LES Approaches to combustion

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LES Approaches to Combustion

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SIG on Combustion Science, Technology and Applications, Imperial College London
28th September 2017

Turbulent Flows: DNS

Inert Flows

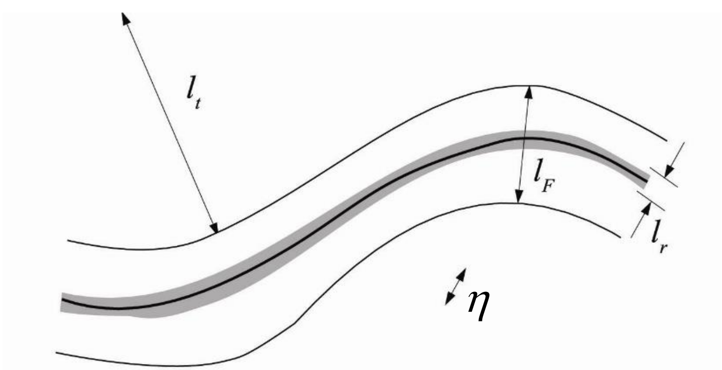
Resolve the smallest scales

Number of mesh points, $N_{xyx} \propto \mathrm{Re}^{\frac{9}{4}}$

Time step $\Delta t \propto \mathrm{Re}^{-\frac{3}{4}}$

$\Rightarrow$ CPU time $\propto \mathrm{Re}^{3}$

Combusting Flows



Many reactions of type $A + B \rightarrow C$

$$\dot{r}_A = -aT^n \exp\left(-\frac{E}{RT}\right)\rho \frac{Y_A Y_B}{W_B}$$

Pressure $\sim$ 1 bar, $\ell_r \sim 0.01$ mm

Pressure $\sim$ 40 bar, $\ell_r \sim 0.001$ mm

Modelling Approaches

Reynold/Favre Averaged Approaches (RANS)

- Quasi-steady and quasi-homogeneous assumptions
- 40-50 years research

Large Eddy Simulation (LES)

- Assumptions: scale separation, i.e. high turbulence Reynolds numbers
- Resolve large scale energy containing motions responsible for transport.
- Model fine scale dissipative motions / replace physical viscosity with sub-grid scale (sgs) viscosity.
- sgs viscosity provides mechanism for dissipation.
- Mean profiles, Reynolds stresses, turbulent kinetic energy etc. insensitive to sgs viscosity.

Large Eddy Simulation

Introduce a spatial filter:

$$\bar{\phi}(\mathbf{x},t) = \int_\Omega \phi(\mathbf{x}',t) G(\mathbf{x}-\mathbf{x}',\Delta) d^3\mathbf{x}'$$

$$\tilde{\phi}(\mathbf{x},t) = \int_\Omega \frac{\rho(\mathbf{x}',t)}{\bar{\rho}(\mathbf{x},t)} \phi(\mathbf{x}',t) G(\mathbf{x}-\mathbf{x}',\Delta) d^3\mathbf{x}'$$

where $\int G(\mathbf{x}-\mathbf{x}',\Delta) d^3\mathbf{x}' = 1$; $G(\mathbf{x}-\mathbf{x}',\Delta) \geq 0$

Generalised moments: $\overline{\varphi\psi} - \bar{\varphi}\bar{\psi},\ \overline{\varphi^2} - \bar{\varphi}^2,\ \overline{u_i u_j} - \bar{u}_i \bar{u}_j$ etc.

The filter width is given by: $\Delta = (\Delta x \Delta y \Delta z)^{1/3}$

Filtered Equations

Continuity

$$\frac{\partial \bar{\rho}}{\partial t} + \frac{\partial \bar{\rho}\tilde{u}_i}{\partial x_i} = 0$$

Momentum

$$\frac{\partial \bar{\rho}\tilde{u}_i}{\partial t} + \frac{\partial \bar{\rho}\tilde{u}_i\tilde{u}_j}{\partial x_j} = -\frac{\partial \bar{p}}{\partial x_i} + \frac{\partial}{\partial x_j}\mu\left(\frac{\partial \tilde{u}_i}{\partial x_j} + \frac{\partial \tilde{u}_j}{\partial x_i} - \frac{2}{3}\frac{\partial \tilde{u}_k}{\partial x_k}\delta_{ij}\right) - \frac{\partial \tau_{ij}^{sgs}}{\partial x_j} + \bar{\rho} g_i$$

