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- EST.1943 ------

Mixing and Turbulence: Are we there yet?





extremefluids.lanl.gov

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We are developing predictive models for complex, multiphysics flows that can't be simulated directly.

Models With the essential physics (often discovered through experiments) Code implementation With parameters set via experiments

Validation With fundamental and complex experiments



Most turbulence at LANL does not fall into the idealized Kolmogorov 1941 (K41) conditions

Assumptions from K41:

- Gradual cascade from large to small scales, where the flow doesn't retain memory of how it started (initial conditions)
- Isotropy at small scales (statistics invariant to rotations of axes)
- Homogeneous (statistics invariant to translations of axes)
- In transitional flows, large-scale mixing exists concurrently with smallscales
- Initial conditions are usually remembered
- Shock-driven mixing is transitional, inhomogeneous and anisotropic
- Variable-density flows can have homogeneity in the velocity fields but not the density fields

How do we model these difficult flows?



The LANL Reynolds-Averaged Navier-Stokes (RANS) model is designed to distinguish between homogeneous and inhomogenous flows

LANL Turbulence Model Quantities are:

Reynolds stress, R_{ij} $\tilde{R}_{ij} = \overline{\rho u_i'' u_j''} / \overline{\rho}$ $u_i'' = u_i' - a_i$ Turbulent decay length scale, S_D Turbulent transport length scale, S_T Density specific-volume correlation, b $b = -\overline{\rho'(1/\rho)'}$ Turbulent mass flux, a_i $a_i \equiv -\overline{u_i''} = \overline{\rho' u_i'} / \overline{\rho}$

Schwarzkopf, Livescu, Baltzer, Gore, Ristorcelli, Flow Turb. Combust. (2016)

Variable-density and non-uniform mixing affect the stresses on the fluid

• Turbulent Mass Flux Transport (exact)

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$$\frac{\partial(\overline{\rho}a_i)}{\partial t} + \left(\rho\tilde{u}_j a_i\right)_{,j} \underbrace{\neq b}_{,i} - \tilde{\tau}_{ki,k} - \tilde{\tau}_{ki,k} - \tilde{\rho}\left(a_k a_i\right)_{,k} - \overline{\rho}a_k \overline{u}_{i,k} - \overline{\rho}\left(\frac{\overline{\rho'u_i'u_k'}}{\overline{\rho}}\right)_{,k} + \overline{\rho}v'(\underline{P_i' - \tau'_{ki,k}})$$



Models are chosen that reflect our best understanding of the physics



Assumptions:

- **Transport** is modeled as a **turbulent flux**. All other transport terms dropped or thought to be covered by this term.
- **Pressure strain** modeled with the isotropization of production model.
- **Dissipation** assumed isotropic.

What kind of flows require this complex modeling?



Inertial Confinement Fusion (ICF) at the National Ignition Facility (NIF)

192 Lasers: 500 trillion watts in 20 ns



NIF uses 192 laser beams to squeeze a tiny capsule to create ignition via fusion



Fuel capsule

deuterium (H with 1 neutron) + tritium (H with 2 neutrons)





LLNL Sci&Tech Review (1999)

ICF capsules are compressed to form a hot spot, creating conditions for fusion



2-D and 3-D simulations can now account for instability growth that happens in these high energy density regimes. Can we predict the instabilities well enough to achieve ignition?

abeth Merritt

Type Ia supernovae are "standard candles" that help determine the age of the universe



Instabilities are important in:

- Pre-ignition conditions
- Triggering ignition
- Final chemical structure

Image from NASA's Chandra X-Ray Observatory chandra.harvard.edu

Initial Conditions affect the supernova's evolution. Turbulence models don't account for the ICs of the flow!



Laboratory-scale experiment



Simulation of IC effects on chemical structure: 8 different ignition and detonation conditions 100 s after ignition



D Kasen et al. (2009) Nature

initial interfaces

Re~ 10⁴

2 differer

2 different post-shock flows

How do we simulate initial conditions effects?

