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Enthalpy Diffusion in Multicomponent Flows

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Disclaimer

Enthalpy Diffusion in Multicomponent Flows

Wake Vortex Study at Wallops Island

The Siege and Destruction of Jerusalem by the Romans Under the Command of Titus, A.D. 70, by David Roberts (1850)

Andrew W. Cook

APS/DFD, Minneapolis, Nov. 22-24, 2009

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UCRL-PRES-??????

Do the multicomponent Euler equations adequately describe turbulent mixing?

$$\frac{\partial \rho Y_i}{\partial t} + \nabla \cdot \left(\rho Y_i \mathbf{u}\right) = 0$$

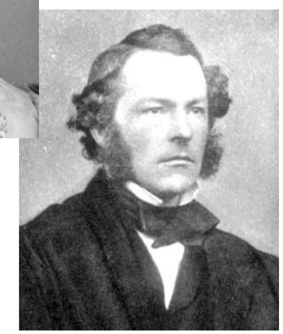
$$\frac{\partial \rho \mathbf{u}}{\partial t} + \nabla \cdot \left(\rho \mathbf{u}\mathbf{u} + p\underline{\ddot{\mathbf{a}}}\right) = 0$$

$$\frac{\partial \rho E}{\partial t} + \nabla \cdot \left[\left(E + p\right)\mathbf{u}\right] = 0$$

Can these equations accurately predict temperature?

Can the multicomponent Navier-Stokes equations accurately predict temperature?

$$\frac{\partial \rho Y_i}{\partial t} + \nabla \cdot \left(\rho Y_i \mathbf{u}\right) = -\nabla \cdot \mathbf{J}_i$$

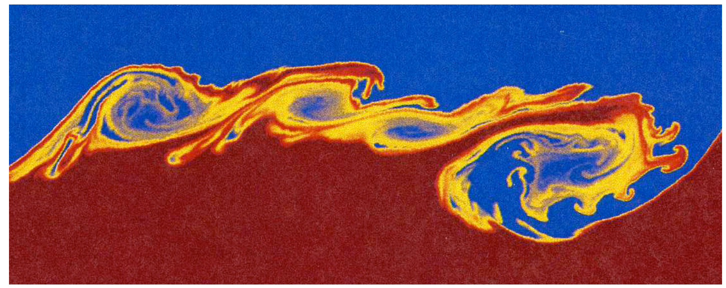


$$\frac{\partial \rho \mathbf{u}}{\partial t} + \nabla \cdot \left(\rho \mathbf{u}\mathbf{u} + p\underline{\mathbf{\ddot{a}}}\right) = \nabla \cdot \underline{\hat{\mathbf{o}}}$$

$$\frac{\partial \rho E}{\partial t} + \nabla \cdot \left[\left(E + p\right)\mathbf{u}\right] = \nabla \cdot \left(\underline{\hat{\mathbf{o}}} \cdot \mathbf{u} - \mathbf{q}_c - \mathbf{q}_d\right)$$

Enthalpy Diffusion: $\mathbf{q}_d = h_i \mathbf{J}_i$

The species diffusion flux (J_i) is present in any simulation wherein mixing occurs.



$\mathbf{J}_i$ can represent:

- molecular diffusion (DNS, physical diffusivity)
- numerical diffusion (Euler solvers, ILES)
- subgrid-scale diffusion (LES, grid-scale transfer)
- turbulent diffusion (RANS, k-ε & k-l models)

q_d must balance J_i

The role of q_d is illustrated through a simple gedanken experiment.

Light gas	Heavy gas
Molecular weight: M_L	Molecular weight: M_H
Mass fraction: $Y_L = 1$	Mass fraction: $Y_H = 1$
Temperature: $T^< = T_0$	Temperature: $T^> = T_0$

$n_L \longrightarrow$

$\longleftarrow n_H$

If q_d=0 there can be no net mass flux; hence, $n_L M_L = n_H M_H$

Mixed gas in left partition	Mixed gas in right partition
$T^< = T_0/(Y_L+Y_H M_L/M_H) > T_0$	$T^> = T_0/(Y_L M_H/M_L+Y_H) < T_0$
$\Delta S^< > 0$	$\Delta S^> < 0$

$$\boxed{\Delta S = \Delta S^< + \Delta S^> < 0}$$

Shear layers evolve differently, depending on the presence of q_d.

