Zababakhin Scientific Talks

Modeling of turbulent mixing induced by hydrodynamic instabilities

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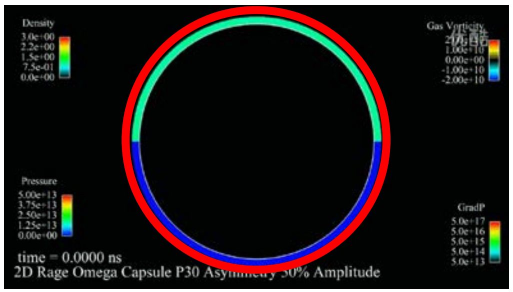
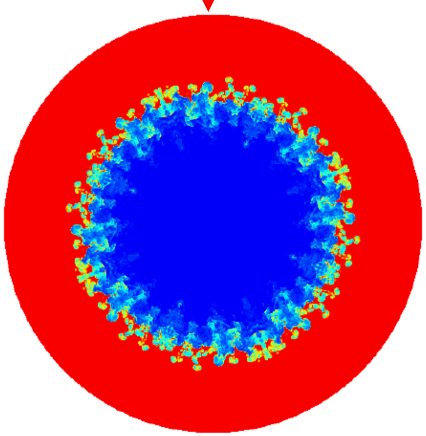
Background

- Turbulent mixing broadly occurs in both natural phenomena, e.g. supernova explosions, and engineering applications, e.g. inertial confinement fusion (ICF).

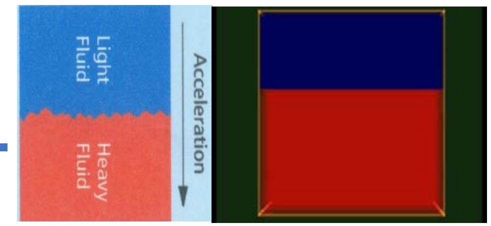
ICF



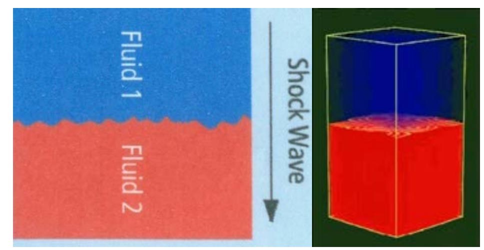


Turbulent mixing significantly affects the nuclear reaction rate

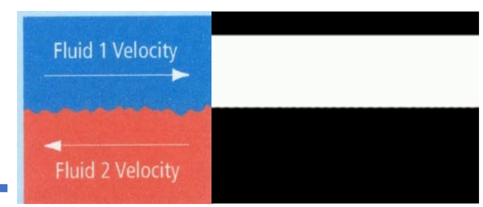
Induced by hydrodynamic instabilities



Rayleigh-Taylor (RT) : acceleration



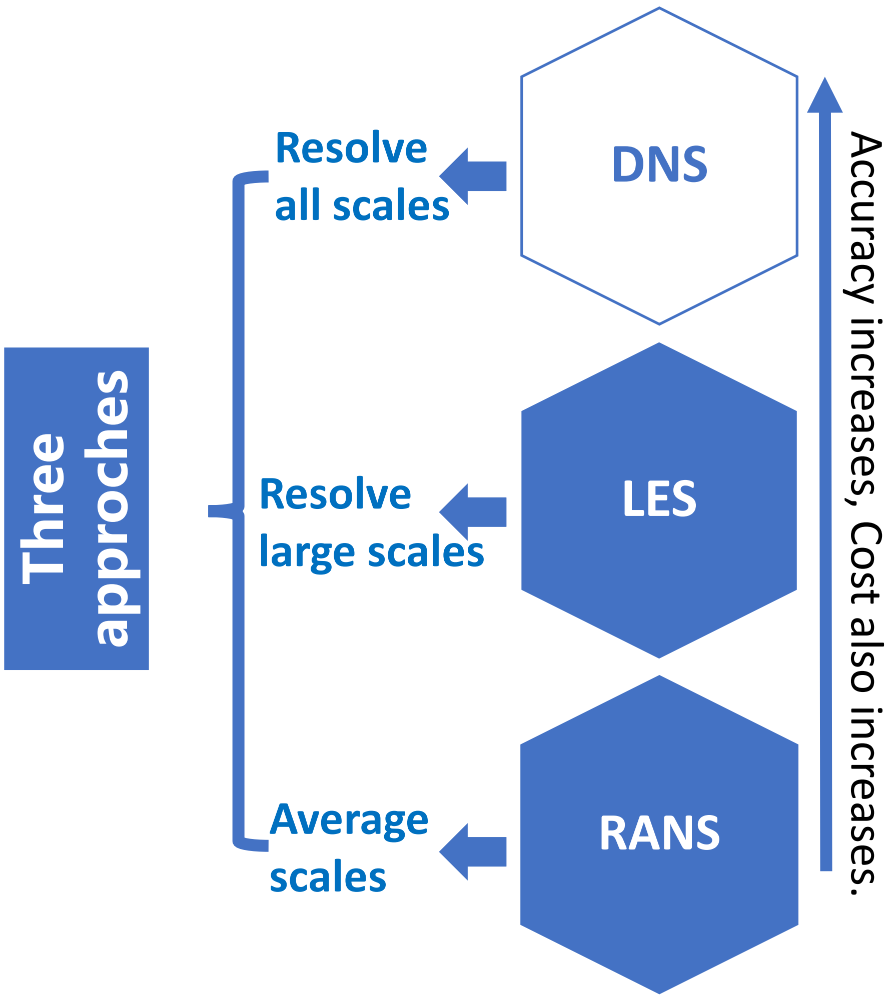
Richtmyer-Meshkov (RM): shock



Kelvin-Helmholtz (KH): shear

Numerical simulation

- **The RANS models remain the most viable approach for the solution of practical problems.**



