Investigation of the effects of body forces on flame-turbulence interactions in turbulent premixed combustion

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Introduction: Motivation

- Ducted turbulent premixed flames → subjected to external pressure gradients
- Considerable difference in density between unburned reactants and burned products → Buoyancy is expected influence flame characteristics
- Last well-known DNS study → Veynante and Poinsot[1] → 2D, emphasis was on scalar flux
- Application: Industrial combustors under low turbulence intensities, large fires/explosions

[1] D. Veynante and T. Poinsot, J. Fluid Mech., vol. 353, pp. 83-114, 1997

Introduction: Objectives

- Investigate the effects of body force on evolutions of:
  - *Vorticity and enstrophy*
  - *Turbulent kinetic energy*
  - *Flame Surface Density*
  - *Turbulent scalar flux*
- Modelling of unclosed terms in the context of RANS (not covered)
- Modification of existing models, wherever necessary (not covered)

Mathematical Background

- Momentum equation under the action of a body force:

$$\frac{\partial(\rho u_i)}{\partial t} + \frac{\partial(\rho u_i u_j)}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \boldsymbol{S_i} + \frac{\partial \tau_{ij}}{\partial x_j}$$

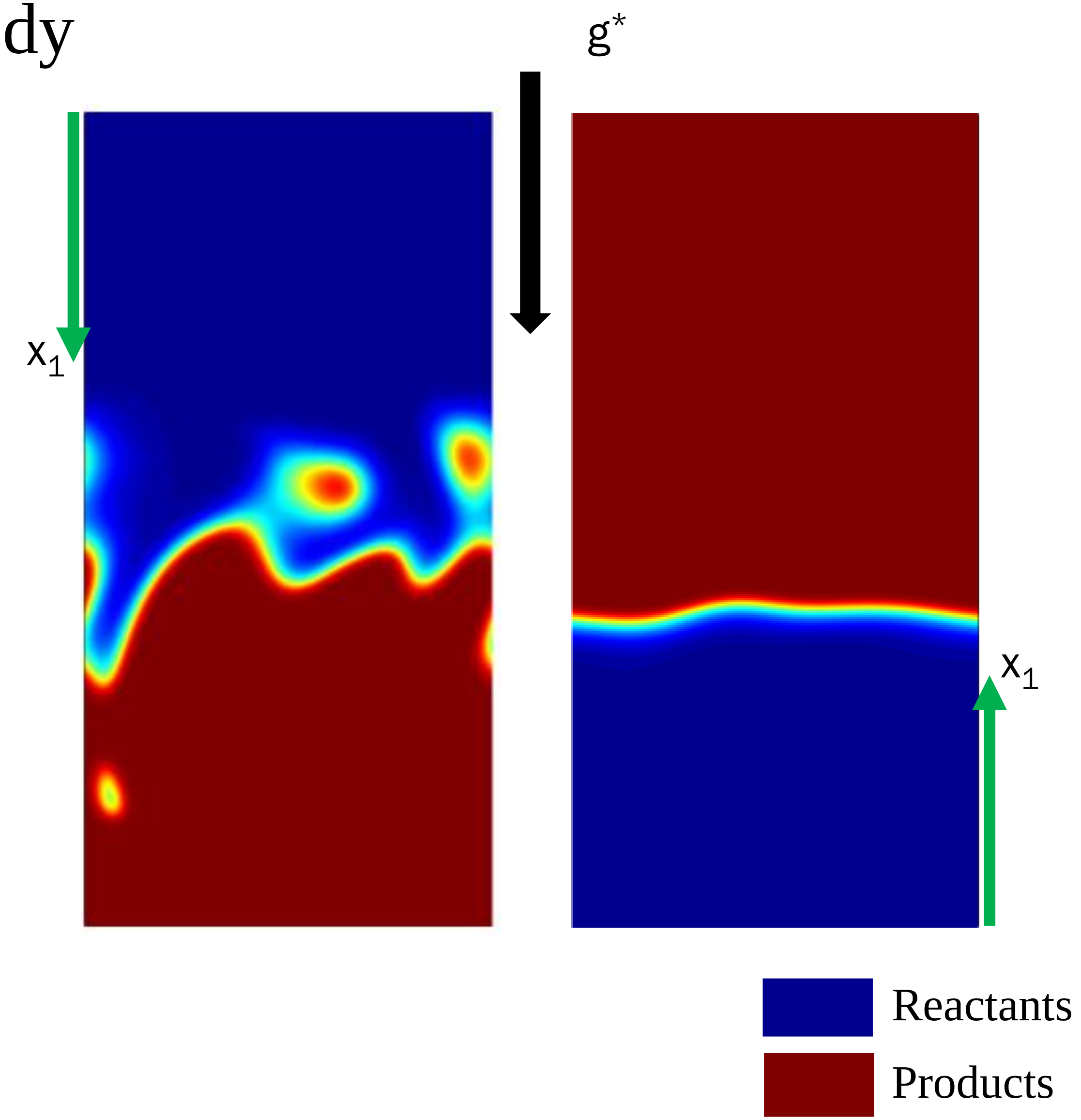
$S_i = \rho\Gamma_i$ is the source/sink term in the i^{th} direction

$$\boldsymbol{S_1 = \rho\Gamma_1 = \frac{\rho g^* S_L^2}{\delta_Z}}$$

g^* represents inverse of Froude number-squared ($g^* = Fr^{-2}$)

δ_Z is the Zel'dovich flame thickness

- Positive g^* → Unstable stratification
- Negative g^* → Stable stratification



Mathematical Background

- Progress variable c

$$c = (Y_P - Y_{P0})/(Y_{P\infty} - Y_{P0})$$

Y_P - suitable product mass fraction

- Transport equation of Favre averaged progress variable $\tilde{c}$:

$$\frac{\partial(\bar{\rho}\tilde{c})}{\partial t} + \frac{\partial(\bar{\rho}\tilde{c}\tilde{u}_j)}{\partial x_j} = \overline{\frac{\partial}{\partial x_j}\left(\rho D \frac{\partial c}{\partial x_j}\right)} + \bar{\dot{w}} - \frac{\partial(\overline{\rho u_j'' c''})}{\partial x_j}$$

Beyond the scope of this presentation

Negligible in statistically planar flames in the context of RANS

Usually expressed in terms of the generalized FSD[1]
$\bar{\dot{w}} = \overline{(\rho S_d)}_s \Sigma_{gen}$

[1] M. Boger, D. Veynante, H. Boughanem, A. Trouvé, Proc. Combust. Inst. 27, pp. 917-925, 1998.