OFF

ON

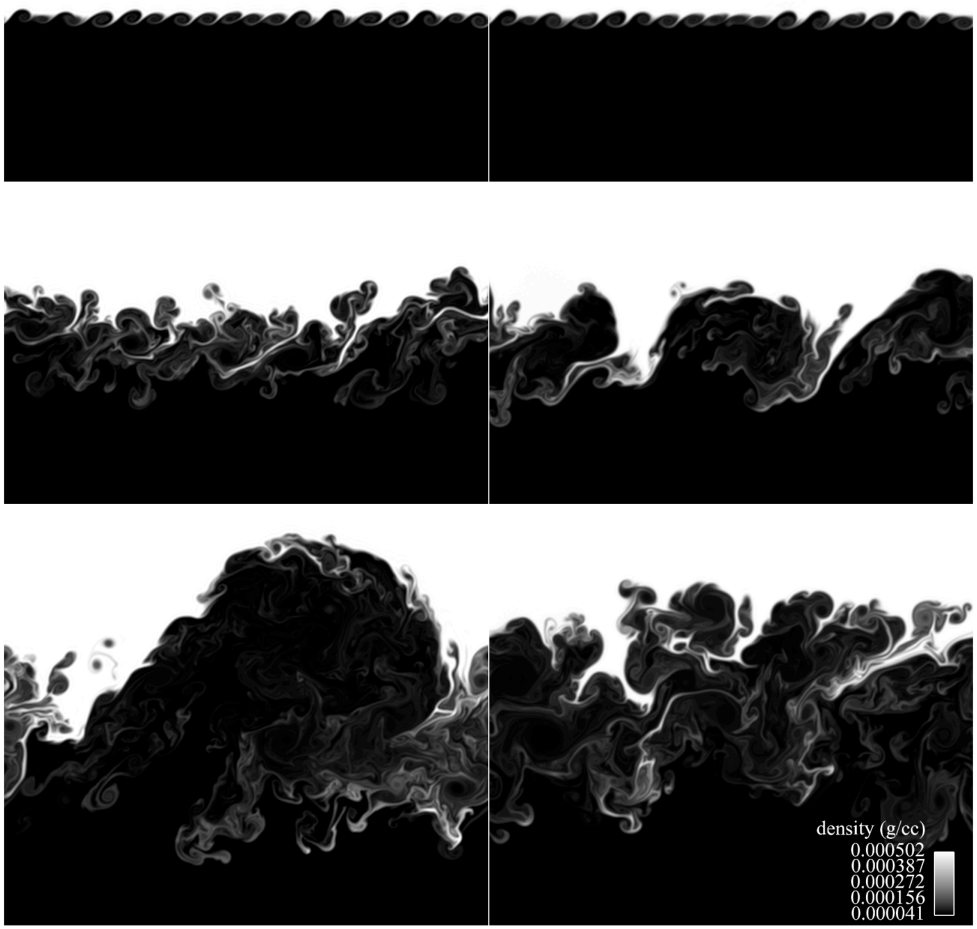
Air

H_2

1 ms

5 ms

10 ms



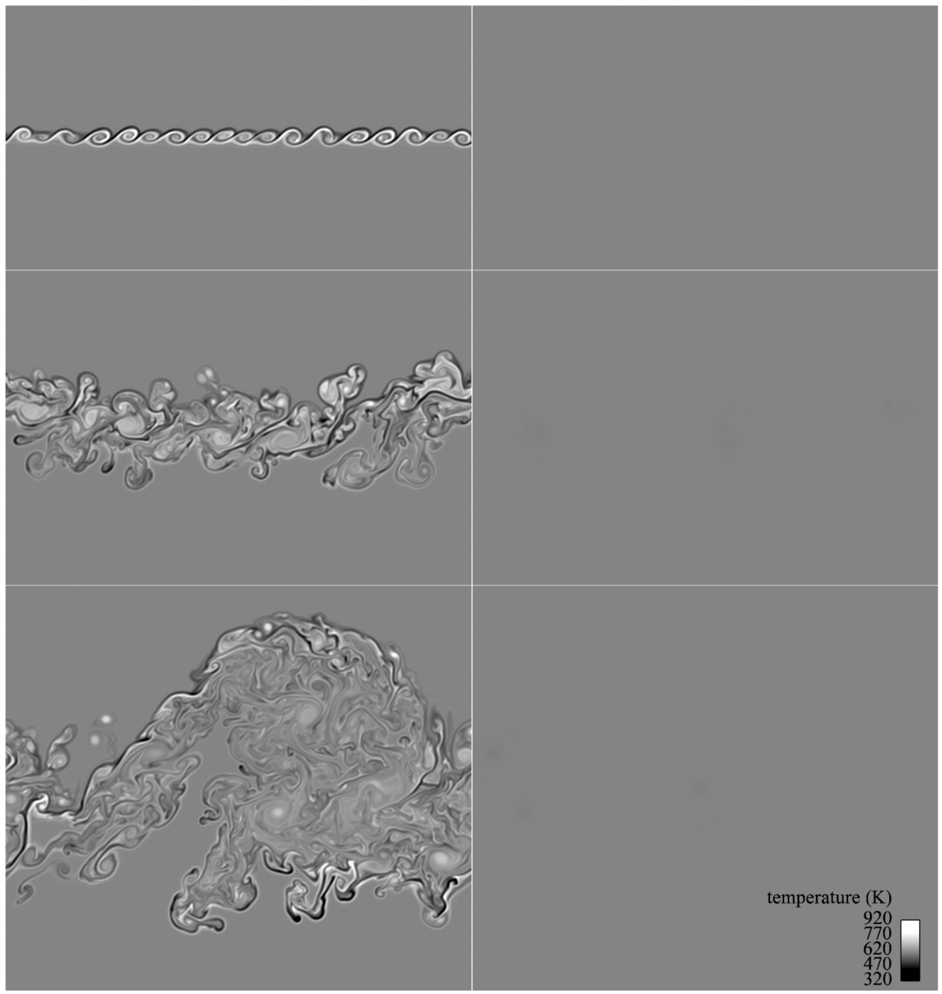
Temperature can be extremely sensitive to enthalpy diffusion.