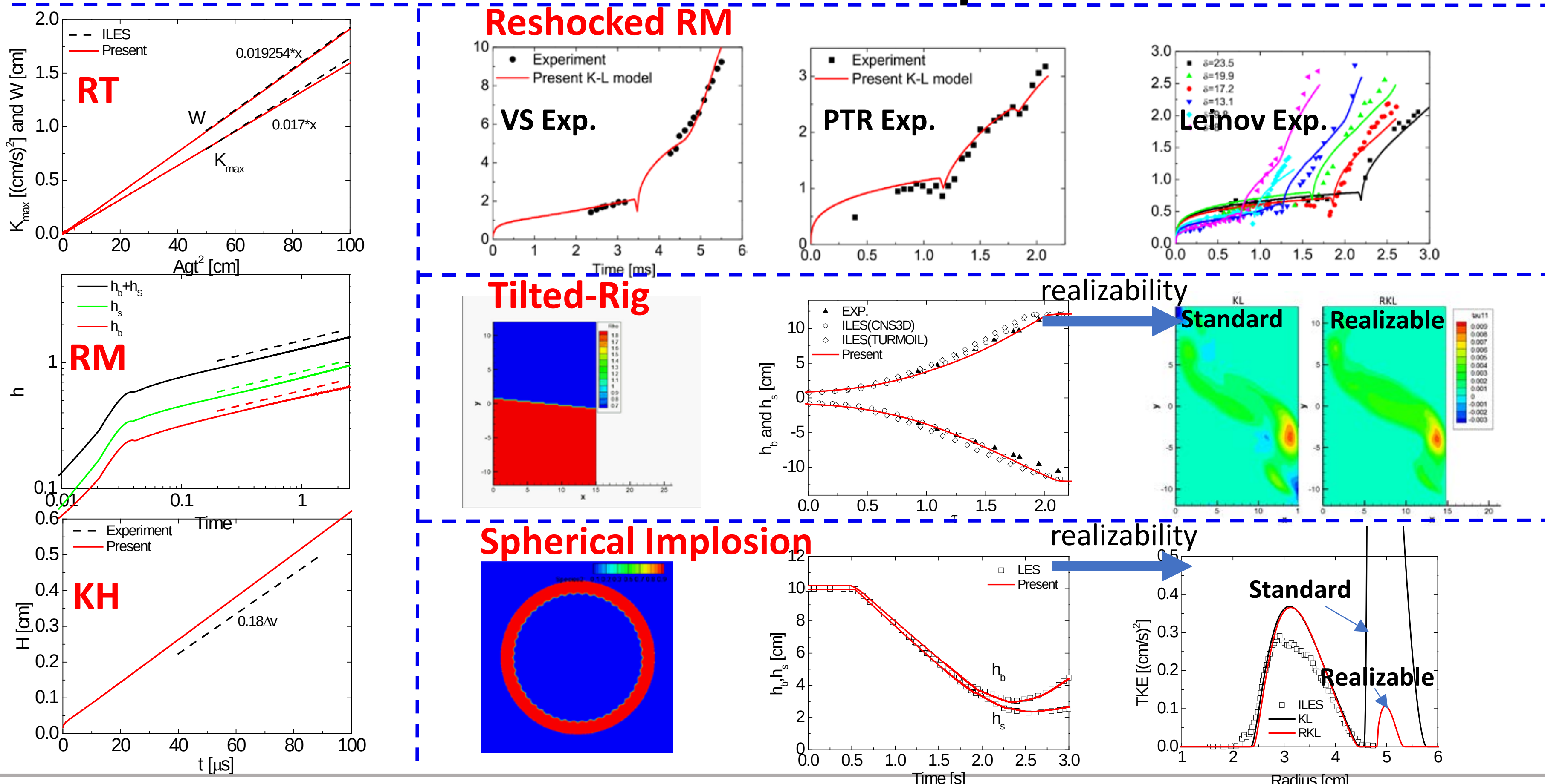
Grids for reaching minimum state turbulence[1]	Cost
$>10^{10}$ 3D	Expensive
$10^{7} \sim 10^{9}$ 3D	Affordable
$10^{2} \sim 10^{4}$ 1D/2D	Cheap

DNS: Direct Numerical Simulation; LES: Large Eddy Simulation;
RANS: Reynolds-Averaged Navier-Stokes; [1] https://doi.org/10.1063/1.5088745

Works on RANS models

- **Our series of works on RANS models, yielding a unified and realizable prediction of both canonical and complex mixings.**

Canonical | **Complex**

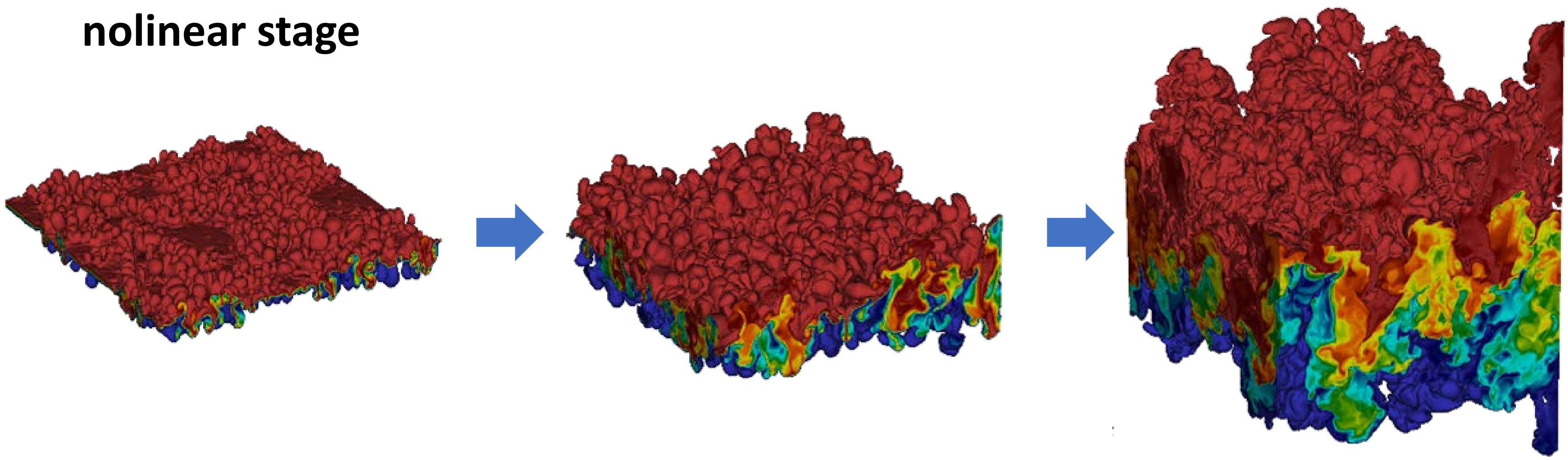


K-L(JFM2020;PoF2020a,b;PoF2021a,AMS2023), **K-ε**(AIPA2021b), **BHR** (PoF2021b)

Challenge for RANS models

- The present RANs models can only describe the fully turbulence stage. However, instabilities will evolve through different stages before transitioning to fully turbulence.

