 questions: Pr. 1/3 (2 views)
The mean wind breaks symmetry, with its own consequences.

large-scale circulation ("mean wind")

the container

E:\videoplayback(2).wmv

Segment of 120 hr record

E:\videoplayback(2).wmv
How are the reversals distributed?

\( \tau_1 = \text{time between subsequent switches in the velocity signal} \)

power-law scaling of the probability density function for small \( \tau_1 \)

for large \( \tau_1 \):

\[ p(\tau_t) : \exp\left[-\left(\frac{\tau_t}{\tau_m}\right)\right] \]

\( \tau_m = 400 \text{ s} \)


-1 power law scaling characteristic of SOC systems (see papers in *Europhys. Lett.*, *Physica A* and *PRE*)
Summary of major points

• Despite the enormous importance of the problem of mixing, there are numerous problems (which can be posed sharply) for which there are no sharp answers. There is an enormous opportunity here.

• The large scale features of the scalar depend on initial and boundary conditions, and each of them has to be understood on its own merits. In the absence of full-fledged theory, models are very helpful to understand the essentials.

• The Kraichnan model explains the appearance of anomalous scaling.

• The best-understood part corresponds to large Sc, for which classical predictions of the past have been confirmed (e.g., those relating to the -1 power). There is, however, no theory for the numerical value of the spectral constant and its behavior for Sc < 1 remains unexplained.
thanks
Non-dimensional parameters and scales

Reynolds number: \( \text{Re} = \frac{uL}{\nu} \gg 1 \)
\( \eta = (\nu^3/\varepsilon)^{1/4}: \text{Re based on } \eta = 1 \)
Schmidt number, \( \text{Sc} = \frac{\nu}{\kappa} \)

inertial range
\( \phi(k) = C_k k^{-5/3} \)
\( C_k \approx 0.5 \)
[PoF, 7, 2778 (1995)]

For \( \text{Sc} = O(1) \),
\( \phi_\theta(k) = C_{OC} k^{-5/3} \)
\( C_{OC} \approx 0.35 \)
[PoF, 8, 189 (1996)]
Brownian motion

Robert Brown, a botanist, discovered in 1827, that pollen particles suspended in a liquid execute irregular and jagged motion, as shown.

Einstein 1905 and Smoluchowski 1906 provided the theory.

- The Brownian motion of pollen grain is caused by the exceedingly frequent impacts of the incessantly moving molecules of the liquid.
- The motion of the molecules is quite complex but the effect on the pollen occurs via exceedingly frequent and statistically independent impacts.
Langevin’s derivation

- Consider a small spherical particle of diameter ‘a’ and mass ‘m’ executing Brownian motion.

- Equipartition: $<\frac{1}{2}mv^2> = \frac{1}{2}kT$; \( v = \frac{dx}{dt} \)

Two forces: viscous (Stokes) drag = $6\pi \eta av$ and the fluctuating force $X$ due to bombardment of molecules; $X$ is negative and positive with equal probability.

- Newton’s law: \( m \frac{d^2x}{dt^2} = -6\pi \eta a \frac{dx}{dt} + X \)

- Multiply by $x$

\[
\frac{m}{2} \frac{d^2(x^2)}{dt^2} = -6\pi \eta a \frac{dx^2}{dt} + Xx
\]

Average over a large number of different particles

\[
\frac{m}{2} \frac{d^2<x^2>}{dt^2} + 6\pi \eta a \frac{dx^2}{dt} = kT
\]

We have put $<Xx> = 0$ because $x$ fluctuates too rapidly on the scale of the motion of the Brownian particle.

- Solution: $\frac{d<x^2>}{dt} = \frac{kT}{3\pi \eta a} + C \exp(-6\pi \eta at/m)$

The last term approaches zero on a time scale of the order $10^{-8}$ s.

We then have: $\frac{d<x^2>}{dt} = \frac{kT}{3\pi \eta a}$

Or, \( <x^2> - <x_0^2> = (kT/3\pi \eta a)t \)

Comparing with the result:

Mean square displacement \( <x^2>^{1/2} = (2\kappa t)^{1/2} \), we have \( \kappa = \frac{kT}{6\pi \eta a} \)

quantum fluid

superfluidity

classical liquid

classical gas

Helium I: $v = 2 \times 10^{-8} \text{ m}^2/\text{s}$ (water: $10^{-6} \text{ m}^2/\text{s}$, air: $1.5 \times 10^{-5} \text{ m}^2/\text{s}$)

obvious interest in model testing.

4.4 K, 2 mbar: $\alpha/\nu \kappa = 6.5 \times 10^9$

5.25 K, 2.4 bar: $\alpha/\nu \kappa = 5.8 \times 10^{-3}$

Superfluids flow without friction and transport heat without temperature gradients.
moment orders 2, 4, 6, 8, 10, 12; $k_{max} \eta = 11$

$k_{max} \eta = 1.5 - 33.6$
$R_\lambda = 10 - 690$
$Sc = 1 - 1024$
$k_{max} \eta_B = 1.5 - 6$
box-size: 512-2048
(some preliminary results for 4096)
At high Ra, the temperature gradient is all at the wall and their self-organization into a large scale flow in a confined apparatus.