Mathematical Background

- Transport equation of vorticity ($\vec{\omega} = \nabla \times \vec{u}$):

$$\frac{\partial \omega_i}{\partial t} + u_k \frac{\partial \omega_i}{\partial x_k} = \underbrace{\omega_k \frac{\partial u_i}{\partial x_k}}_{t_{1i}} \underbrace{- \epsilon_{ijk} \frac{1}{\rho^2} \frac{\partial \rho}{\partial x_j} \frac{\partial \tau_{kl}}{\partial x_l}}_{t_{21i}} + \underbrace{\frac{\epsilon_{ijk}}{\rho} \frac{\partial^2 \tau_{kl}}{\partial x_j \partial x_l}}_{t_{22i}} \underbrace{- \omega_i \frac{\partial u_k}{\partial x_k}}_{t_{3i}} + \underbrace{\frac{\epsilon_{ijk}}{\rho^2} \frac{\partial \rho}{\partial x_j} \frac{\partial p}{\partial x_k}}_{t_{4i}}$$

t_{1i} - vortex stretching
t_{21i} - viscous torque term
t_{22i} - vorticity diffusion term
t_{3i} - dilatation term
t_{4i} - baroclinic effects

- Transport equation of enstrophy ($\Omega = \omega_i \omega_i / 2$):

$$\frac{\partial \overline{\Omega}}{\partial t} + \overline{u_k \frac{\partial \Omega}{\partial x_k}} = \underbrace{\overline{\omega_i \omega_k \frac{\partial u_i}{\partial x_k}}}_{T_I} \underbrace{\overline{- \epsilon_{ijk} \omega_i \frac{1}{\rho^2} \frac{\partial \rho}{\partial x_j} \frac{\partial \tau_{kl}}{\partial x_l}}}_{T_{II}} + \underbrace{\overline{\frac{\epsilon_{ijk} \omega_i}{\rho} \frac{\partial^2 \tau_{kl}}{\partial x_j \partial x_l}}}_{T_{III}} \underbrace{\overline{- 2 \frac{\partial u_k}{\partial x_k} \Omega}}_{T_{IV}} + \underbrace{\overline{\epsilon_{ijk} \frac{\omega_i}{\rho^2} \frac{\partial \rho}{\partial x_j} \frac{\partial p}{\partial x_k}}}_{T_V}$$

T_I - vortex stretching term
T_{II} - scalar product of vorticity and viscosity torque
T_{III} - viscous dissipation term
T_{IV} - dilatation rate term
T_V - baroclinic torque term

Mathematical Background

- Transport equation of turbulent kinetic energy:

$$\frac{\partial(\bar{p}\tilde{k})}{\partial t}+\frac{\partial(\bar{\rho}\tilde{u}_j\tilde{k})}{\partial x_j}=\underbrace{-\overline{\rho u_i''u_j''}\frac{\partial\tilde{u}_i}{\partial x_j}}_{K_1}\underbrace{-\overline{u_i''}\frac{\partial\bar{p}}{\partial x_i}}_{K_2}+\underbrace{\overline{p'\frac{\partial u_k''}{\partial x_k}}}_{K_3}+\underbrace{\overline{u_i''\frac{\partial\tau_{ij}}{\partial x_j}}}_{K_4}\underbrace{-\frac{\partial\overline{(p'u_i'')}}{\partial x_i}}_{K_5}\underbrace{-\frac{\partial}{\partial x_i}\left(\overline{\frac{1}{2}\rho u_i''u_k''u_k''}\right)}_{K_6}$$

K_1 - mean velocity gradient term
K_2 - mean pressure gradient term
K_3 - pressure dilatation term
K_4 - viscous dissipation term
K_5 - pressure transport term
K_6 - turbulent transport term

- Generalized FSD $\Sigma_{gen}=\overline{|\nabla c|}$

- Transport equation of generalized FSD:

$$\frac{\partial\Sigma_{gen}}{\partial t}+\frac{\partial(\tilde{u}_j\Sigma_{gen})}{\partial x_j}=\underbrace{-\partial\{[\overline{(u_k)_s}-\tilde{u}_k]\Sigma_{gen}\}/\partial x_k}_{T_1}+\underbrace{\overline{\left((\delta_{ij}-N_iN_j)\,\partial u_i/\partial x_j\right)_s}\Sigma_{gen}}_{T_2}\underbrace{-\partial[\overline{(S_dN_k)_s}\Sigma_{gen}]/\partial x_k}_{T_3}$$

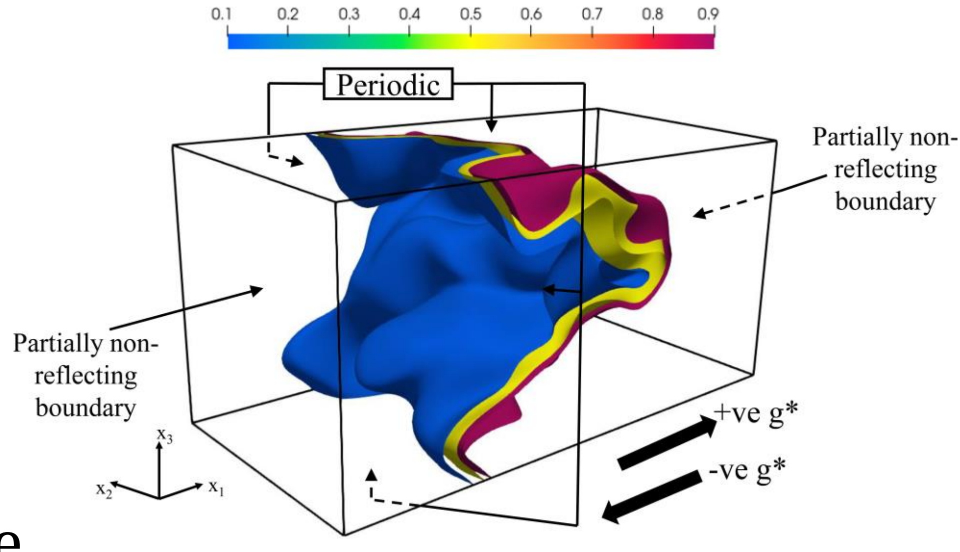
$$+\underbrace{\overline{(S_d\,\partial N_i/\partial x_i)_s}\Sigma_{gen}}_{T_4}$$