I. Linear and weakly nolinear stage **II.Transition** **III.Turbulence**



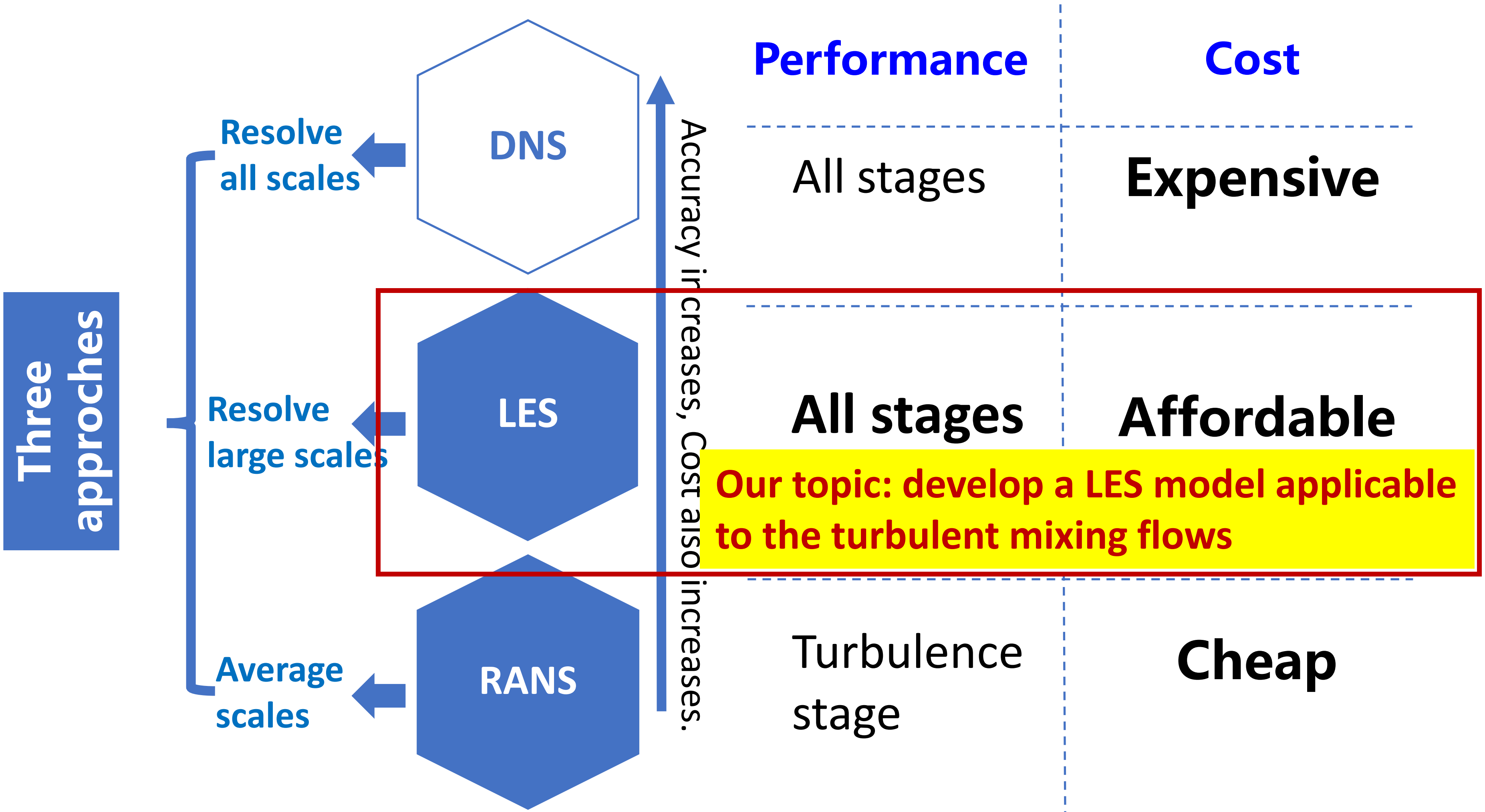
How to describe the mixing transition stage?

➢ Develop a transition RANS model? (Difficult in short term)

➢ Or …

Numerical simulation

- **LES is the most comprehensive method as it can capture different evolving stages with affordable computational cost..**



DNS: Direct Numerical Simulation; LES: Large Eddy Simulation;
RANS: Reynolds-Averaged Navier-Stokes

Introduction of the LES model

- Governing equations based on the closure form of a eddy viscosity LES model:

	Resolved terms：		Introduced terms by filterings:
Mass	$\frac{\partial \bar{\rho}}{\partial t}+\frac{\partial \bar{\rho}\tilde{u}_j}{\partial x_j}$	$=$	0
Momentum	$\frac{\partial \bar{\rho}\tilde{u}_i}{\partial t}+\frac{\partial \bar{\rho}\tilde{u}_i\tilde{u}_j}{\partial x_j}+\frac{\partial \bar{p}}{\partial x_i}-\bar{\rho}g_i$	$=$	$\frac{\partial \tau_{ij}^{sgs}}{\partial x_j}$ sgs: sub-grid scale
Energy	$\frac{\partial \bar{\rho}\tilde{E}}{\partial t}+\frac{\partial \tilde{u}_j\left(\bar{\rho}\tilde{E}+\bar{p}\right)}{\partial x_j}-\bar{\rho}\tilde{u}_i\bar{g}_i$	$=$	$\frac{\partial}{\partial x_j}\left(\frac{\mu^{sgs}}{\Pr_t}\frac{\partial \tilde{T}}{\partial x_j}\right)+\frac{\partial}{\partial x_j}\left(\mu^{sgs}\frac{\partial K^{sgs}}{\partial x_j}+\tau_{ij}^{sgs}\tilde{u}_i\right)$
Mass fraction	$\frac{\partial \bar{\rho}\tilde{Y}_a}{\partial t}+\frac{\partial \bar{\rho}\tilde{u}_j\tilde{Y}_a}{\partial x_j}$	$=$	$\frac{\partial}{\partial x_j}\left(\frac{\mu^{sgs}}{Sc_t}\frac{\partial \tilde{Y}_a}{\partial x_j}\right)$

sub-grid stress: $\tau_{ij}^{sgs}=-2\bar{\mu}^{sgs}\left(\tilde{S}_{ij}-\frac{1}{3}\tilde{S}_{kk}\delta_{ij}\right)+\frac{2}{3}\bar{\rho}k^{sgs}\delta_{ij}$

The key lies in how to accurately model these two quantities?

