# Direct numerical simulations of high speed reactive mixing layers


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# Contents

# Introduction

## Problem description

- Direct numerical simulations: no turbulence models.
- High speed combustion regimes: Scramjet engines.
    - Gas mixtures: hydrogen, air . . .
    - Multicomponent transport.
    - Detailed reaction mechanisms.
- Compressibility effects.
- Shocked configurations.

# Introduction

## Previous works

- Previous works dealt mainly with temporally evolving mixing layers, i.e. parallel flow assumption.
- Few examples of spatially developing mixing layers referred only to non reactive conditions (air flows).
- Infinitely fast chemistry assumptions/tabulated chemistry simplifications.

# Governing equations

Fully compressible formulation, multicomponent reactive mixtures:

$$\partial_t(\rho) + \nabla \cdot (\rho u) = 0, \tag{1}$$

$$\partial_t(\rho u) + \nabla \cdot (\rho u \otimes u + PI) = \nabla \cdot \tau, \tag{2}$$

$$\partial_t(\rho e_t) + \nabla \cdot [(\rho e_t + P)\, u] = \nabla \cdot (\tau u - q), \tag{3}$$

$$\partial_t(\rho Y_\alpha) + \nabla \cdot (\rho Y_\alpha u) = -\nabla \cdot (\rho Y_\alpha V_\alpha) + \rho \dot{\omega}_\alpha, \quad \alpha \in \mathcal{S}. \tag{4}$$

$$e_t = u \cdot u/2 + \Sigma_{\alpha \in \mathcal{S}} h_\alpha Y_\alpha - \mathcal{R} T, \tag{5}$$

$$\tau = \mu \left( \nabla u + (\nabla u)^t \right) + (\kappa - 2\mu/3)(\nabla \cdot u)\, I, \tag{6}$$

$$q = \Sigma_{\alpha \in \mathcal{S}} \rho Y_\alpha V_\alpha (h_\alpha + \mathcal{R} T \tilde{\chi}_\alpha / \mathcal{W}_\alpha) - \lambda \nabla T, \tag{7}$$

$$\rho Y_\alpha V_\alpha = -\rho Y_\alpha \Sigma_{\beta \in \mathcal{S}} D_{\alpha\beta} (d_\beta + X_\beta \tilde{\chi}_\beta \nabla T / T), \tag{8}$$

$$d_\alpha = \nabla X_\alpha + (X_\alpha - Y_\alpha) \nabla P / P. \tag{9}$$

# Governing equations

$$P = \rho \mathcal{R} T / \mathcal{W}, \quad \mathcal{W} = \left(\Sigma_{\alpha \in \mathcal{S}} Y_\alpha / \mathcal{W}_\alpha\right)^{-1}, \tag{10}$$

$$c_{p\alpha}(T) = \mathcal{R} \mathcal{W}_\alpha^{-1} \phi_\alpha, \tag{11}$$

$$h_\alpha(T) = \mathcal{R} T \mathcal{W}_\alpha^{-1} \varphi_\alpha. \tag{12}$$

## Remarks

- $\phi_\alpha$ and $\varphi_\alpha$: polynomial representation (JANAF tables).
- Multicomponent transport (Soret and Dufour): EGLIB library[a].
- Chemical reactions: DVODE (CHEMKIN II library[b]).

[a] A. Ern and V Giovangigli. Fast and accurate multicomponent transport property evaluation. J. Comput. Physics **120**, 105-116, (1995).

[b] R. J. Kee, F. M. Rupley and E. Meeks. CHEMKIN-III: A Fortran Chemical Kinetics Package for the Analysis of Gas-Phase Chemical and Plasma Kinetics. Sandia National Laboratories (1996).

# Numerical methods

## Spatial discretization

- Convective fluxes: $7^{th}$ order accurate Weighted Essentially Non Oscillatory (WENO) scheme[a].
- Molecular fluxes: $8^{th}$ order accurate centered difference scheme.