T_1 - turbulent transport term
T_2 - tangential strain rate term
T_3 - propagation term
T_4 - curvature term

Numerical Implementation

- 3D compressible DNS code SENGA+
- Boundary conditions – NSCBC technique[1]
- Turbulence field – pseudo spectral method of Rogallo[2], Batchelor-Townsend energy spectrum[3]
- u'/S_L values: 3.0, 5.0, 7.5, 10.0 → Decaying turbulence
- g^* values[4]: -3.12, -1.56, 0.0, 1.56, 3.12
- Total of 20 simulation cases

2000 Pa/m



u'/S_L	l_T/δ_{th}	Da	Ka	*Domain size*	*Grid size*
3.0	3.0	1.0	3.0	$70.2\delta_Z \times (35.1\delta_Z)^2$	$400 \times (200)^2$
5.0	3.0	0.6	6.45	$70.2\delta_Z \times (35.1\delta_Z)^2$	$400 \times (200)^2$
7.5	3.0	0.4	11.86	$70.2\delta_Z \times (35.1\delta_Z)^2$	$400 \times (200)^2$
10.0	3.0	0.3	18.26	$70.2\delta_Z \times (35.1\delta_Z)^2$	$400 \times (200)^2$

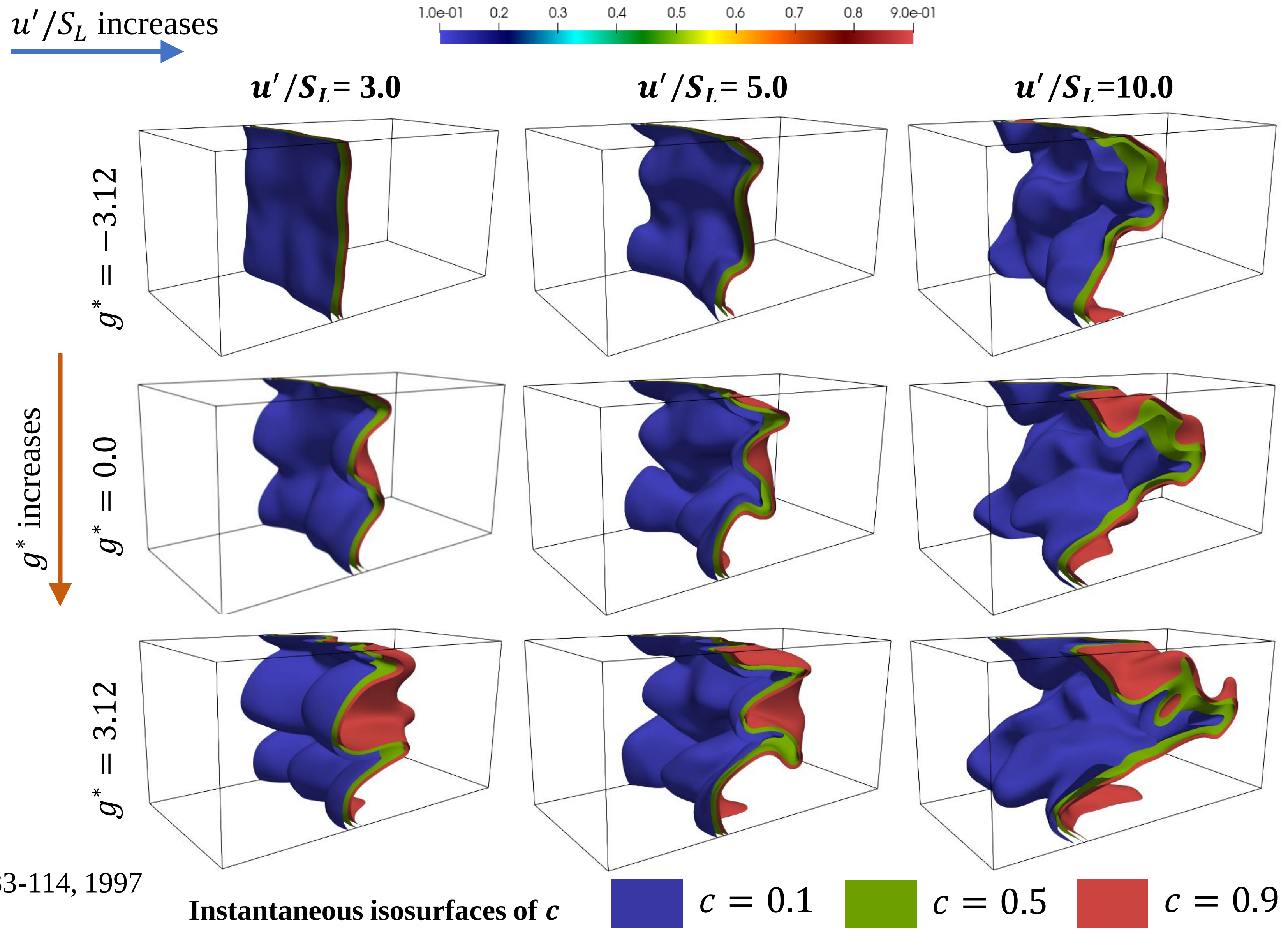
[1] T. Poinsot, S.K. Lele, J. Comp. Phys., 101, 104-129, 1992.
[2] R. S. Rogallo, NASA Technicla Memorandum 81315, NASA AMES Research Centre, California, 1981.
[3] G. K. Batchelor and A. Townsend, Proc. Roy. Soc. A, Volume 194, Issue 1039, London, 1948.
[4] Shepherd, I. G., Moss, J. B. & Bray, K. N. C., Proc. Combust. Inst, 19, 423-431, 1982.