Sparrow, Husar & Goldstein


(for flow visualization and quantitative work, see K.-Q. Xia et al. from Hong Kong)
4. Schmidt number effects on anisotropy

fixed Reynolds number
The case of large Schmidt number

Schmidt number, \( \text{Sc} = \frac{\nu}{\kappa} \sim O(1000) \)

\[ N = \text{Re}^3 \text{Sc}^2 \]

\( \text{Sc} \gg 1 \)

Batchelor regime
\( \phi_\theta(k) \sim q k^{-1} \)
\( q = O(1) \)
Resolution matters!

\[ k_{\text{max}} \eta_B = 1.5 \]

\[ k_{\text{max}} \eta_B = 6 \]

Low scalar dissipation

Not much difference
Sensitivity of low dissipation regions

(Schumacher, KRS & Yeung, JFM 2005)

Regular resolution

High resolution

\[
D_q \quad \text{vs.} \quad q
\]

\[
\left\langle \varepsilon_\theta \right\rangle < \frac{1}{40}
\]

\[
128^3, \quad 512^3
\]
2. The effect of Schmidt number on dissipative anomaly
3. Anisotropy of small scales
5. Effective diffusivity

![Graph showing the relationship between Sc and \( \frac{u' L}{K_T} \)](image)
6. Frisch’s excitement

a. Normal scaling

\[ S_n \sim (r/L)^{\zeta_n}, \text{ where } \zeta_n = n/3. \]

b. Anomalous scaling

\[ \zeta_n \neq n/3, \quad 2\zeta_n > \zeta_{2n}. \]

c. Importance

Contrast to critical scaling

d. \[ M_n \neq M_2^n \]
The iron core becomes nuclear matter and cannot shrink anymore. The matter from outside continues to be attracted and rebounds off the nuclear matter. The acoustic waves created coalesce to an outward moving shock wave which stirs up and, eventually blasts out, the matter. This is the supernova.

All calculations show that the shock wave stalls. We read from G.E. Brown, *Physics Today* 58, 62 (2005): “To this day, calculated explosions have yet to work. Investigators are refining ideas about convection and relaxing assumptions about the explosion.”

Supernova 1987A provided strong evidence of turbulence emanating from the core of the exploded star because core materials were observed well before they were predicted. The turbulence caused mixing among the layers and greatly complicated the tidy ‘onion’ model of dying stars. [Image reproduced from Muller, Fryxell, and Arnett. *Astronomy & Astrophysics* 251, 505 (1991).]
(i) dissipative anomaly for both low and high Sc
(ii) clear inertial-convective scaling for low and moderate Sc
(iii) viscous-convective $k^{-1}$ for scalars of high Sc, which has received mixed support from the experiments and simulations
(iv) clear tendency to isotropy with Sc to a lesser degree with Re which may be a big issue now that we found that with high resolution the latter appears to be true
(v) saturation of moments of scalar gradients with Sc; I also used a very simple model for large gradient formation to explain saturation of intermittency. This analysis, leads to $(R_\lambda^2 \cdot Sc)$ as the important parameter and the data show a high degree of universality when normalized by this parameter (see the paper I submitted to Physica D)
(vi) systematic study of resolution effects for scalars and derivation of analytic expressions to estimate errors.
Schumacher & KRS: numerical simulations

Corrsin (1959): schematic
\[ <u(x;t) \nabla(\theta)> = -(\kappa_T \cdot \nabla(\theta(x;t))) \]

\[ \approx \approx <\pm \Sigma \partial_x \equiv \chi \Delta \nabla \]

\[ \partial_t a = v \cdot \nabla a + \kappa \Delta a + F_a \]

\[ V_i(x;t) = \int dy \ G_i(x,y) \ a(y,t) \]
**Other cases**

1. **Velocity field stationary, scalar field decaying**
   Main result known: initially non-G PDFs tend to a Gaussian (Yeung & Pope)

2. **Velocity field decaying, scalar field stationary**: unlikely to be practical, nothing known

3. **Both velocity and scalar fields are stationary**: some results are the same for the scalar whether sustained by random forcing or through mean gradients, but there are differences as well.

*Large-scale features depend on details of forcing, initial conditions and perhaps geometry. Only some of these features are understood well.*

*Are small-scales universal?*
Other cases

1. Velocity field stationary, scalar field decaying
   Numerical result: initially non-G PDFs tend to a Gaussian (Yeung & Pope)

2. Velocity field decaying, scalar field stationary:
   unlikely to be practical, nothing known

3. Both velocity and scalar fields are stationary:
   some results are the same whether the scalar is sustained by random forcing or through mean gradients (dissipation).

Length-scale ratio? (autocorrelation times?)

Shear flow ref
DISSIPATIVE ANOMALY

microscale Reynolds number

Sc > 1

normalized dissipation rate

[Graph showing normalized dissipation rate vs. microscale Reynolds number (Sc) with data points and trend lines for Sc > 1.]

[Color plots showing variations in a parameter across different conditions, labeled 1, 3, and 8.]
The problem is simple if the velocity field is simple (e.g., \( u \) = constant, or periodic in 2d)

Not many results are known if \( u \) is turbulent in 3d, but this is what we consider here: the equation is linear for each realization but statistically nonlinear because of \( \langle u \cdot \nabla \theta \rangle \).
The turbulent velocity field is analytic only in the range \( r < \eta \), and only Hölder continuous, or “rough,” \((\Delta_r u \sim r^h, h < 1)\), in the scaling range, which introduces various subtleties.

\( h = 1/3 \) for Kolmogorov turbulence, in practice, \( h \) has a distribution: multiscaling.


A quantity such as a structure function.
DISSIPATIVE ANOMALY

No theory exists!