

Volume fraction profiles of transport structures in Rayleigh-Taylor turbulent mixing zone: evidence of enhanced diffusion processes

Antoine Llor¹, Pascal Bailly² & Olivier Poujade²

1. CEA/Siège, 31-33, rue de la Fédération, 75752 Paris Cedex 15, France,
antoine.llor@cea.fr

2. CEA/DAM, BP12, 91680 Bruyères le Châtel, France,
pascal.bailly@cea.fr, olivier.poujade@cea.fr

I. Motivations: 2SFK modeling

A Two-Structure Two-Fluid Two-Turbulence (2SFK) model was first presented in 2001 by A. Llor & P. Bailly at the 8th IWPCTM in Pasadena, which:

- had all the **basic physics** deemed important,
- but was obtained
by **assembling separate independent elements**,
- and involved
an **empirical enhanced diffusion** for stability.

Today, our new version of 2SFK:

- has the **same basic physics**,
- follows from a **unified derivation**
(least action principle
and extended thermodynamics of irreversible processes,
see other presentation by A. Llor, P. Bailly & O. Poujade),
- and still involves **enhanced diffusion** which is

here shown to be a *general feature*
of *any* Two-Structure Two-Fluid (2SF) model.

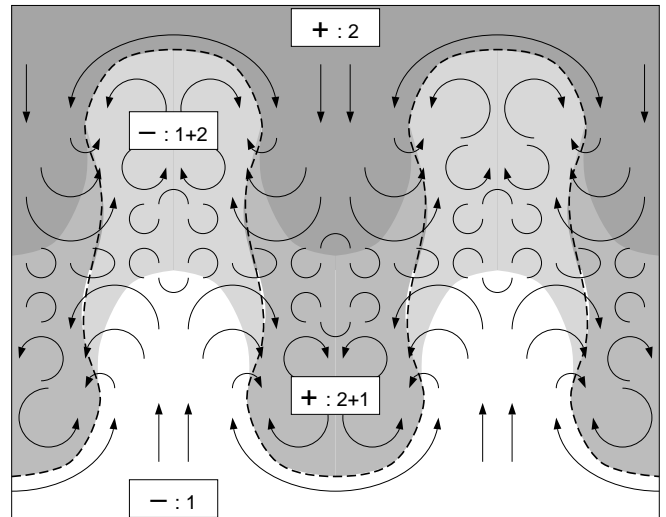
Well-known example of 2SF model other than 2SFK:

Youngs' model (1995).

II. Basic mass transport equations in two-structure two-fluid models

Most models of Rayleigh–Taylor turbulent mixing involve:

- i) light − and heavy + structures as basic transport entities,
- ii) made of mixed or entrained light 1 and heavy 2 fluids.



Examples: Youngs', Bubble models, Dimonte's, Dalziel's... and 2SFK.

Mass conservation equations gives transport (1D):

$$D_t^\pm \alpha^\pm \rho^\pm c^{m\pm} = -\Phi_{x,x}^{m\pm} \mp \Psi^m,$$

$$D_t^\pm a = \partial_t a + (aU_x^\pm)_{,x},$$

U_x^\pm = velocity of structure \pm ,

α^\pm = volume fraction of structure \pm ,

ρ^\pm = density of structure \pm ,

$c^{m\pm}$ = mass fraction of fluid m in structure \pm ,

$\Phi_x^{m\pm}$ = flux of fluid m in structure \pm ($\Phi_x^{2\pm} + \Phi_x^{1\pm} = 0$),

Ψ^m = exchange of fluid m between structures \pm .

Assuming incompressibility:

$$D_t^\pm \alpha^{m\pm} = - \left(\frac{\Phi_x^{m\pm}}{\rho^m} \right)_{,x} \mp \frac{\Psi^m}{\rho^m}.$$

$\alpha^{m\pm}$ = volume fraction of fluid m of structure \pm ,
 ρ^m = density of fluid m (constant),

$$\alpha^{m\pm} \rho^m = \alpha^\pm \rho^\pm c^{m\pm}.$$

“Solve” these equations using experimental data and basic assumptions:

- $At \rightarrow 0$, zero Atwood limit,
- $L(t) = 2\alpha Atgt^2$, $2\alpha \approx .08$
 TMZ width self-similar growth, $\xi = x/L$,
- $\alpha^m(\xi) = \alpha^{m+} + \alpha^{m-}$,
 self-similar fluid fraction profiles (linear),
- $\Theta \approx .8 \approx 6 \left\langle \frac{\alpha^{2+}\alpha^{1+}}{\alpha^{2+} + \alpha^{1+}} + \frac{\alpha^{2-}\alpha^{1-}}{\alpha^{2-} + \alpha^{1-}} \right\rangle$, molecular mixing ratio,
- $\Phi_x^{m\pm} = -D^\pm(\xi)(LL') \times \alpha^\pm(\rho^1\rho^2/\rho^\pm) (\alpha^{m\pm}/\alpha^\pm)_{,x}$,
 usual “first gradient” closure, $D^\pm \geq 0$,
- $\Psi^m = C(\xi)(L'/L) \times \alpha^+\alpha^-\rho^m(\alpha^{m+} - \alpha^{m-})$,
 “first gradient” closure, $C \geq 0$,
- $\alpha^{m\pm}$, assumed profiles,
 simplest consistent with previous constraints.
- $C(\xi) = C$, uniform exchange rate.