Numerical Implementation

- Single-step Arrhenius type irreversible chemical reaction is considered
- Standard value of parameters:
  - *Unity Lewis number*
  - *Prandtl number Pr= 0.7*
  - *Zel'dovich number* β *= 6.0*
  - *Heat release parameter* $\tau = (T_{ad} - T_0)/T_0$ *= 4.5 (methane flames preheated to 415K)*
- Simulation time $\boldsymbol{t_s}$ **= 3.0**$\boldsymbol{t_e}$, where $\boldsymbol{t_e}$ is the initial eddy turnover time (greater than 2 chemical time scales for all cases, comparable to several previous studies)

Results: Isosurfaces of c

- Flame wrinkling ↑
  Flame brush thickness ↑ } g^* ↑
- Flame wrinkling ↑
  Flame brush thickness ↑ } u'/S_L ↑
- Consistent with previous findings of Veynante and Poinsot[1] and the theory of Libby[2]

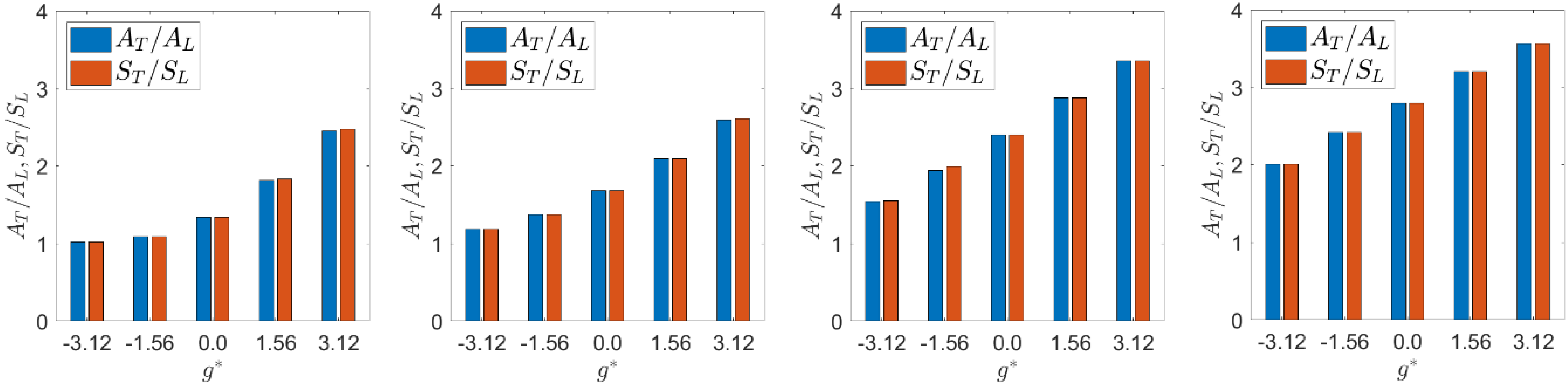


Instantaneous isosurfaces of c

[1] D. Veynante and T. Poinsot, J. Fluid Mech., vol. 353, pp. 83-114, 1997
[2] Libby, P.A., Combust. Sci. Tech. 68, 15–33, 1989

Results: Normalized flame surface area and turbulent flame speed

u'/S_L = 3.0 **u'/S_L = 5.0** **u'/S_L = 7.5** **u'/S_L = 10.0**



- $A_T/A_L \uparrow$ $S_T/S_L \uparrow$ → $g^* \uparrow$
- $A_T/A_L \uparrow$ $S_T/S_L \uparrow$ → $u'/S_L \uparrow$

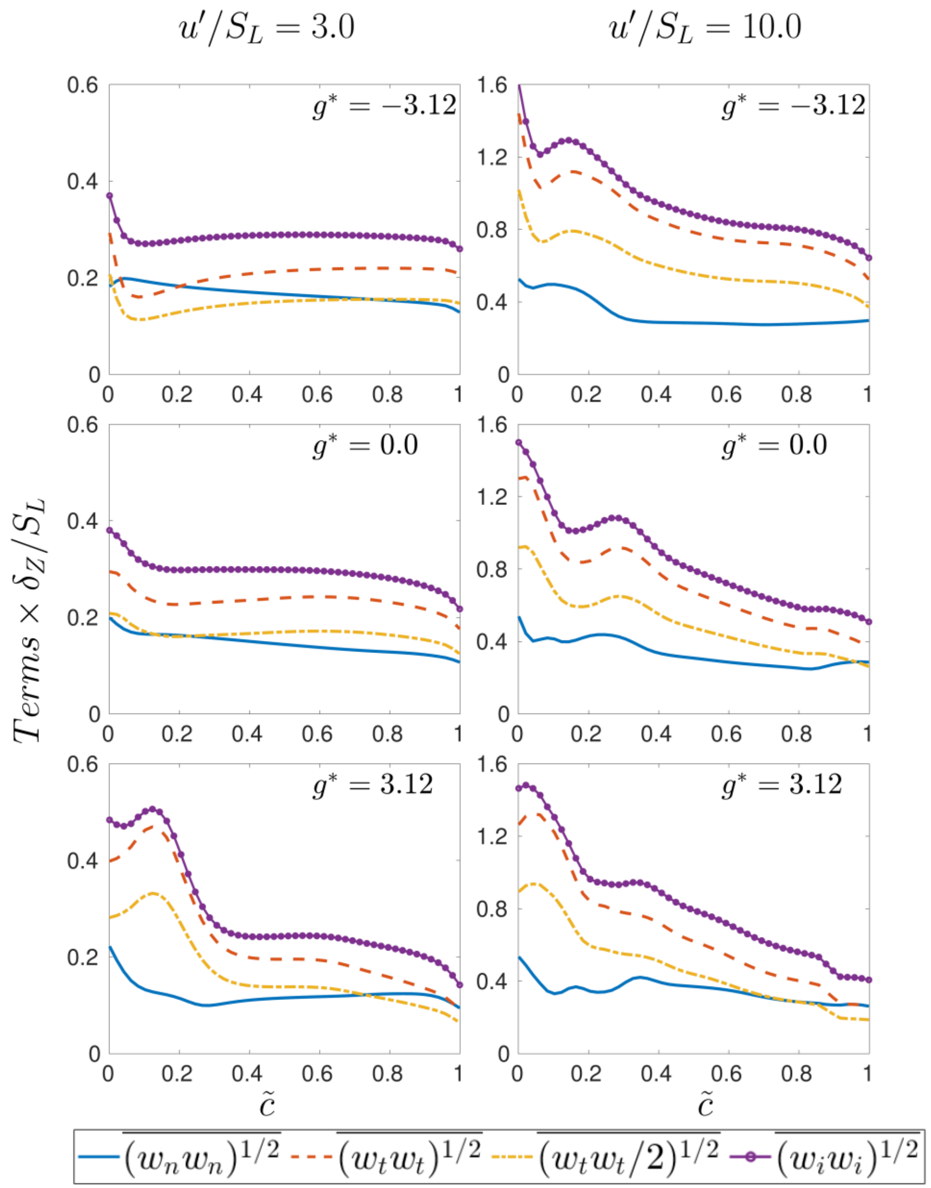
$$A_T = \int_V |\nabla c| \, dV = \int_V \Sigma_{gen} \, dV$$