Modification1: one-equation model

- One-equation model introduces a transport equation of sub-grid kinetic energy, more suitable for the case of large strain rate (shock)

$$\tau_{ij}^{sgs} = -2\bar{\mu}^{sgs}\left(\tilde{S}_{ij} - \frac{1}{3}\tilde{S}_{kk}\delta_{ij}\right) + \frac{2}{3}\bar{\rho}k^{sgs}\delta_{ij}$$

Algebraic (Smogrinsky)

$C_d\bar{\rho}\bar{\Delta}^2|\tilde{S}|$

$C_I\bar{\Delta}^2|\tilde{S}|^2$

$|\tilde{S}| = \sqrt{\tilde{S}_{ij}\tilde{S}_{ij}}$

Note: yielding non-physical results in the case of large strain rate (shock of RM)

One-equation

$C_d\bar{\rho}\bar{\Delta}\sqrt{K^{sgs}}$

equation

$$\frac{\partial\bar{\rho}}{\partial t} + \frac{\partial\bar{\rho}\tilde{u}_j K^{sgs}}{\partial x_j} = \tau_{ij}^{sgs}\frac{\partial\tilde{u}_i}{\partial x_j} + \frac{\partial}{\partial x_j}\left(\mu^{sgs}\frac{\partial K^{sgs}}{\partial x_j}\right) - C_\varepsilon\bar{\rho}\frac{\left(\sqrt{2K^{sgs}}\right)^3}{\bar{\Delta}}$$

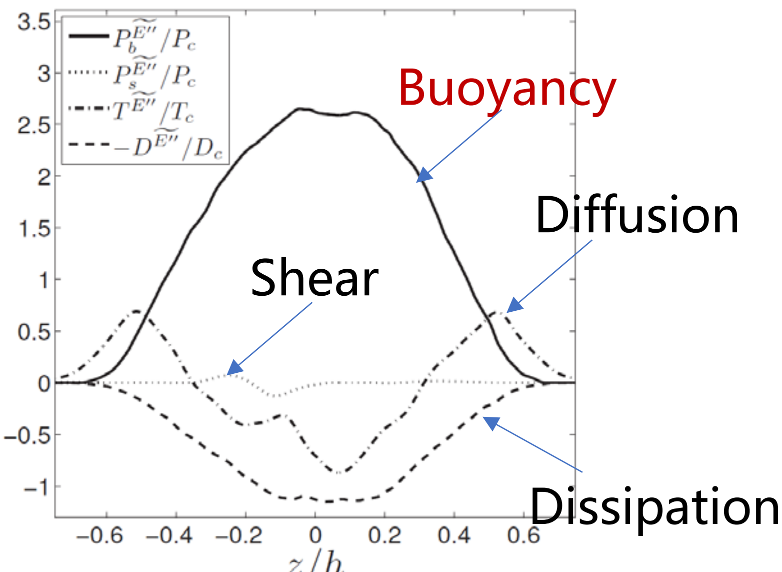
+?

What else needs to be considered different from the general model?

Modification2: buoyancy production

- Buoyancy production plays an dominant role for buoyancy-driven flows, e.g. RT and RM turbulent mixing[1], and it remains important at the smallest scales[2].

$$\frac{\partial \bar{\rho}}{\partial t}+\frac{\partial \bar{\rho}\tilde{u}_j K^{sgs}}{\partial x_j}=\underbrace{\tau_{ij}^{sgs}\frac{\partial \tilde{u}_i}{\partial x_j}}_{\text{Shear production}}+\underbrace{\frac{\partial}{\partial x_j}\left(\mu^{sgs}\frac{\partial K^{sgs}}{\partial x_j}\right)}_{\text{Diffusion}}\underbrace{-C_\varepsilon \bar{\rho}\frac{\left(\sqrt{2K^{sgs}}\right)^3}{\bar{\Delta}}}_{\text{Dissipation}}\underbrace{-C_B\frac{\mu^{sgs}}{\rho^2}\frac{\partial \bar{\rho}}{\partial x_k}\frac{\partial \bar{p}}{\partial x_k}}_{\text{Buoyancy production}}$$



(LLNL-Schilling et al., 2010 RT)

This term is usually neglected in aeronautical or wall-bounded flows.

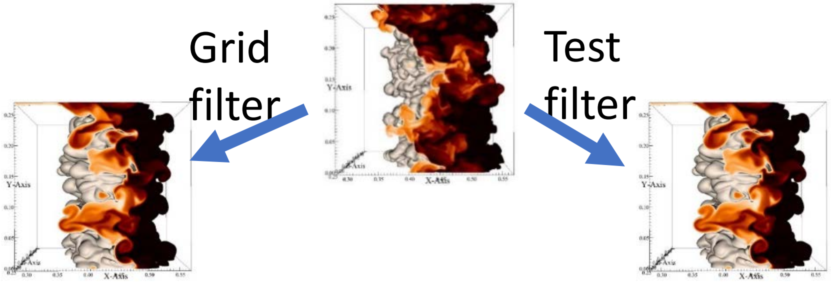
Its importance has also been proven in the modeling of RANS models.

[1]: LLNL-Schilling et al., 2010 RT;
[2]:LANL-Livescu et al., 2009

Modification3: dynamic coefficients

- Five coefficients (Cμ, Prt, Sct,Cε,CB) are dynamically computed in order to adapt the models better to the local structure of mixing flows and can be easily generalized to engineering flows.