4 equations with $\alpha^{m\pm}$ given



4 unknown profiles (U_x^\pm, D^\pm) and 1 constant (C)

III. Characteristic volume fraction profiles

Algebraically-simplest density profiles of structures of zero slope with pure fluids at TMZ edges, and adjusted by pole at ξ_0 for mixing level:

$$\frac{\rho^+ - \rho^2}{\rho^2 - \rho^1} = -\frac{(\frac{1}{2} - \xi)^2}{\xi_0 + \frac{1}{2} - \xi},$$

$$\frac{\rho^- - \rho^1}{\rho^2 - \rho^1} = \frac{(\frac{1}{2} + \xi)^2}{\xi_0 + \frac{1}{2} + \xi}.$$

Fluid volume fractions:

$$\alpha^2 = \frac{1}{2} + \xi,$$

$$\alpha^1 = \frac{1}{2} - \xi.$$

$$\alpha^{2+} = (\frac{1}{2} + \xi) \frac{\xi_0 + \frac{1}{4} - \xi^2}{\xi_0 + \frac{1}{2} - 2\xi^2},$$

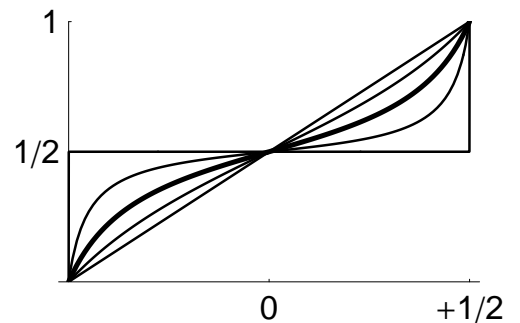
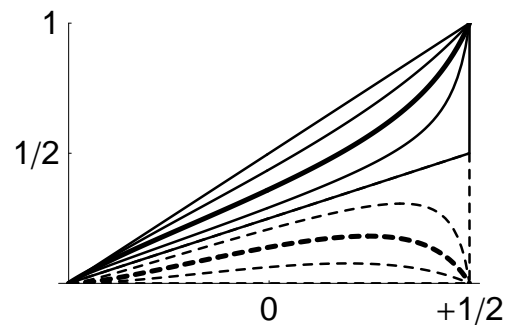
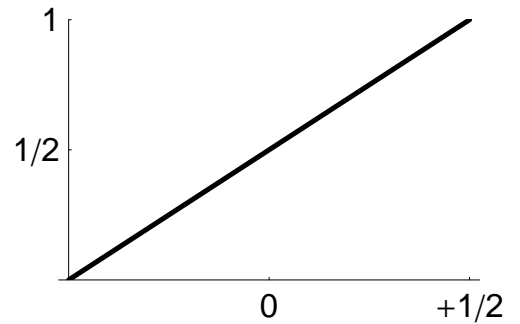
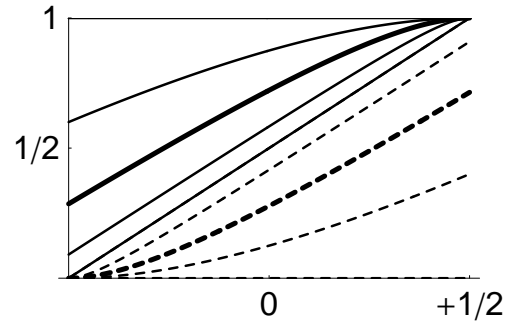
$$\alpha^{2-} = (\frac{1}{2} + \xi) \frac{\frac{1}{4} - \xi^2}{\xi_0 + \frac{1}{2} - 2\xi^2},$$

$$\alpha^{1+} = (\frac{1}{2} - \xi) \frac{\frac{1}{4} - \xi^2}{\xi_0 + \frac{1}{2} - 2\xi^2},$$

$$\alpha^{1-} = (\frac{1}{2} - \xi) \frac{\xi_0 + \frac{1}{4} - \xi^2}{\xi_0 + \frac{1}{2} - 2\xi^2}.$$

Structure volume fractions:

$$\alpha^\pm = (\frac{1}{2} \pm \xi) \frac{\xi_0 + \frac{1}{2} \mp \xi}{\xi_0 + \frac{1}{2} - 2\xi^2}.$$



$\Theta = .8$ obtained at $\xi_0 \approx .38$ (thick lines).