$$S_T = \int_V \dot{w} \, dV / \rho_0 A_P$$

A_P is flame area projected in x_1 direction

Results: Vorticity evolution[1]

- Vorticity magnitude mostly decays from the unburned to burned gas side
- Tangential component first decays, but rises again for -g^* values at low turbulence intensities
- Localized augmentation of vorticity
- Anisotropic nature



[1]Varma, A. R., Ahmed, U., Chakraborty, N., Phys. Fluids 33, 035102 (2021).

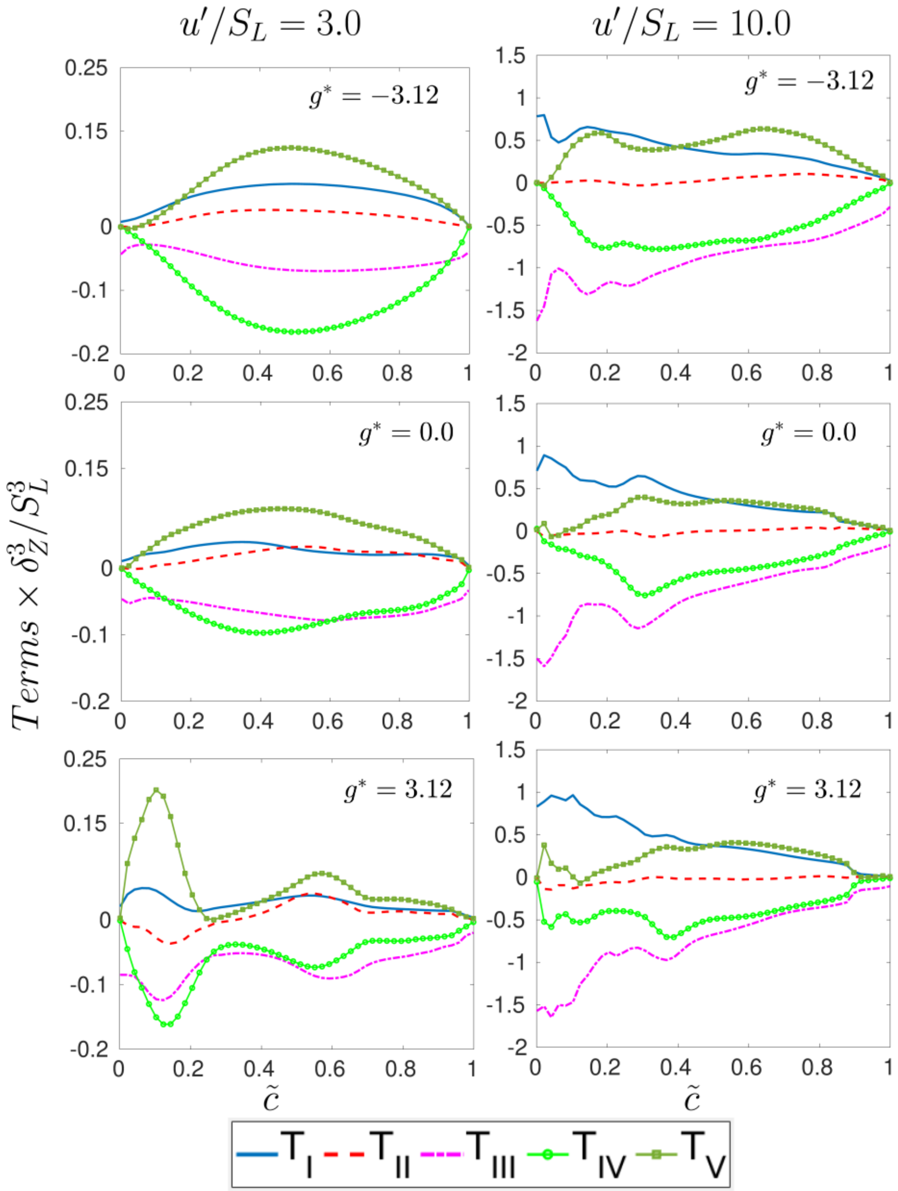
Results: Enstrophy budget[1]

$$\frac{\partial \overline{\Omega}}{\partial t} + \overline{u_k \frac{\partial \Omega}{\partial x_k}} = \underbrace{\overline{\omega_i \omega_k \frac{\partial u_i}{\partial x_k}}}_{T_I} \underbrace{- \overline{\epsilon_{ijk} \omega_i \frac{1}{\rho^2} \frac{\partial \rho}{\partial x_j} \frac{\partial \tau_{kl}}{\partial x_l}}}_{T_{II}} + \underbrace{\overline{\frac{\epsilon_{ijk} \omega_i}{\rho} \frac{\partial^2 \tau_{kl}}{\partial x_j \partial x_l}}}_{T_{III}} \underbrace{-2 \overline{\frac{\partial u_k}{\partial x_k} \Omega}}_{T_{IV}} +$$

$$\underbrace{\overline{\epsilon_{ijk} \frac{\omega_i}{\rho^2} \frac{\partial \rho}{\partial x_j} \frac{\partial p}{\partial x_k}}}_{T_V}$$