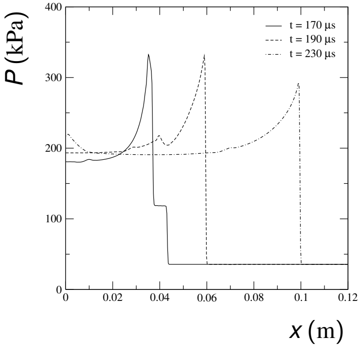
[a] Y. Shen and G. Zha. Improved seventh-order WENO scheme. AIAA Paper 2010-1451 (2010).

## Temporal integration: Strang splitting technique[a]

[a] R. P. Fedkiw, B. Merriman and S. Osher. High accuracy numerical methods for thermally perfect gas flows with chemistry. J. Comput. Phys. **132**, 175–190, (1997).

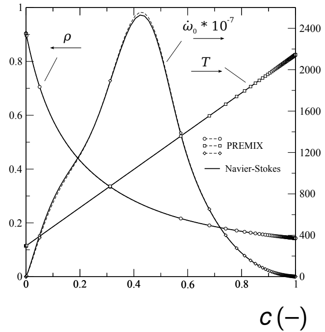
1. $t \to t + \Delta t/2$ : DVODE solver.
2. $t \to t + \Delta t$ : $3^{th}$ order accurate Total Variation Diminishing (TVD) Runge Kutta scheme.
3. $t + \Delta t/2 \to t + \Delta t$ : DVODE solver.

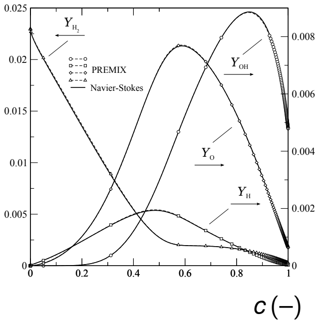
# Multi-species reactive shock tube




- Riemann problem with a discontinuity at t=0.
- Focus on the competition between convection and reaction terms.
- Shock hits a solid wall boundary and reflects off.
- A reaction wave kicks in picking up steam and merges with the shock.

# One-dimensional hydrogen/oxygen laminar premixed flame




- Similar orders of magnitude for convection, diffusion and reaction.
- PREMIX reference solution retained as the initial condition.
- Progress variable defined as: $c = (T - T_u)/(T_b - T_u)$.

# Cheng approximate conditions

## Overview

- Conditions representative of Scramjet engine operations.
- A reference benchmark for supersonic combustion modeling.
- Available experimental data[a].
- Different reaction mechanisms:
    1. Marinov reaction mechanism: 3 species, 1 step calibrated reaction.
    2. Jachimowski reaction mechanism: 13 species, 33 reactions.
    3. O' Conaire reaction mechanism: 9 species, 19 reactions.

[a] T. S. Cheng, J. A. Wehrmeyer and R. W. Pitz. Raman measurement of mixing and finite-rate chemistry in a supersonic hydrogen-air diffusion flame. Combustion and Flame **99**, 157-173, (1994).

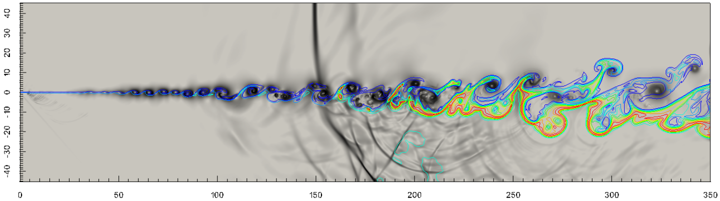
# Shear layer configuration


$L_x \times L_y = 350\delta_\omega^0 \times 90\delta_\omega^0$ with $N_x \times N_y = 2085 \times 455$.
$R_\omega = \bar{\rho}\Delta u \delta_\omega^0 / \bar{\mu} = 640$, $M_c = \Delta u/(c_f + c_o) = 0.4$.