Scalars

$$\frac{\partial \bar{\rho}\tilde{\phi}_\alpha}{\partial t} + \frac{\partial \bar{\rho}\tilde{u}_j\tilde{\phi}_\alpha}{\partial x_j} = \frac{\partial}{\partial x_j}\left[\bar{\rho} D \frac{\partial \tilde{\phi}_\alpha}{\partial x_j}\right] + \overline{\rho\dot{\omega}_\alpha(\boldsymbol{\phi}, T)} - \frac{\partial J_{\alpha,j}^{sgs}}{\partial x_j}$$

Closures are required for the sub-grid stress τ_{ij}^{sgs}, sub-grid flux $J_{\alpha,j}^{sgs}$ and the filtered rate of formation $\overline{\rho\dot{\omega}_\alpha(\boldsymbol{\phi}, T)}$ terms.

$\mu_{sgs} = \overline{\rho}\,(C_S\Delta)^2\,||\tilde{e}_{ij}||$ with C_S determined dynamically *i.e.* $C_S = C_S(\mathbf{x},t)$

LES: Justification

Large scale energy containing motions responsible for turbulent transport.

Energy transfer from large to small scales.

Energy Dissipation via viscosity at the smallest scales.

Energy dissipation rate and hence turbulent transport independent of viscosity and indeed the precise dissipation mechanism, (Kolmogorov).

LES

- resolve large scale energy containing motions responsible for transport.
- model fine scale dissipative motions / replace physical viscosity with sub-grid scale (sgs) viscosity.
- sgs viscosity provides mechanism for dissipation.
- mean profiles, Reynolds stresses, turbulent kinetic energy etc insensitive to sgs viscosity

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Numerical Requirements

Discretisation:-

- **Spatial Derivatives**

  Convection terms: the use of 'dissipation free' schemes is desirable if excessive CPU times/memory are to be avoided.

  $\Rightarrow$ at least second order accurate central differences. Asymmetric approximation such as QUICK and upwind schemes are too diffusive!

  Diffusion and Pressure gradient Terms: Second order accurate central approximations yield reasonable results.

- **Time**

  At least second order accurate: Crank-Nicholson, Adams-Bashforth 3-step Runge-Kutta and three-point backward difference approximations have all been used to good effect.

Solution Methods

- If Δ is linked to the mesh spacing then the solution will not be 'smooth' on the mesh $\Rightarrow$ high frequency 'noise'

Numerical Accuracy

Grid independence

- If Δ is linked to the mesh spacing then the only truly grid independent solution will be a DNS.
- Resolve 80-90% of turbulence energy ⇒ mean quantities, Reynolds stresses etc independent of mesh size.

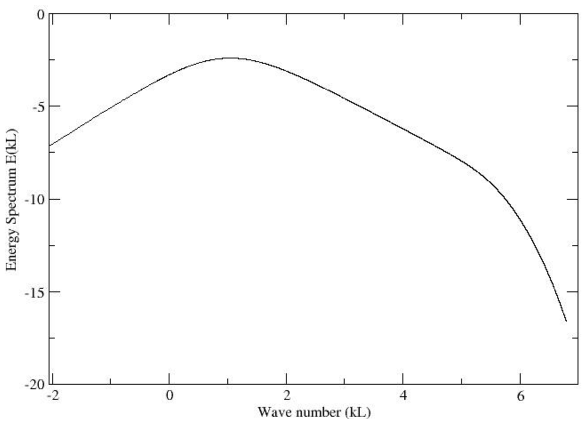
Mesh Quality Indicators??