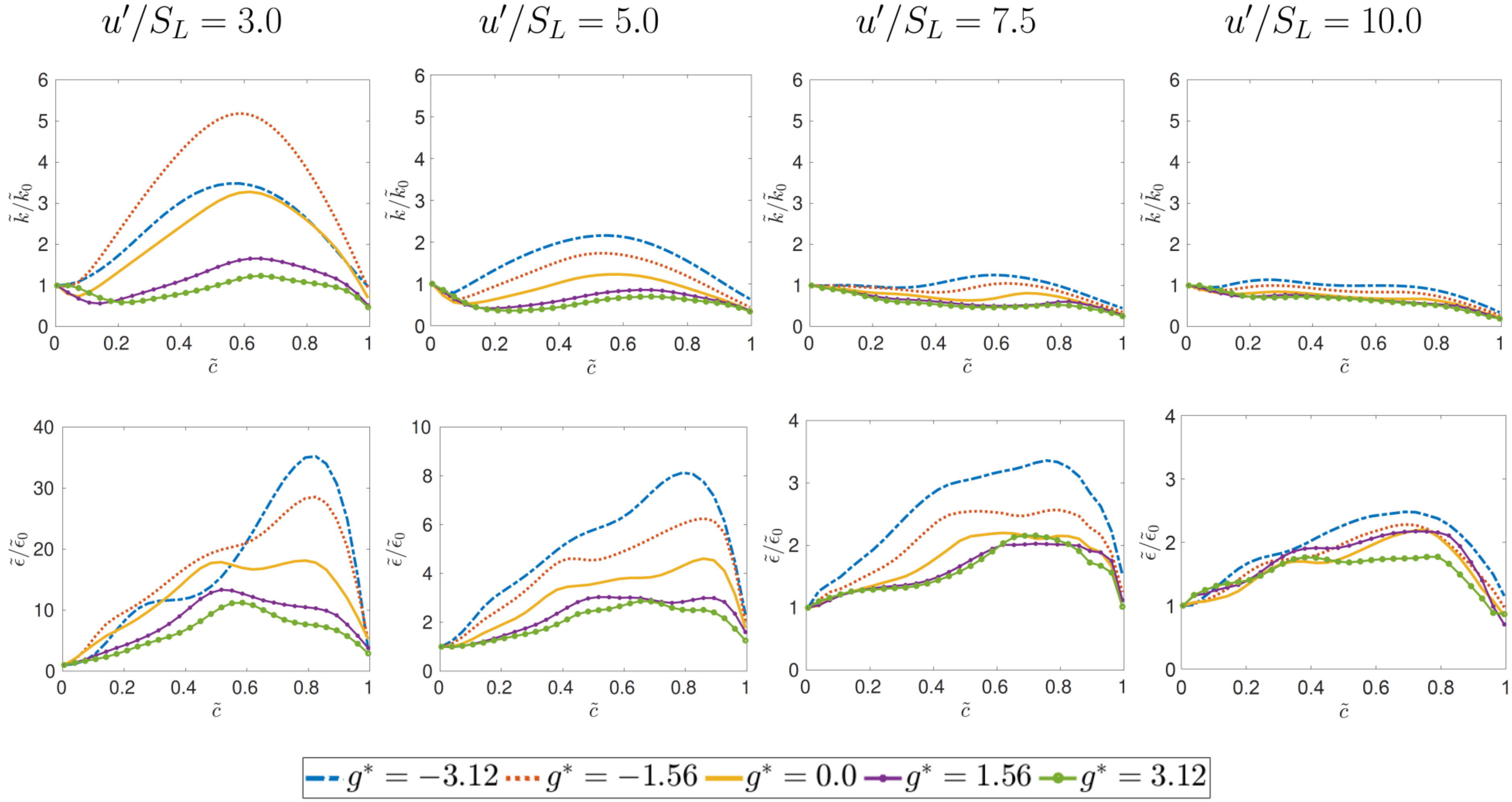
T_I - vortex stretching term
T_{II} - scalar product of vorticity and viscosity torque
T_{III} - viscous dissipation term
T_{IV} - dilatation rate term
T_V - baroclinic torque term

- Main source term - T_I, main sink term - T_{III}
- T_{IV} and T_V remain significant for all cases
- T_{IV} and T_V more important for the low turbulence intensities



[1]Varma, A. R., Ahmed, U., Chakraborty, N., Phys. Fluids 33, 035102 (2021).

Results: Kinetic Energy evolution



- Variations of both normalised kinetic energy and the normalised dissipation rate are affected by magnitude and direction of g^*