Taking C_μ as a example:



$$\tau_{ij}^{sgs}(\Delta) \equiv \overline{\rho u_i u_j} - \overline{\rho u_i}\,\overline{\rho u_j} / \overline{\rho} = \frac{1}{3}\tau_{kk}^{sgs}\delta_{ij} - C_\mu \alpha_{ij}^{sgs}$$

$$\tau_{ij}^{test}(\hat{\Delta}) \equiv \widehat{\overline{\rho u_i u_j}} - \widehat{\overline{\rho u_i}}\,\widehat{\overline{\rho u_j}} / \widehat{\overline{\rho}} = \frac{1}{3}\tau_{kk}^{test}\delta_{ij} - C_\mu \alpha_{ij}^{test}$$

Germano identity:

$$L_{ij} \equiv \widehat{\overline{\rho}\tilde{u}_i\tilde{u}_j} - \widehat{\overline{\rho}\tilde{u}_i}\,\widehat{\overline{\rho}\tilde{u}_j} / \hat{\overline{\rho}} = \tau_{ij}^{test} - \hat{\tau}_{ij}^{sgs}$$

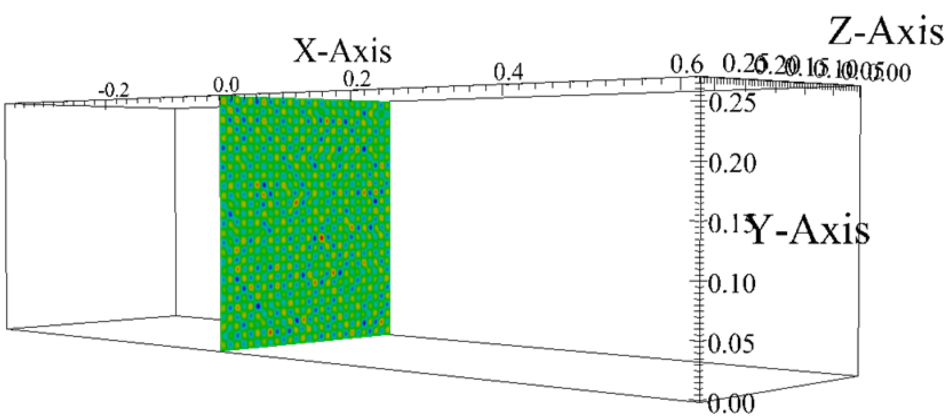
$$C_\mu = \frac{L_{ij}^d \tilde{S}_{ij}}{M_{ij}\tilde{S}_{ij}} \Rightarrow C = \frac{L \cdot Cont}{M \cdot Cont}$$

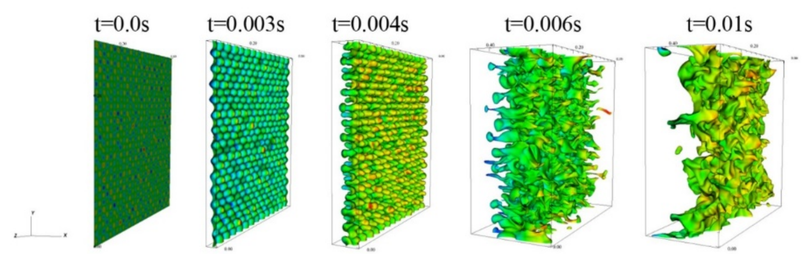
Generialization

Application 1: Reshocked RM

- Reshocked RM involves combined RT, RM and KH effects.

Shocks pass through a perturbed interface separating two materials, and are further reflected by a wall to repeatedly re-shock the mixing zone to a final turbulent state.

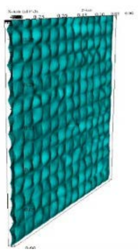


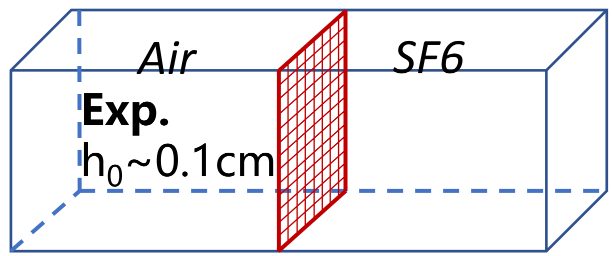


Application 1: Reshocked RM

- Modification of the initial perturbation: using velocity perturbation to produce a initial magnitude of perturbation comparable to the corresponding experiments.

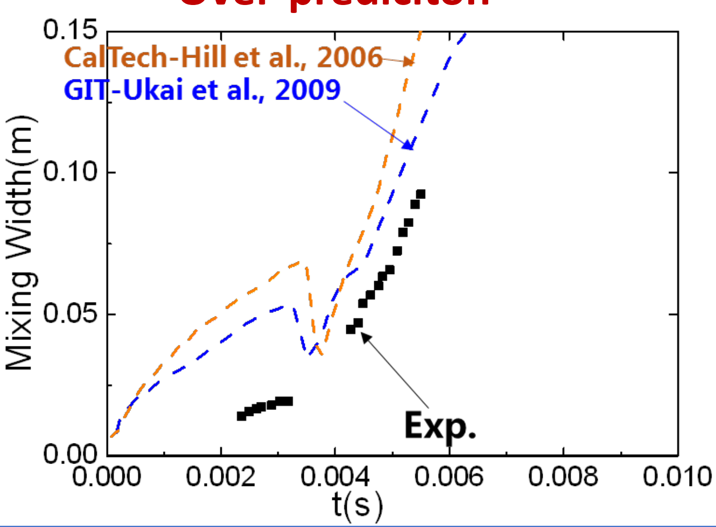
Previous LES
Interface perturbation
h_0~0.25cm