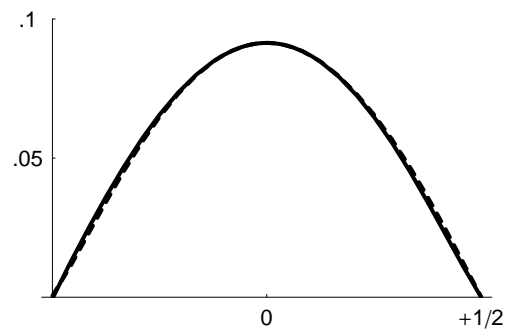
IV. Solution of mass transport equations

With $\alpha^{m\pm}$ as above, solutions given by simple quadratures of algebraic functions, most conveniently computed numerically and not explicit here.

Limit conditions on $\alpha^{m\pm}$ and $\Phi_x^{m\pm}$ give:

$$C = \frac{\int_{-1/2}^{+1/2} \xi \alpha_{,\xi}^{2+} d\xi}{\int_{-1/2}^{+1/2} \alpha^+ \alpha^- (\alpha^{2+} - \alpha^{2-}) d\xi} \approx 2.$$

Scaled diffusion coefficients D^+ (solid) and D^- (dashed) almost identical.

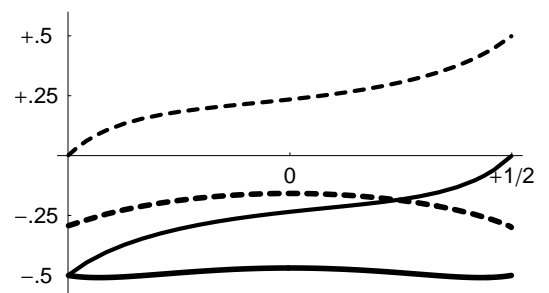


$$D^\pm(0) \approx .0914.$$

Scaled structure velocities U^+/L' (solid) and U^-/L' (dashed) with nearly constant drift (thick):

$$\delta U_x = U_x^+ - U_x^- ,$$

and $\approx 1/4$ diffusive contribution (thick dashed):



$$\delta U_x^o = -D^+ \frac{(\alpha^+ \rho^+)_{,x}}{\alpha^+ \rho^+} + D^- \frac{(\alpha^- \rho^-)_{,x}}{\alpha^- \rho^-}.$$

Structure directed energy larger than fluid directed energy:

$$\int \alpha^+ \alpha^- \frac{(\delta U_x)^2}{2} d\xi \approx 1.19 \times \int \alpha^2 \alpha^1 \frac{(U_x^2 - U_x^1)^2}{2} d\xi = 1.19 \times \frac{(L')^2}{48}.$$

V. General properties of solutions

Basic properties do not depend on:

- $\alpha^{m\pm}$ profile details (if Θ preserved),
- $C(\xi)$ non uniformity (up to factor ≈ 2).

More specifically:

- $D^\pm(\xi) \neq 0$ at $\xi \neq 0$ if $\Theta \neq 0$
(otherwise $\exists \xi$ such that $C(\xi) < 0$),
- $D^\pm(\pm 1/2) = 0$
(otherwise $(\alpha^{2+}/\alpha^+)_{,x} \neq 0$ at $\xi = +1/2$),
- $C(\xi) \approx 2$,
- D^\pm bell shaped, $D^\pm(0) \approx .1$,
- $\delta U_x(\xi)/L' \approx .5$,
- *Structure* directed energy
 $\approx 20\%$ higher than *fluid* directed energy.

VI. Consistency of D^\pm and C with usual $k-\epsilon$ estimates

Observational data (α -group)

on self-similar Rayleigh-Taylor TMZ:

- TMZ growth coefficient $\alpha \approx .04$ ($L = 2\alpha Atgt^2$),
 - reduced potential energy $\frac{K_I}{(L')^2} \approx \frac{1}{96\alpha} = .26$,
 - *fluid* directed/potential energy ratio $\frac{K_D}{K_I} \approx 2\alpha$,
 - kinetic/potential energy ratio $\frac{K_T}{K_I} \approx .48$,
- (consistent selection of α and K_T/K_I values).

Energy balance $\frac{d}{dt}(LK_I) = \frac{d}{dt}(LK_T) + LE$, yields E .