OFF ON

1 ms

5 ms

10 ms



Air →

H_2 ←

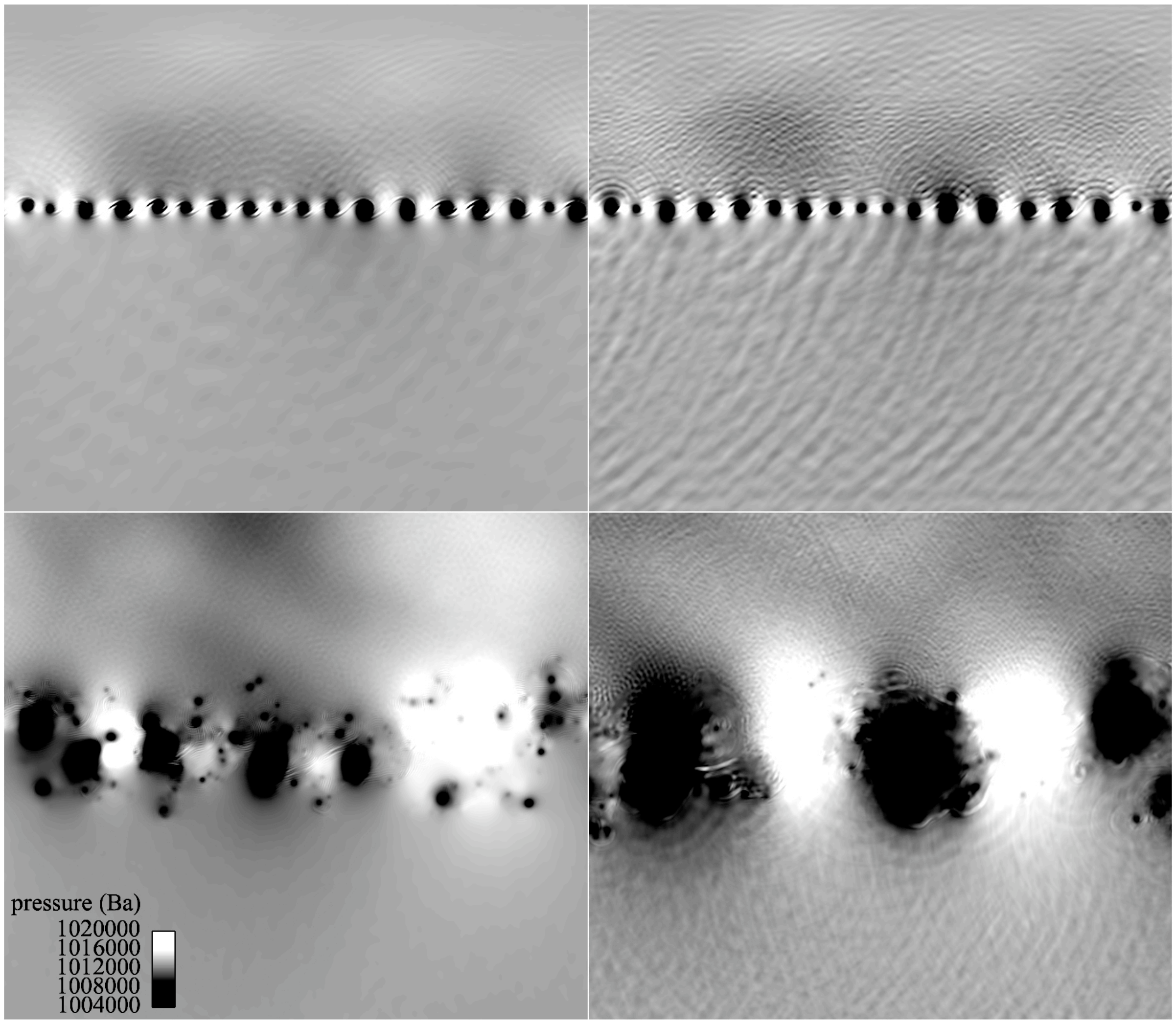
White regions exceed ignition temperature.

Enthalpy diffusion generates acoustic noise.