Gas curtain experiments in a shock tube allow us to carefully control the initial and shock conditions



The nature of the mixing changes with Mach number, even after scaling time. How do we quantify these differences?

Orlicz, S. Balasubramanian, Prestridge (2013) *Phys. Fluids.* Orlicz, S. Balasubramanian, Vorobieff, Prestridge (2015) *Phys. Fluids*

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Reshocking the curtain speeds up mixing, yet sensitivity to initial conditions persists

At=
$$\frac{\rho_2 - \rho_1}{\rho_2 + \rho_1} = 0.6$$
 M=1.2

Reshock timing changes initial condition 170µs

η₀ =15

= 18

385µs

η₀ = 35





$$b = -\rho' \left(\frac{1}{\rho}\right)'$$

Balasubramanian et al. (2012) PoF Tomkins et al. (2013) JFM

Simulations can systematically show us how sensitive the flow is to initial conditions



Collaborations with numerical physicists have driven the experimental conditions and measurements

Multispecies ILES simulations:

Good quantitative comparisons at large scales (e.g., peak vorticity, extent of mixing region).



Experiments Simulations Velocity and Concentration



Vorticity

Improvements/questions driven by validation:

- Always need higher resolution diagnostics!
- Mixing of 2 interfaces is difficult to understand
- Need IC parametric study





We designed new experiments to study the effects of initial conditions and Mach number on shock-driven mixing



Vertical Shock Tube (VST)

Initial conditions

- Single interface, air/SF₆ (At=0.6)
 Diagnostics
- Simultaneous PIV & Quantitative PLIF Mach number
- 1.2<M<3

Powder Gun Shock Tube

Initial conditions

- Single interface, Xe/He (At=0.94) Diagnostics
- Proton Radiography (pRad)
 Mach number
- M=8.8

LES simulations of 2-D initial conditions capture largescale ejections and vorticity

2D perturbations

• Modes in x-z plane







Experimental Initial Conditions used to develop simulation input

Simulations by Nick Denissen using Lagrangian code FLAG



3-D simulations help explain experimental observations

3D perturbations

- Multi-mode in x-z plane
- Single-mode in y direction







The powder gun at LANL's proton radiography facility allows us to drive strong shocks into gases



Proton Radiography:

21 dynamic images (up to 31)
50 ns minimum interframe timing
100 µm spatial resolution
Measurement of areal density

Magnetic lenses focus scattered protons

Test section designed to be impacted by gun projectile, and gases chosen to optimize radiography





Initial Conditions set by membrane supports for each pRad shot



Aluminized Mylar membrane



Goal: Measure timedependent growth of Xe-He turbulent mixing region

Proton Radiography (pRad) provides a movie of areal density of fast events



Movie from pRad experiment with smallest initial perturbations



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Experiments at Mach 8.8 reveal imprint of initial conditions over significant mixing times







13 µs

17 µs







14 µs

17.5 µs

In multiphysics environments, variable-density mixing is important at critical times

Counter-shear of an Al foil turned into a plasma



Variable-density jet mixing

Turbulent Mixing Tunnel At=0.6



He-shell flash convection. Jet into ¹²C He-burning layers leads to a regime of H-¹²C combustion. At≈0.6

> Woodward, Herwig, Lin (2013) arXiv:1307.3821

The Turbulent Mixing Tunnel is designed improve our understanding of subsonic variable-density mixing

Measurements: 10,000 velocity & density fields of the flow per station

Jet conditions: *Re* = 20,000 *At* = 0.1, 0.6 *M* = .09, .02





Air & SF₆ jet turbulence can be compared in shear region and in momentum/buoyant regions



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velocity fields (PLIF/PIV) ations per field



Using experimental data, we can calculate quantities such as the turbulent kinetic energy, tke



A comparison of the turbulent kinetic energy terms between the two jets shows spatial variations



Air jet: Higher advection SF₆ jet: Negative production Positive Turbulent Flux

Negative production slows down total energy transfer compared to the Boussinesq (single density) case.