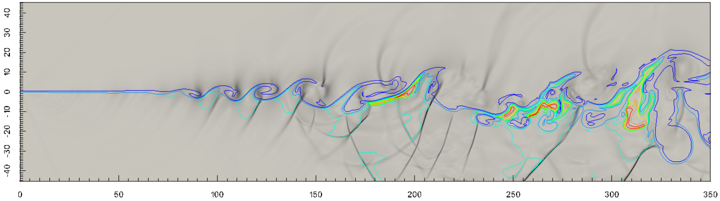
| Fuel (top) | Oxidizer (bottom) |
|---|---|
| $u_f = 1949.08\,\mathrm{m/s}$ | $u_o = 954.55\,\mathrm{m/s}$ |
| $P_f = 109\,\mathrm{KPa}$ | $P_o = 109\,\mathrm{KPa}$ |
| $T_f = 545\,\mathrm{K}$ | $T_o = 1250\,\mathrm{K}$ |
| $Y_{\mathrm{H_2}} = 1.0$ | $Y_{\mathrm{O_2}} = 0.245,\ Y_{\mathrm{N_2}} = 0.58,\ Y_{\mathrm{H_2O}} = 0.175$ |
| $\rho_f = 0.049\,\mathrm{Kg/m^3}$ | $\rho_o = 0.28\,\mathrm{Kg/m^3}$ |
| $c_f = 1949\,\mathrm{m/s}$ | $c_o = 955\,\mathrm{m/s}$ |
| $M_f = 1.1$ | $M_o = 1.34$ |

# Instantaneous fields

Numerical Schieleren of the pressure field.
Temperature iso-contours: $T_{min} = 400\,\mathrm{K}$, $T_{max} = 3100\,\mathrm{K}$.



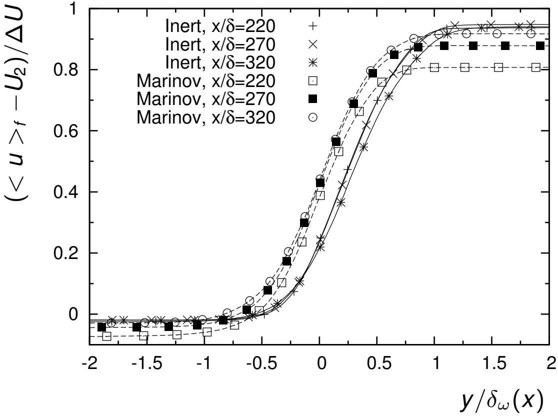

$M_c = 0.4$




$M_c = 0.8$

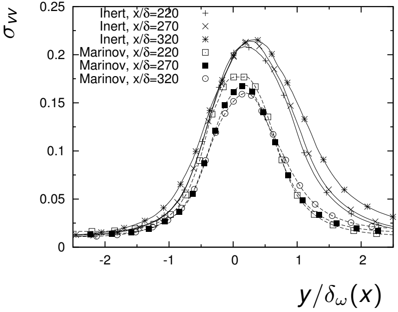
# Self-similarity profiles ($M_c = 0.4$)

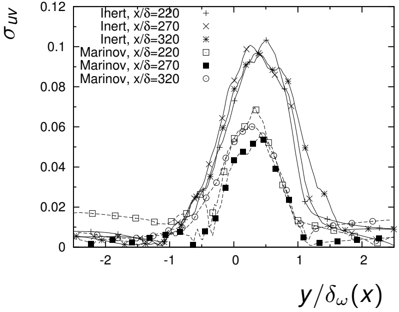
Favre averaged streamwise velocity component