Then standard $k-\epsilon$ closures of rate and diffusion:

$$C_t = \frac{E}{K_T} \times \frac{L}{L'} = 2 \left(\frac{K_I}{K_T} - 1 \right),$$

$$D_t(0) = \frac{3}{2} \frac{C_\mu}{\sigma_c} \frac{K_T^2}{E} \times \frac{1}{LL'} = \frac{3}{4} \frac{C_\mu}{\sigma_c} \frac{K_T}{(L')^2} \left(\frac{K_I}{K_T} - 1 \right)^{-1},$$

and with observed ratios and $C_\mu/\sigma_c \approx .09/.7$:

$$C_t \approx 1.04 \times C,$$

$$D_t(0) \approx .111 \times D(0).$$

Exchange rate correctly captured by $k-\epsilon$ approach, diffusion *underestimated by an order of magnitude!*

VII. Energy budget analysis of RT TMZ in adapted k - ϵ approach

Question: are velocity fluctuations responsible for enhanced D^\pm associated with new specific turbulent energy reservoir?

Simple model adapted from k - ϵ (similar to 2SFK) where large-scale non-turbulent energies (K_D , added mass...) *are not mirrored in E* :

$$\begin{aligned}\frac{d}{dt}(LK_I) &= L\Pi_I, \\ \frac{d}{dt}(LK_{DA}) &= L\Pi_I - L\Pi, \\ \frac{d}{dt}(LK) &= L\Pi - LE, \\ \frac{d}{dt}(LE) &= LC_{\epsilon 1} \frac{E}{K} \Pi - LC_{\epsilon 2} \frac{E^2}{K}, \\ &(\Pi_I \text{ and } \Pi = \text{gravity and drag works}).\end{aligned}$$

Under self similar RT growth, yields:

$$\begin{aligned}\frac{K_{DA}}{K_I} &= C_\epsilon \frac{K_T}{K_I} - C_\epsilon + 1, \quad \text{where } C_\epsilon = \frac{4C_{\epsilon 2} - 3}{4C_{\epsilon 1} - 3}, \\ &\approx .118 \text{ for } K_T/K_I \text{ as above, } C_{\epsilon 2} \approx 1.92, C_{\epsilon 1} \approx 1.44.\end{aligned}$$

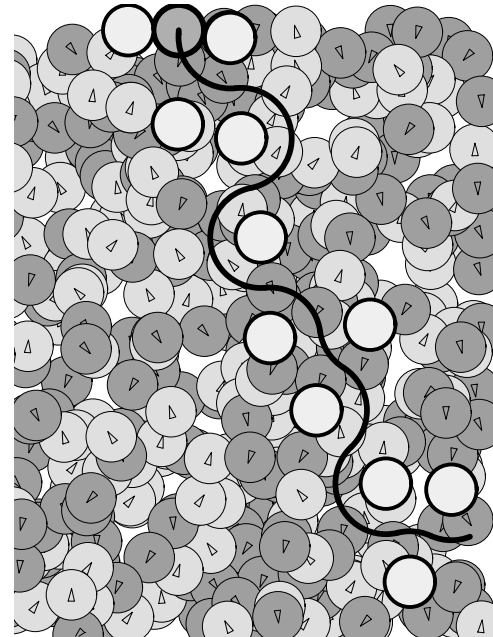
Observed: $K_{DA}/K_I = 1.2 \times 1.5 \times (K_D/K_I) \approx .144$
with corrections for structure/fluid and added mass.

No significant energy reservoir other than directed and added mass is expected to be associated with enhanced diffusion.

VIII. Modeling and experiment suggestions

Possible consistent diffusion process:

sifting diffusion or
 “Pachinko” effect between
 opposite flowing structures.



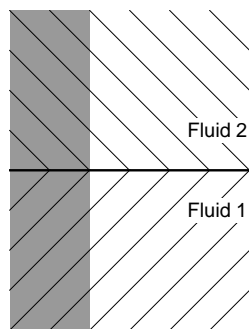
Consistent closure:

$$D^\pm = D = 4C_s\alpha^+\alpha^-\lambda\|\delta\vec{U}\|,$$

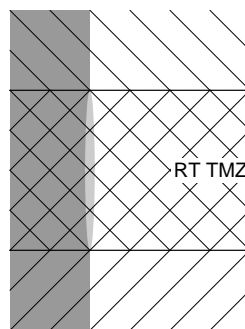
where λ is characteristic structure size and $C_s \approx 1$.
 $\lambda \approx L/5$ in RT (α -group).

May stabilize models by making them parabolic.

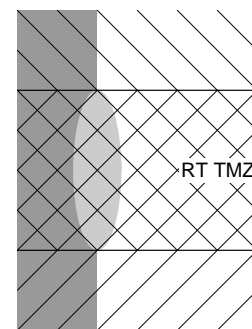
Observationnal confirmation of enhanced diffusion could be achieved despite lack of structure determination methods:



Initial state



Standard
 $k-\epsilon$ diffusion



Consistent
 enhanced diffusion

Ultimately, structure analysis techniques will provide global insight (not only on diffusion).