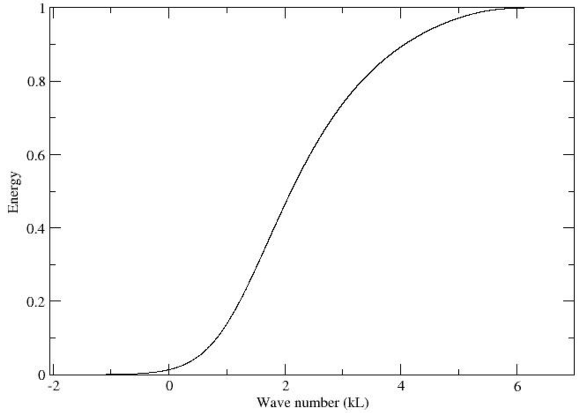
- There is no reliable single mesh accuracy indicator

Mesh size – 'a rule of thumb'

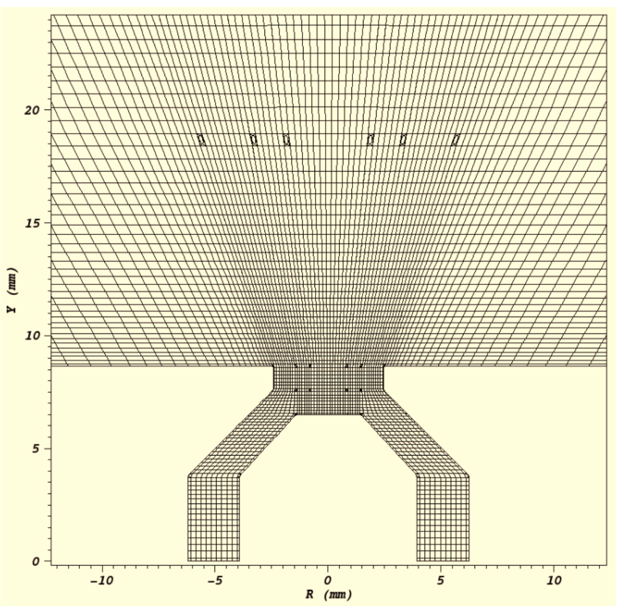
- Equal mesh spacing, *i.e*. $\Delta x \approx \Delta y \approx \Delta z$, expansion ratios close to unity; sufficiently fine to resolve mean motion