# Self-similarity profiles ($M_c = 0.4$)

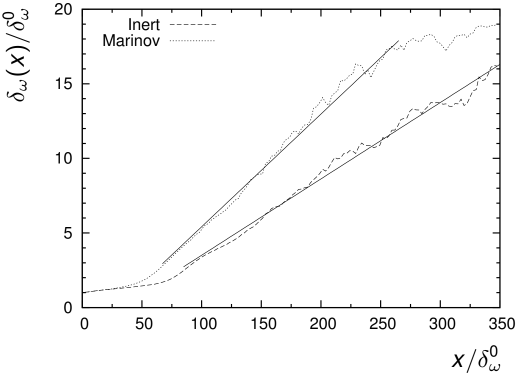
## Reynolds shear stresses




- $\sigma_{vv} = \sqrt{< v''v'' >_f}/\Delta U.$
- $\sigma_{uv} = \sqrt{< u''v'' >_f}/\Delta U.$

# Vorticity thickness growth rate ($M_c = 0.4$)




$$\mathrm{d}\delta_\omega/\mathrm{d}x = K_\delta(U_1 - U_2)/(U_1 + U_2), \quad K_\delta^I = 0.15, \quad K_\delta^R = 0.22$$

$$K_\delta^R/K_\delta^I \approx 1.47$$

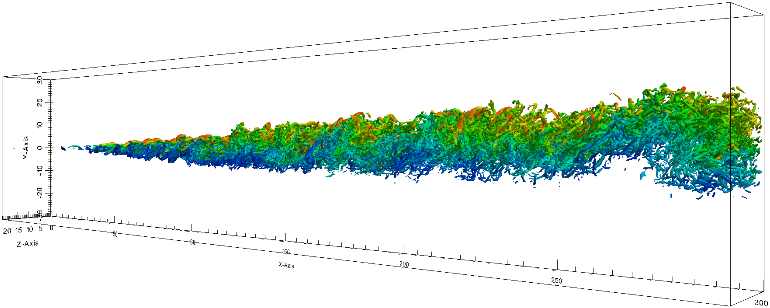
# Cheng approx. conditions: conclusion

| $Re_\theta$ | $\sigma_{uu_{max}}$ | $\sigma_{vv_{max}}$ | $\sigma_{uv_{max}}$ | $K_\delta$ | Type | Reference |
|---|---|---|---|---|---|---|
| – | 0.176 | 0.138 | 0.097 | 0.190 | Experimental | Wygnanski & Fiedler (1970) |
| – | 0.190 | 0.120 | 0.114 | 0.160 | Experimental | Spencer & Jones (1971) |
| 450 | 0.180 | 0.140 | 0.100 | 0.163 | DNS-3D | Bell & Mehta (1990) |
| 800 | 0.160 | 0.130 | 0.100 | 0.130 | DNS-3D | Rogers & Moser (1994) |
| 90 | 0.200 | 0.290 | 0.150 | 0.143 | DNS-2D | Stanley & Sarkar (1997) |
| 160 | 0.220 | 0.220 | 0.110 | 0.150 | DNS-2D | Inert simulation ($M_c = 0.4$) |
| 160 | 0.220 | 0.180 | 0.070 | 0.220 | DNS-2D | Reactive simulation ($M_c = 0.4$) |

## Concluding remarks

- Self-similarity in both inert and reactive cases.
- Shear stresses overestimated in 2D inert simulations.
- Heat release decreases significantly the Reynolds shear stresses and modifies $K_\delta$.

# 3D simulations




- Iso-contour of $Q = 0.01 \times Q_{max}$ colored by the mixing variable, inert case at $M_c = 0.4$.
- $L_x \times L_y \times L_z = 300\delta_\omega^0 \times 60\delta_\omega^0 \times 22\delta_\omega^0$, $N_x \times N_y \times N_z = 1441 \times 307 \times 131$.

# Conclusions and future works

## Conclusions

- Cheng approximate conditions case confirms reduction of the Reynolds shear stresses.
- Moderate heat released effect with detailed reaction mechanisms compared to one step reactions.

## Future works

- Influence of the inflow conditions (inflow oxidizer temperature, convective mach number. . . ).
- 3D turbulent numerical simulations.
- Turbulent kinetic energy budget.
- Scalar turbulent transport.