Present LES: Velocity perturbation
h_0~0.1cm

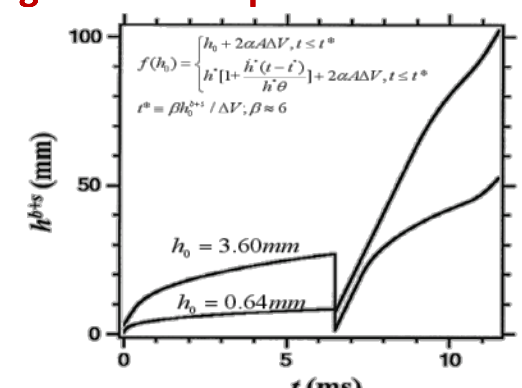
Over-prediciton



reason

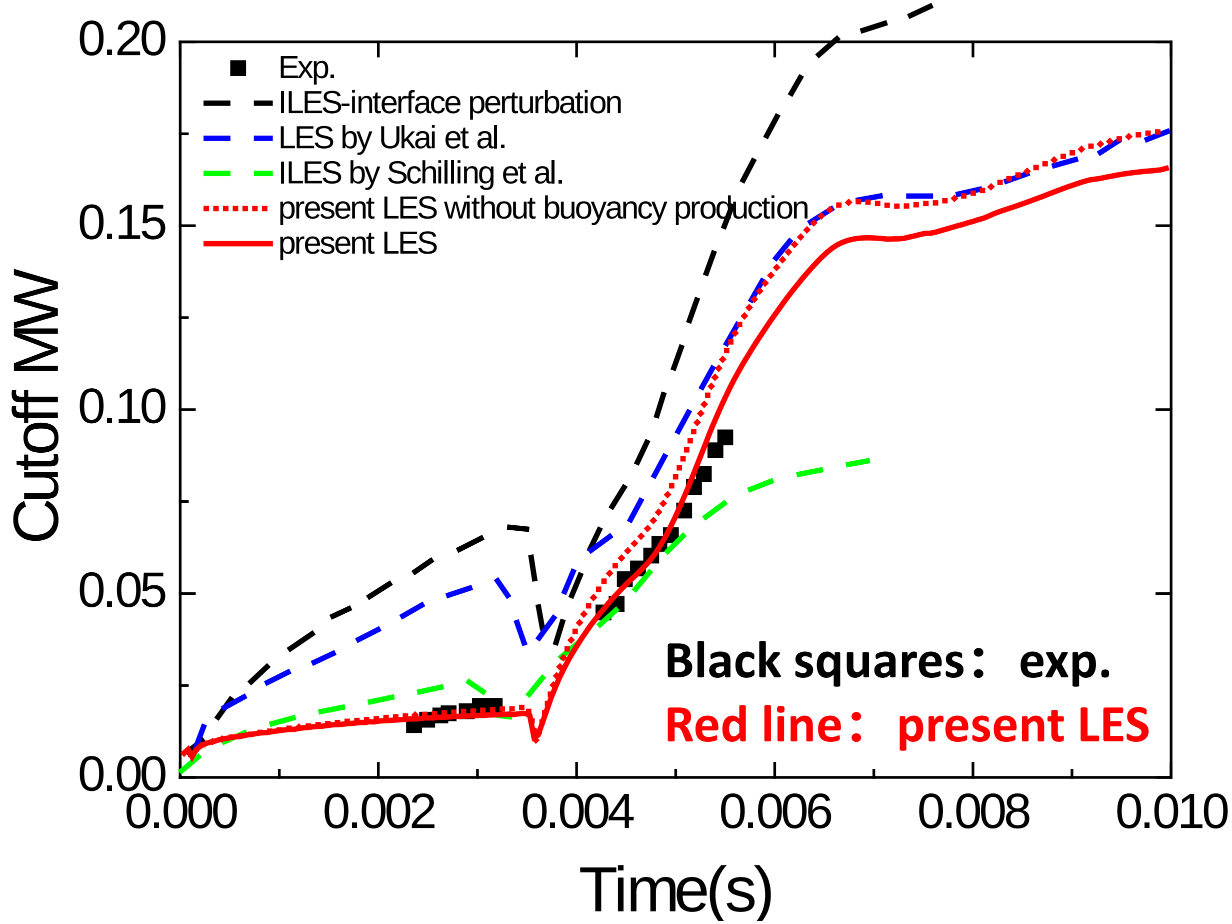
Mikaelian (1990,2011,2015,2020) :

There is a positive correlation between mixing width and perturbation amplitude

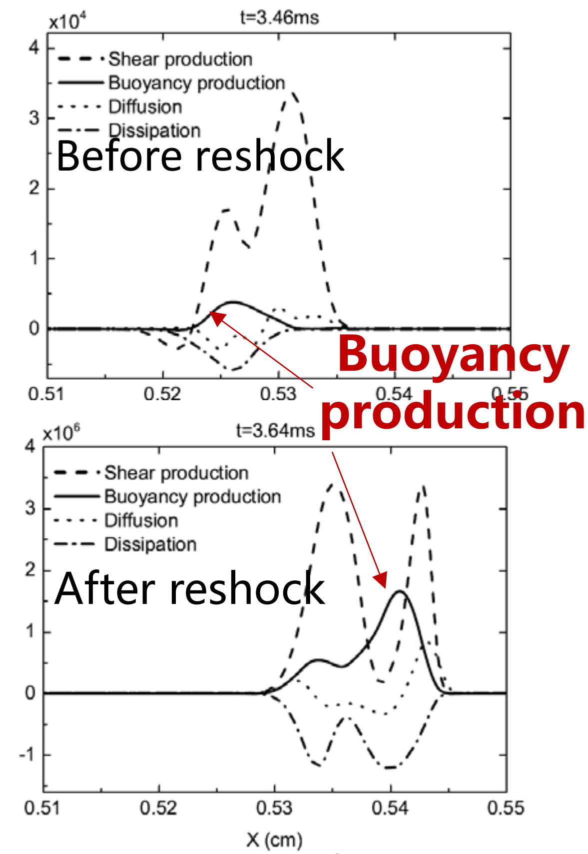


Application 1: Reshocked RM

- The present results are in good agreement with the experimental measurements.