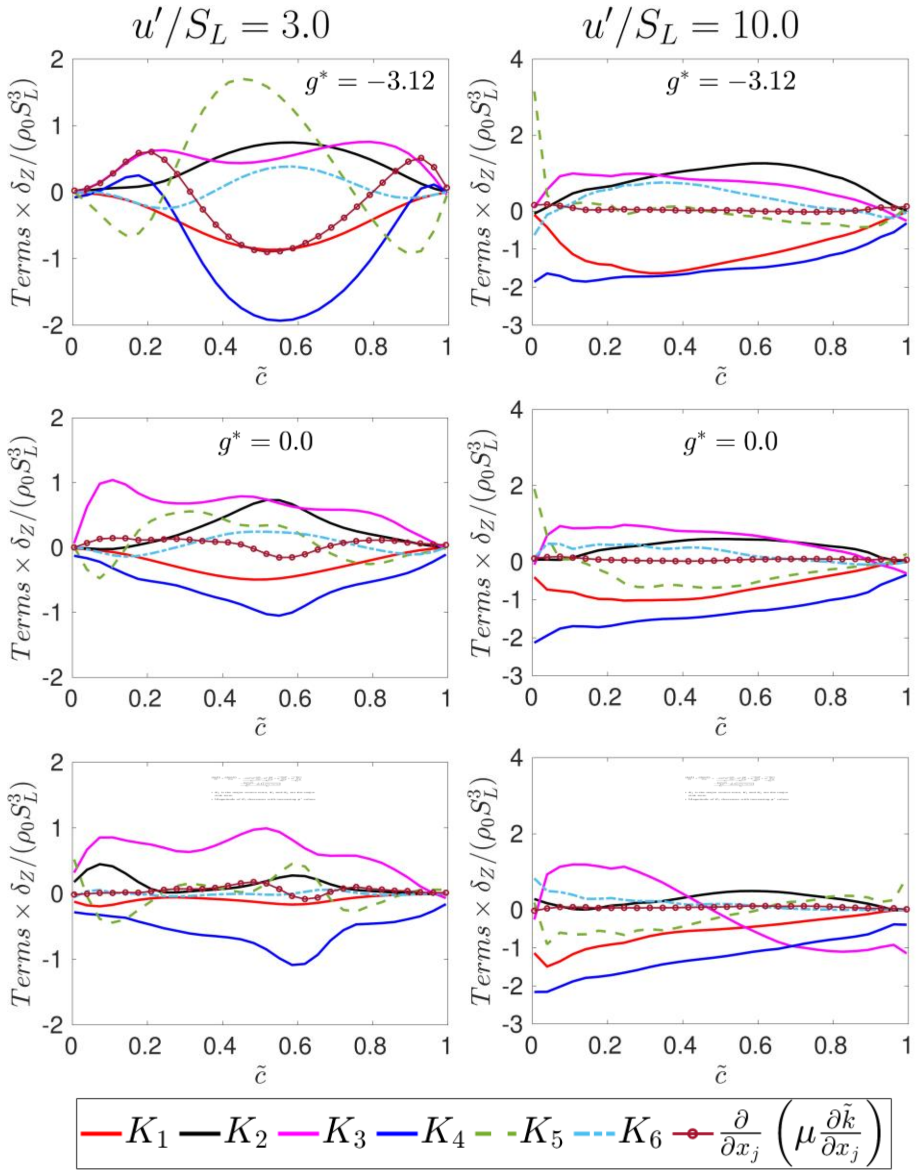
Results: Kinetic Energy budget

$$\underbrace{\frac{\partial(\bar{\rho}\tilde{k})}{\partial t}+\frac{\partial(\bar{\rho}\tilde{u}_j\tilde{k})}{\partial x_j}}\; = \underbrace{-\overline{\rho u_i'' u_j''}\frac{\partial \tilde{u}_i}{\partial x_j}}_{K_1}\underbrace{-\overline{u_i''}\frac{\partial \bar{p}}{\partial x_i}}_{K_2}+\underbrace{\overline{p'\frac{\partial u_k''}{\partial x_k}}}_{K_3}+\underbrace{\overline{u_i''\frac{\partial \tau_{ij}}{\partial x_j}}}_{K_4}$$

$$\underbrace{-\frac{\partial\overline{(p'u_i'')}}{\partial x_i}}_{K_5}\underbrace{-\frac{\partial}{\partial x_i}\left(\overline{\frac{1}{2}\rho u_i'' u_k'' u_k''}\right)}_{K_6}$$

K_1 - mean velocity gradient term
K_2 - mean pressure gradient term
K_3 - pressure dilatation term
K_4 - viscous dissipation term
K_5 - pressure transport term
K_6 - turbulent transport term

- K_3 is the major source term, K_1 and K_6 are the major sink term
- Magnitude of K_1 decreases with increasing g^* values



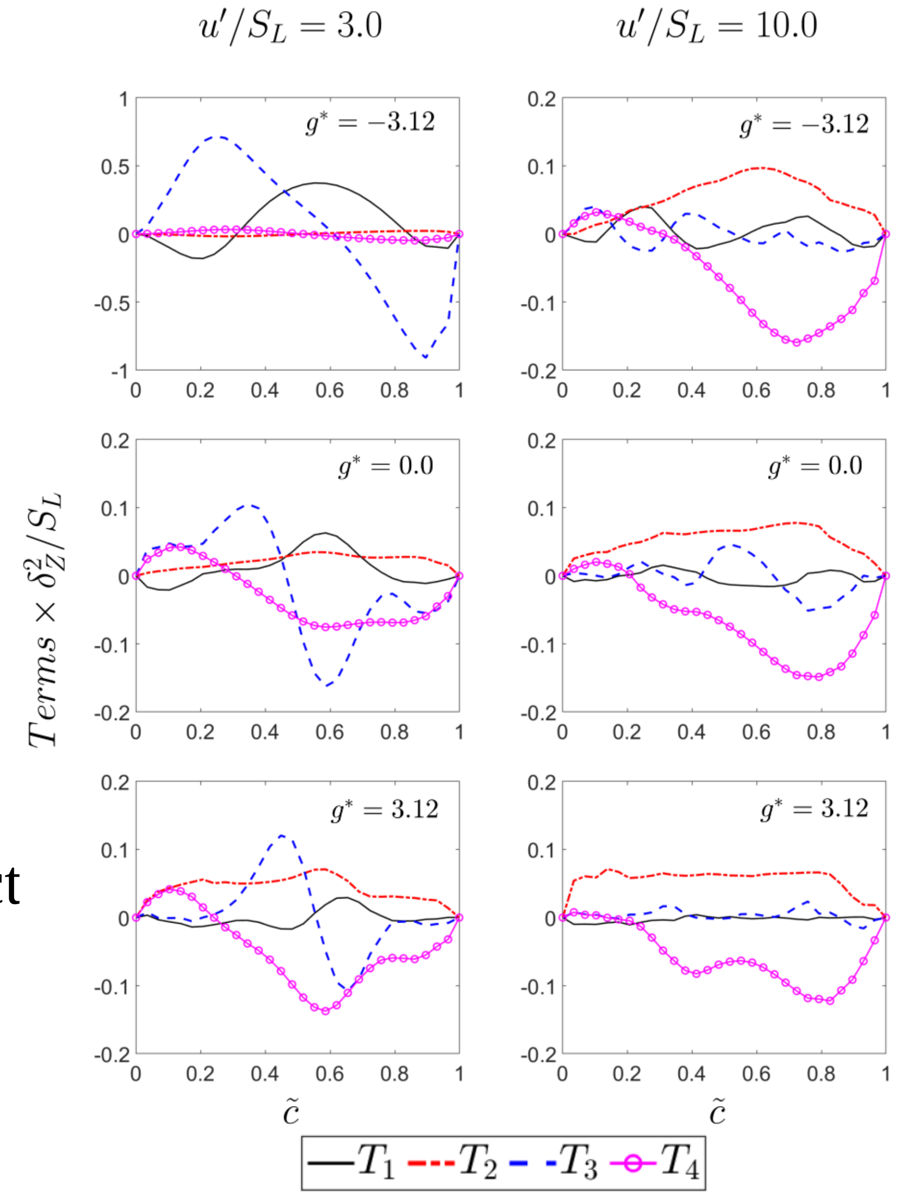
Results: FSD budget

$$\frac{\partial \Sigma_{gen}}{\partial t} + \frac{\partial(\tilde{u}_j \Sigma_{gen})}{\partial x_j} = \underbrace{-\partial\{[\overline{(u_k)_s} - \tilde{u}_k]\Sigma_{gen}\}/\partial x_k}_{T_1} + \underbrace{\overline{\left((\delta_{ij} - N_i N_j)\,\partial u_i/\partial x_j\right)_s}\,\Sigma_{gen}}_{T_2}$$