 Simulations will help us understand how this affects the jet behavior

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What mechanisms are retarding the energy cascade in the dense jet?

Scale energy at two points:
$$\overline{\delta q^2} = \overline{(\delta u_i)^2}$$

Constant density assumptions: $\overline{u_i'^2} + \overline{u_i'^2} - 2\overline{u_i'u_i'}$
Constant density flows: $\overline{u_i'^2} + \overline{u_i'^2} - 2\overline{u_i'u_i'}$
Variable-density flows: $\overline{\rho u_i''^2} + \overline{\rho u_i''^2} - 2\left(\frac{1}{2}\left[\underline{\rho + \rho}\right]\underline{u_i''u_i''}\right)$
Variable-density assumptions
i. Incompressible
ii. No shocks
iii. No magnetic field
 $\overline{(\delta u_i'')_\rho^2} \coloneqq \overline{(u_i'' - \underline{u_i''})(\rho u_i'' - \rho u_i'')}$

What do the energy transfer terms mean physically?

 Π – energy transfer due to local turbulent velocity fluctuations Π_U – energy transfer due to deformation of eddies by mean-flow gradients

$$\Pi = \frac{\partial \overline{\delta u_k''(\delta u_i'')_\rho^2}}{\partial r_k} \qquad \Pi_U =$$

$$\Pi_U = \frac{\partial \delta \widetilde{U}_k (\delta u_i^{\prime\prime})_\rho^2}{\partial r_k}$$





The scale-by-scale energy budgets (spherically averaged) show us differences between the two jets



Production Advection Turbulent Transport Pressure Transport Viscous diffusion Mass flux pressure

The total energy transfer is similar in both jets, but the different mechanisms have modeling implications



SF₆ jet - Π_U (linear interscale energy transfer) strengthens the mean flow by deforming small eddies into larger ones



Boussinesq (air)

 $-(\Pi_U + \Pi) + P \approx \bar{\epsilon}$

Production at large scales sets dissipation (the turbulent cascade)



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Non-Boussinesq (SF₆)

 $-\Pi + P \approx \Pi_U + \bar{\epsilon}$

 Π_{U} causes energy to move from small to large scales

Lai, Charonko, Prestridge (2018) JFM

Exact and modeled terms can be compared using experimental data



- convection
 production
 turb. flux
 pr. flux
 dissipation
 pr. strain
- Formally, the modeled transport term corresponds only to the turbulent flux. Is it correct to lump in the pressure flux?
- The Pressure Strain was computed in the budgets from the balance, assuming isotropic dissipation

Transport: Pressure flux changes the shape (yellow lines)—can't lump pressure and turbulent flux together



The jet experiments are helping us identify potential modeling issues with variable-density flows



t.k.e. dissipation

energy

direct calculation
$$\varepsilon = -2\mu \frac{\partial u_i''}{\partial x_j} \frac{\partial u_i''}{\partial x_j}$$

energy balance $\varepsilon = -(C + P + D + T_P)$

The **pressure flux** term in the energy balance is modeled from turbulent flux:

$$T_P = -\frac{\partial}{\partial x_i} \overline{u_i^{\prime\prime} P^{\prime}} \approx -\frac{2}{5} D$$

Lumley's pressure flux model is not matching measured dissipation when density gradients are large

Lab-scale variable-density mixing experiments help us understand how to better model mixing

• What we know:

- Mixing and turbulence applications require some sort of model for scales that aren't resolved in the simulations
- Physical mechanisms—and the length scales at which they occur--are important to understand and model

What we don't know:

- How to best model pressure flux in variable-density flows!
- How to incorporate initial conditions effects in shock-driven flows
- How to incorporate energy transfer from small to large scales into subgrid models
- How important all of these effects are for specific applications!