OFF ON

1 ms

5 ms

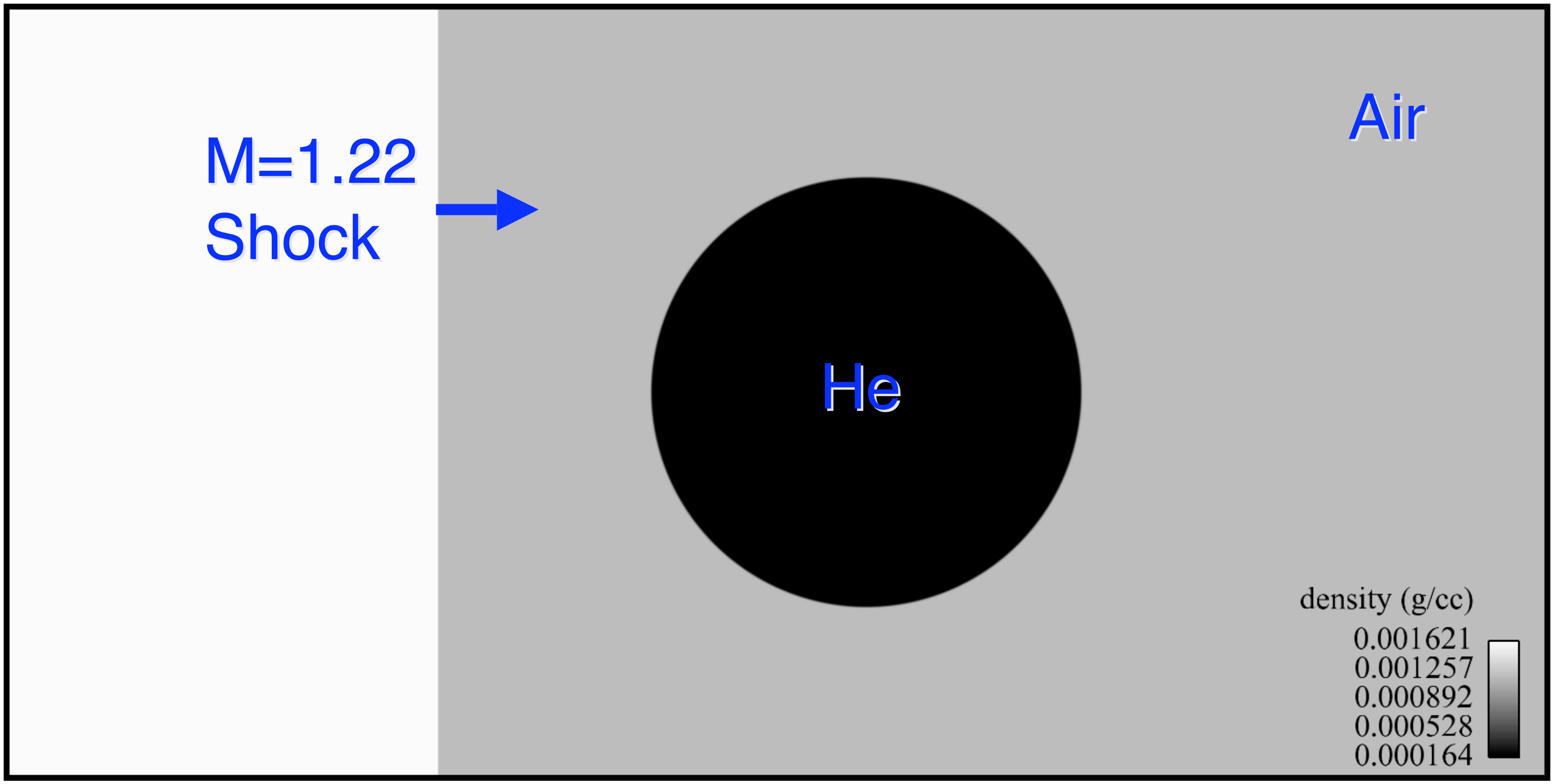


Air

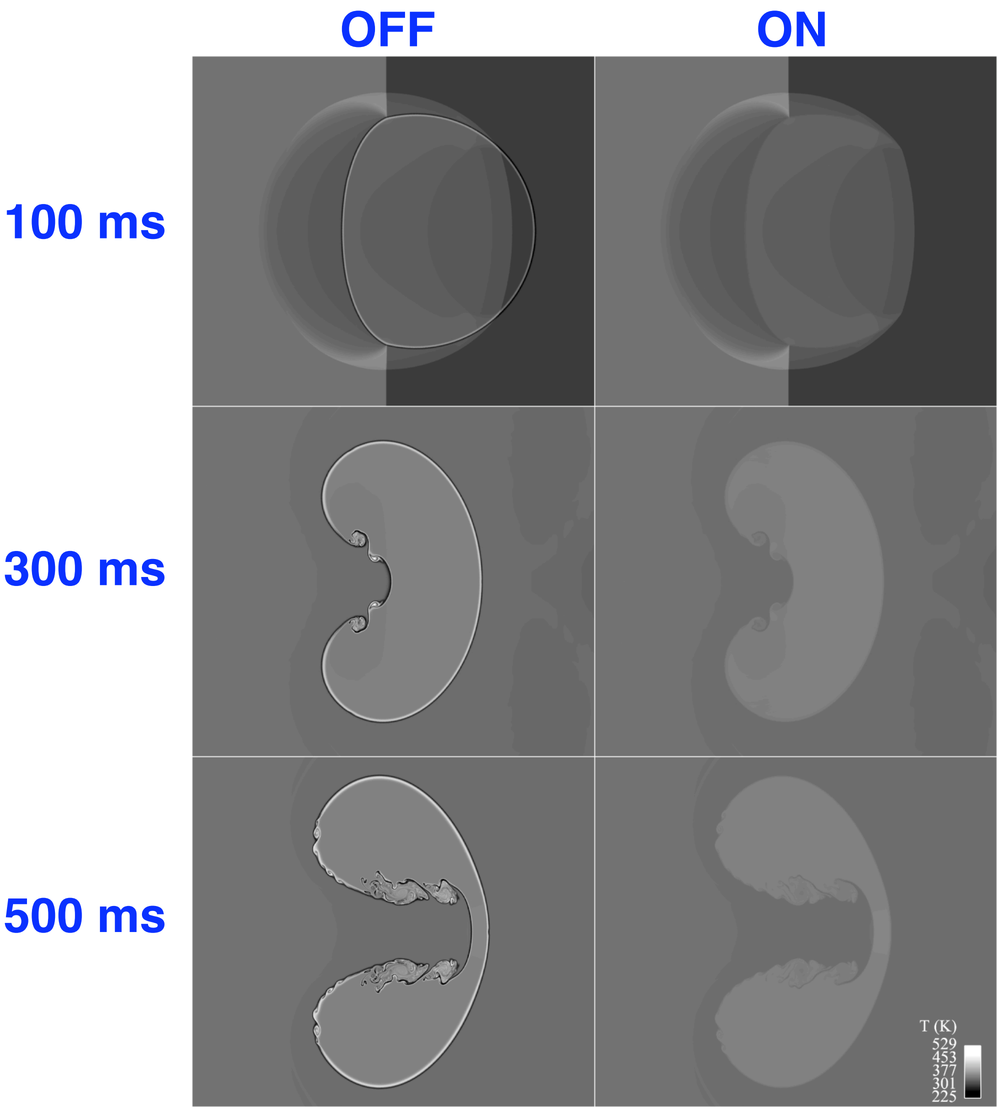
H_2

Recall from the gedanken experiment that q_d perturbs pressure.

The Haas-Sturtevant shock-bubble experiment provides a good test of the importance of q_d.



Temperature can be extremely sensitive to enthalpy diffusion.



W.S. Don and C.B. Quillen, Numerical simulation of shock-cylinder interactions J. Comput. Phys., 122:244-265 (1995)...

“Haas and Sturtevant's shock-helium cylinder interaction is well simulated by an Euler code"