$$\underbrace{-\partial\left[\overline{(S_d N_k)_s}\Sigma_{gen}\right]/\partial x_k}_{T_3} + \underbrace{\overline{(S_d\,\partial N_i/\partial x_i)_s}\Sigma_{gen}}_{T_4}$$

T_1 - turbulent transport term
T_2 - tangential strain rate term
T_3 - propagation term
T_4 - curvature term

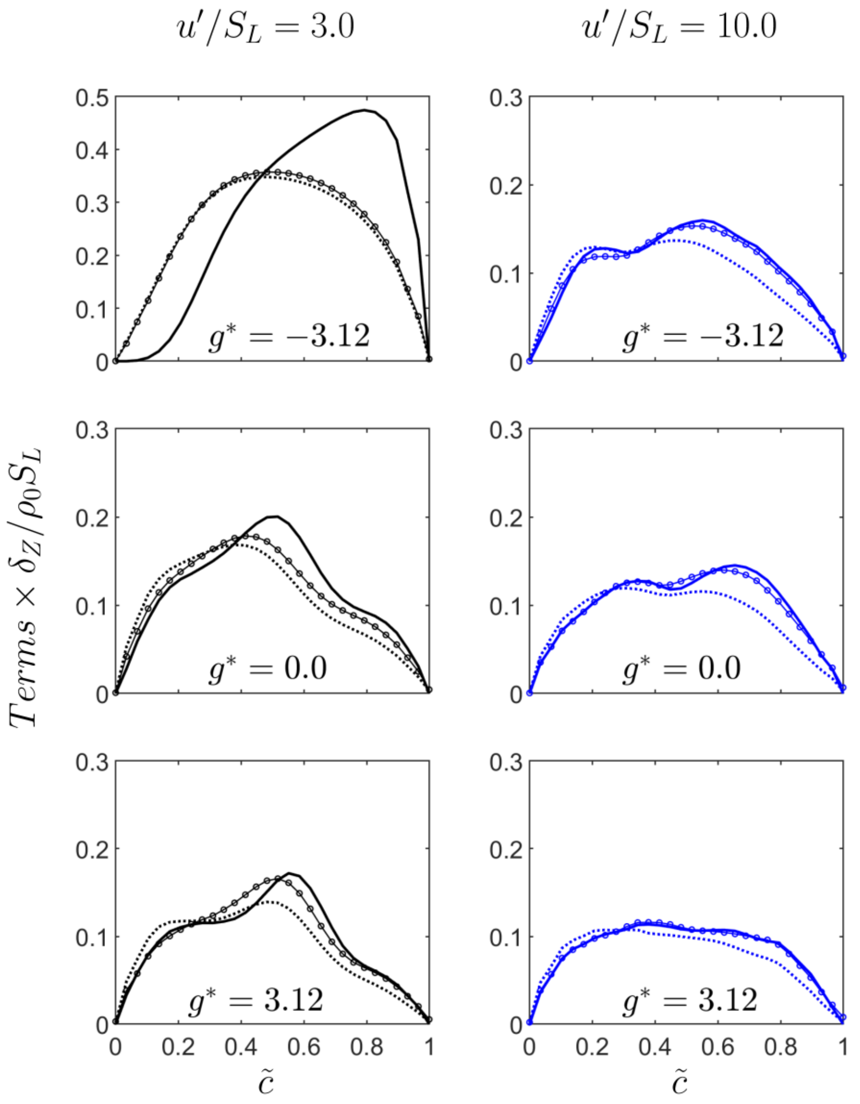
- T_2 acts as a source term in all cases, magnitude increases as g^* and u'/S_L increase
- T_3 is positive towards reactant side, negative towards product side, magnitude decreases as g^* and u'/S_L increase
- T_4 acts as a sink term over the majority of the flame brush



Results: Reaction rate closure

$$\bar{\dot{w}} + \overline{\nabla.(\rho D \nabla c)} = \overline{(\rho S_d)}_s \Sigma_{gen} \text{ [1]}$$

- RANS, $\bar{\dot{w}} \gg \overline{\nabla.(\rho D \nabla c)} \rightarrow \bar{\dot{w}} = \overline{(\rho S_d)}_s \Sigma_{gen}$
- Le = 1, $\overline{(\rho S_d)}_s = \rho_0 S_L$
- The molecular diffusion rate term is not negligible for low turbulence intensity cases



Solid line – $\bar{\dot{w}}$ from DNS Dotted line – $\rho_0 S_L \Sigma_{gen}$

Line with circles - $\left[\bar{\dot{w}} + \overline{\nabla.(\rho D \nabla c)}\right]$

[1] M. Boger, D. Veynante, H. Boughanem, A. Trouvé, Proc. Combust. Inst. 27, pp. 917-925, 1998.

Conclusions

- The effects of body force on the evolutions of vorticity and enstrophy, turbulent kinetic energy, turbulent scalar flux and FSD have been evaluated using a DNS database of three-dimensional statistically planar turbulent premixed flames using the decaying turbulence approach.
  - An unstable (stable) density stratification promotes (weakens) flame wrinkling
  - Vorticity distribution shows anisotropic behaviour due to influence of baroclinic torque
  - Kinetic energy, its dissipation rate and the terms of the kinetic energy transport equation are affected by g^*
  - Contribution of the molecular diffusion rate cannot be ignored for $-g^*$ values, low turbulence intensity cases when behaviour is similar to a laminar flame

Work in progress/Future work

- Effects of g^* on terms of the kinetic energy transport equation and the scalar flux transport equation and their modelling in the context of RANS

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