Temporal evolution of the MW[1]



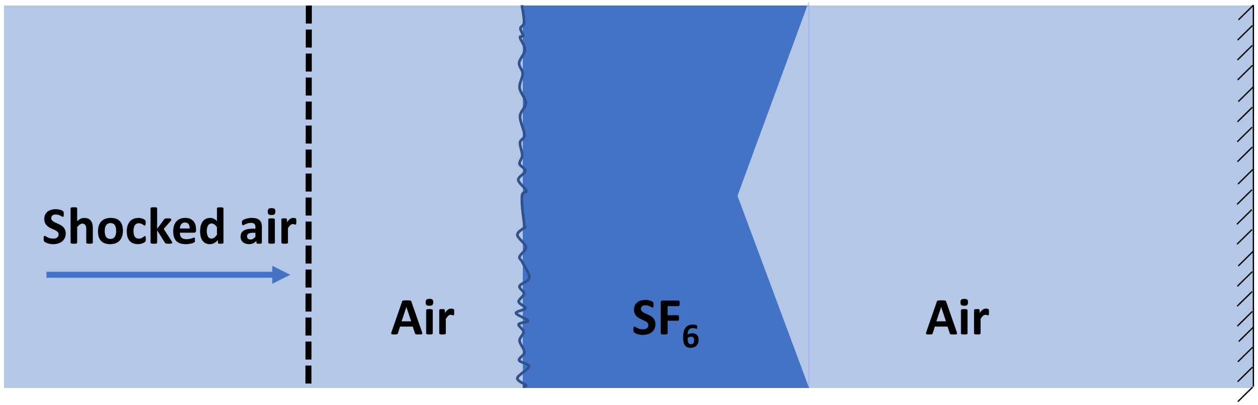
Budgets of TKE

After the reshock, buoyancy production becomes one of the dominant mechanism contributing to turbulent mixing

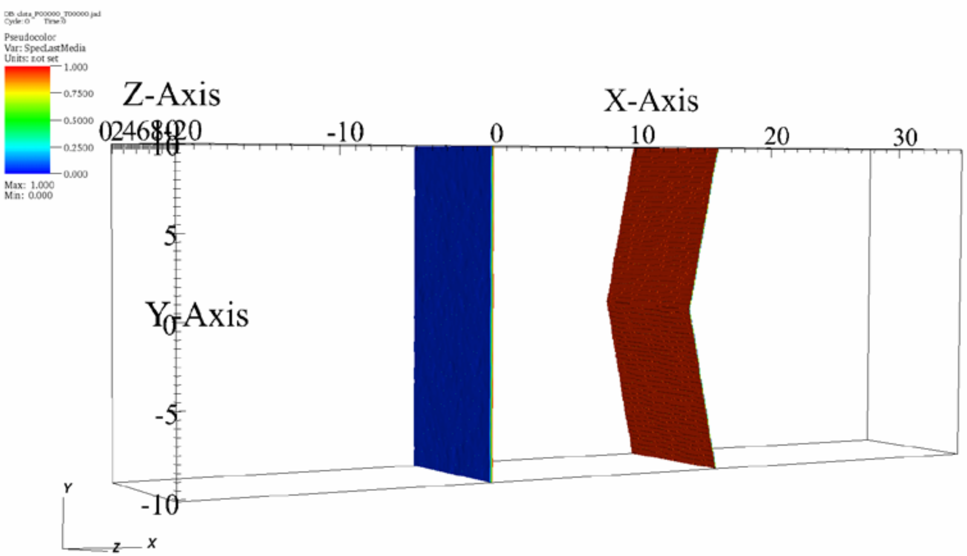
[1]POF2022

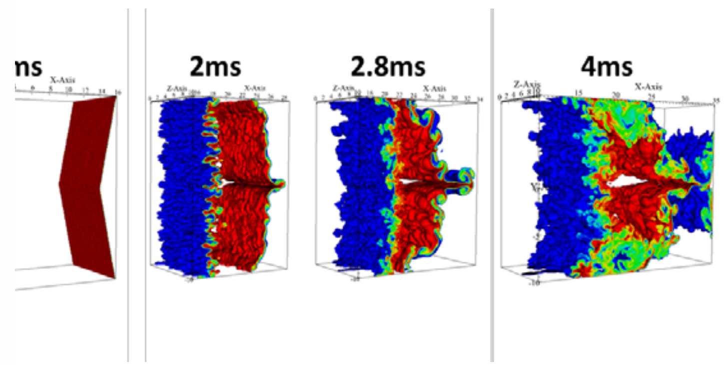
Application 2: inverse chevron

- In this case, the transition process is prominent



Shocks pass through two interfaces, in which the second interface is the shape of a inverse chevron, and are further reflected by a wall to repeatedly re-shock the mixing zone to a final turbulent state.