“the temperature T is found to require a slightly heavier smoothing“

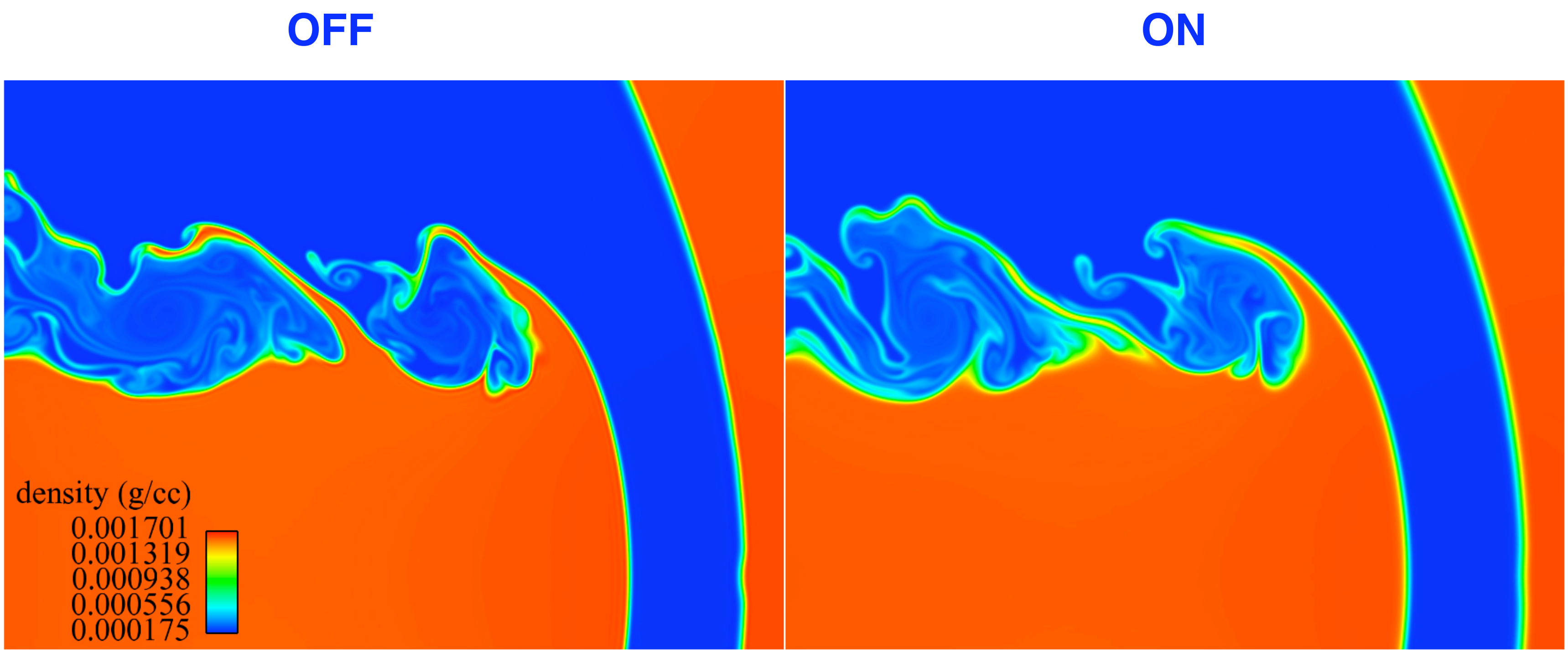
For Hydrogen-Air case…

“the general features are quite similar for both the Euler and the reactive Navier-Stokes simulations”

but

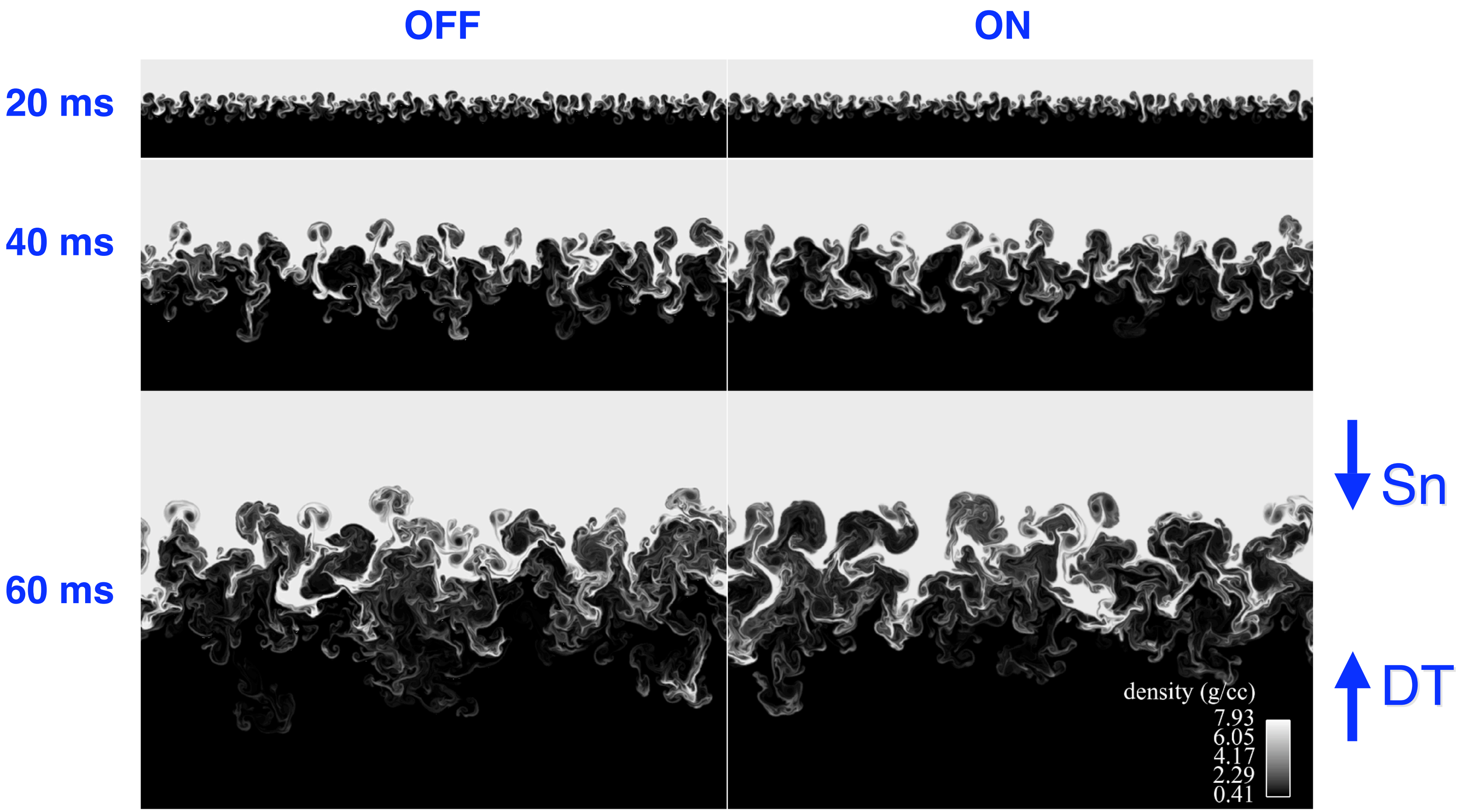
T (ambient) = 1000 K
T (ignition) = 853 K

Enthalpy diffusion indirectly results in a smoother density field.



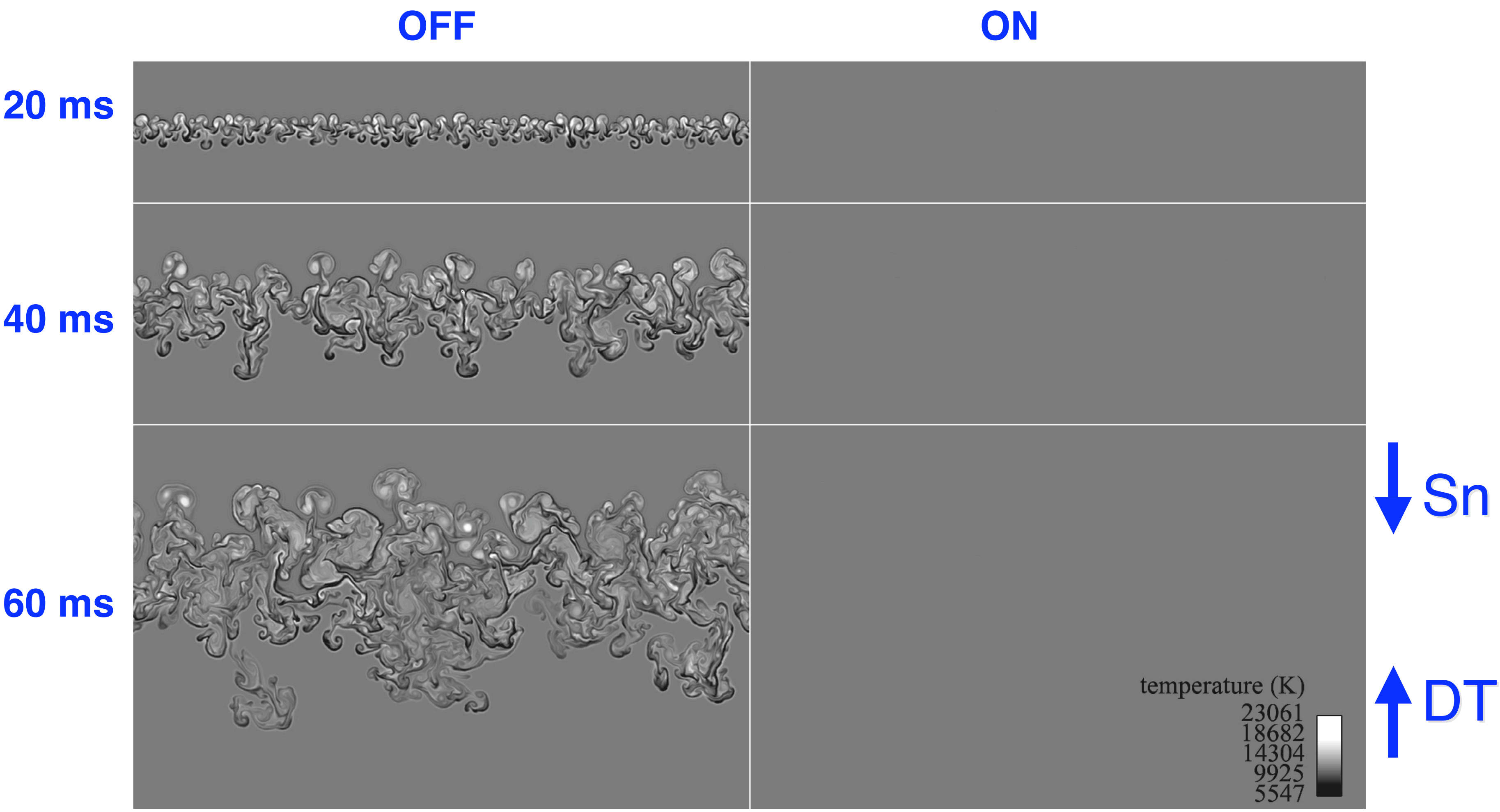
Density does not diffuse! Smoothing of the density field is brought About by a local divergence in the velocity field, which is here influenced by both heat conduction and enthalpy diffusion.

The Rayleigh-Taylor instability evolves differently, depending on the presence of q_d.