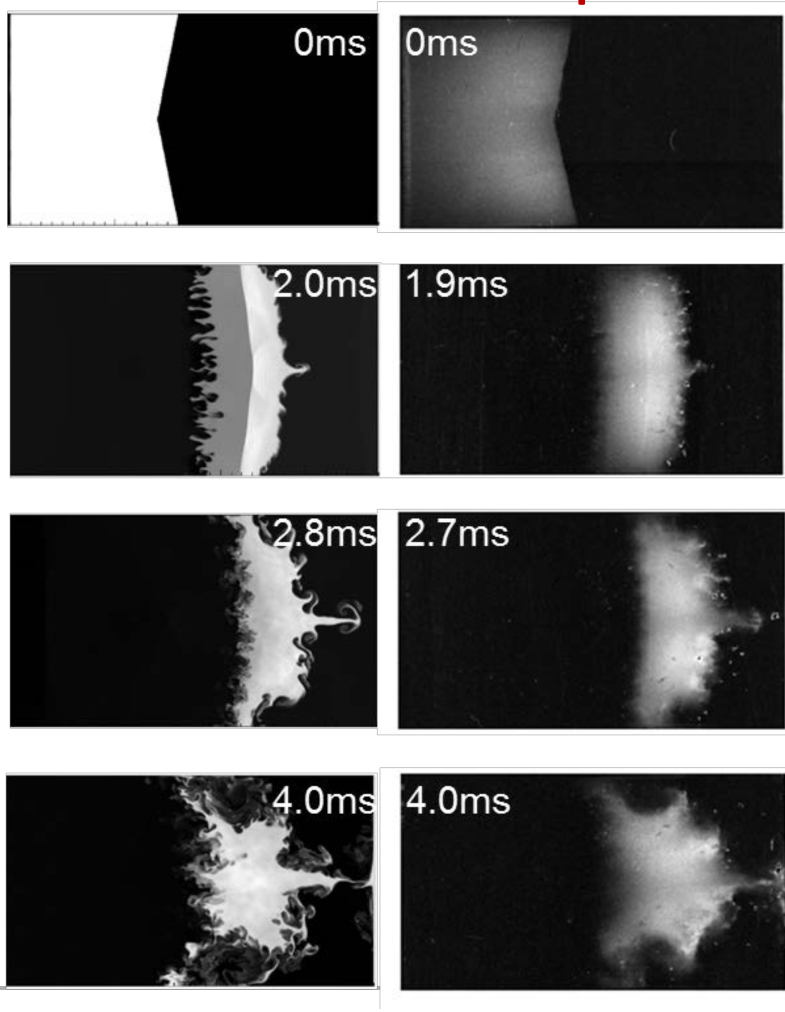




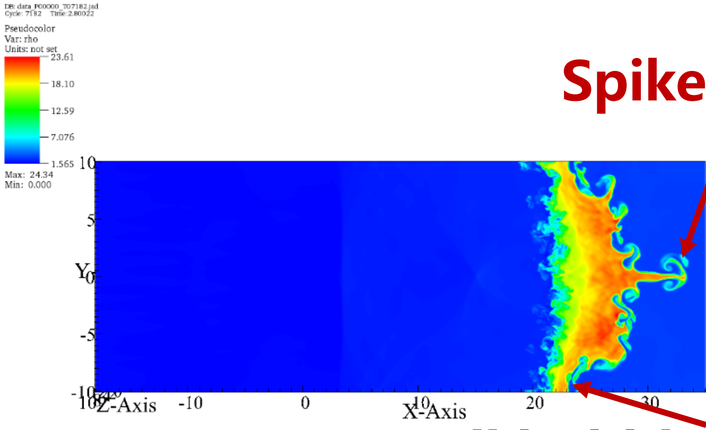
Application 2: inverse chevron

- The present results are qualitatively and quantitatively consistent with the experimental data.

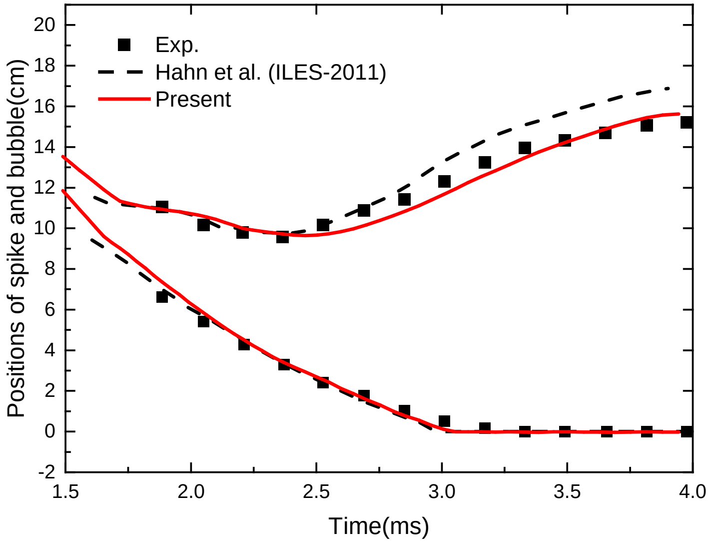
Present LES **Exp.**



Spike height

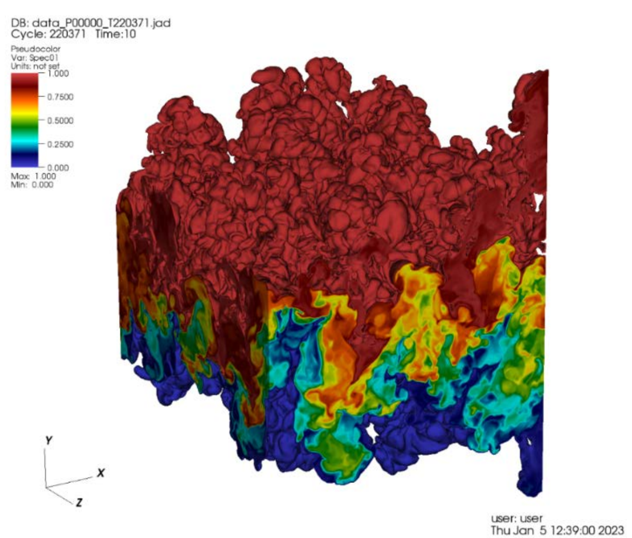


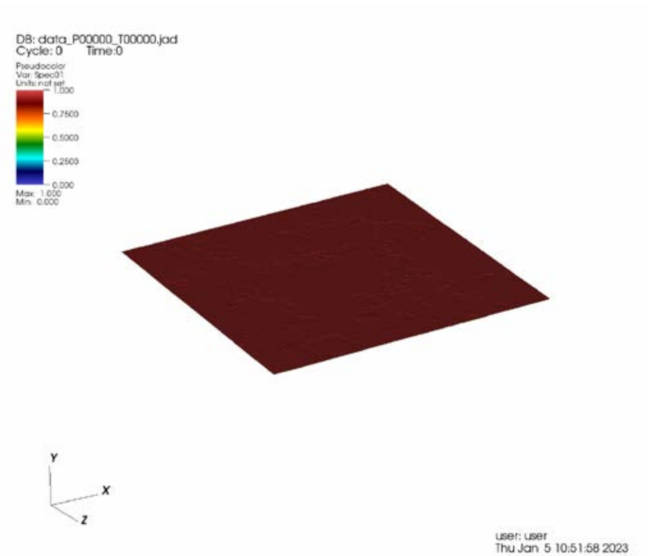
Wall bubble height



Conclusions

- We have developed a new LES model reflecting the characteristics of the turbulent mixing flows;
- This new LES model has been applied to two benchmarks, yielding good results consistent with the corresponding experimental measurements;
- This model can be further utilized to investigate the transition mechanism and to develop mixing transition models, as it can provide the detailed characteristics, structures and quantities not provided by experiments.





Ongoing work: study mixing transition based on RT turbulent mixing

Thanks for listening!

Any questions?