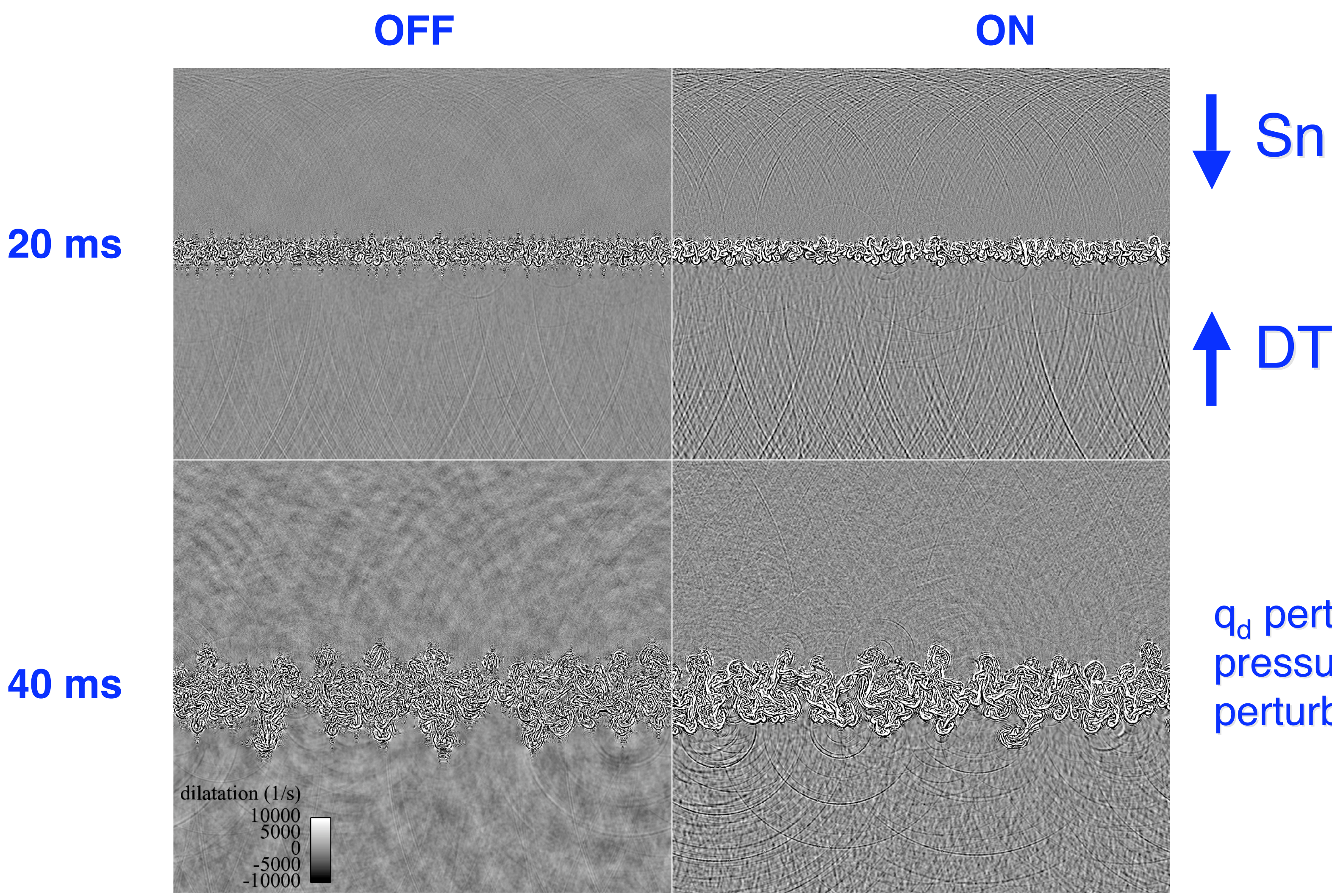
A = 0.87

Including q_d, $\Delta T<0.0052$ eV
Excluding q_d, 0.5 eV < T < 2 eV



T_o=1 eV (to match Dimonte-Tipton, PF 18:085101)

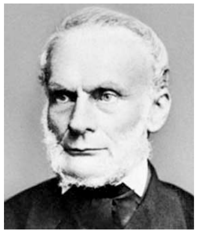
Enthalpy diffusion generates acoustic noise in R-T instability.



q_d perturbs pressure which perturbs velocity

Conclusions

Rudolf Clausius
Originator of the
concept of entropy



1. Enthalpy diffusion preserves the second law.
2. Euler solvers will not produce correct temperatures in mixing regions.
3. Navier-Stokes solvers will only produce correct temperatures if q_d is included.
4. Errors from neglecting enthalpy diffusion are most severe when differences in molecular weights are large.
5. In addition to temperature, enthalpy diffusion affects density, dilatation and other fields in subtle ways.
6. Reacting flow simulations that neglect the term are a dubious proposition.
7. Turbulence models for RANS and LES closures should preserve consistency between energy and species diffusion.