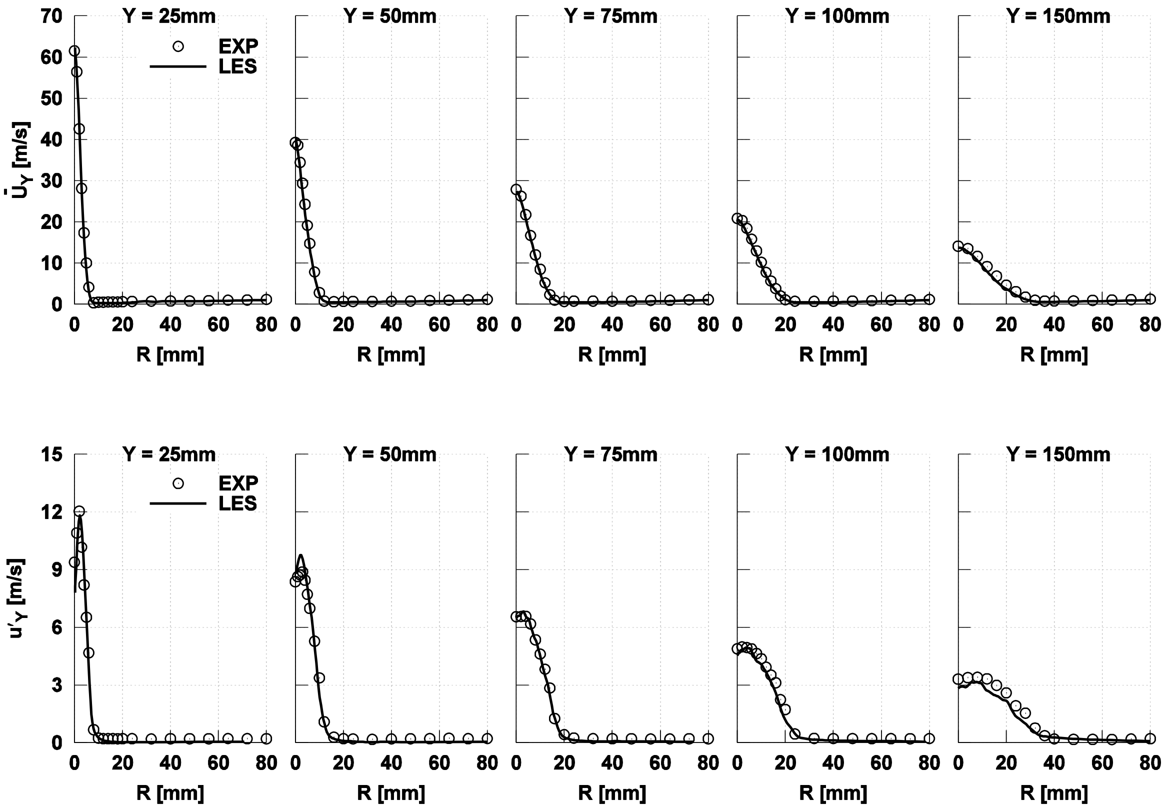
Energy Spectrum





LES of an isothermal Jet





Combustion LES: Approaches

Turbulent transport, e.g. Reynolds stresses, turbulence kinetic energy, scalar fluxes etc., is likely to remain insensitive to the sgs eddy viscosity.

Combustion will take place predominantly within the sub-grid scales. Thus sgs combustion models are likely to exert a more important influence in the LES of turbulent flames.

Approaches:

One/two Scalar Descriptions

Non-premixed Flames

- Conserved scalar/unstrained flamelets/CMC.

Premixed Flames

- Thin flame approach (flame approximated as a propagating ‘material’ surface). Models: flame surface density, level set methods (‘G’ equation), scalar dissipation.

Partially Premixed/Stratified Flames

- Thickened Flame Model, FGM, FSD, Scalar Dissipation,CMC, unsteady flamelets
- Sub-grid scale or Filtered joint scalar pdf transport equation method.

Non-Premixed Combustion

Conserved Scalar Formalism

Assumptions:

- High Reynolds Number
- Adiabatic Flame
- ‘Fast’ Reaction

Mixture Fraction

- Normalized element mass fraction

$$\xi \equiv \frac{Z_\alpha - Z_{\alpha,1}}{Z_{\alpha,2} - Z_{\alpha,1}} \quad \text{air stream}: \ \xi = 0, \quad \text{fuel stream}: \ \xi = 1$$

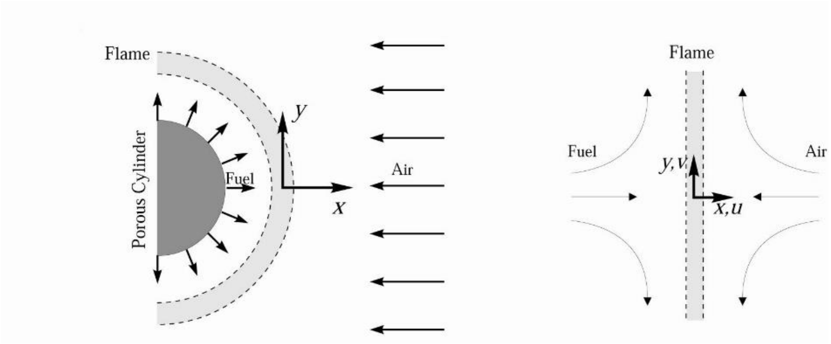
- ξ is a strictly conserved quantity

$$\frac{\partial \tilde{\xi}}{\partial t} + \bar{\rho}\tilde{u}_j \frac{\partial \tilde{\xi}}{\partial x_j} = \frac{\partial}{\partial x_j}\left\{\left(\frac{\mu}{\sigma} + \frac{\mu_{sgs}}{\sigma_{sgs}}\right)\frac{\partial \tilde{\xi}}{\partial x_j}\right\}$$

Laminar Flamelet Computations

Laminar Flamelets

- Flame Thickness < Kolmogorov length Scale
- Instantaneous Dependence of Composition, Density and Temperature on mixture fraction and some measure of Flame Stretch is the same as that prevailing in a laminar flame



$$T = T(\xi, \dot{s});\;\; Y_\alpha = Y_\alpha(\xi, \dot{s});\;\; \rho = \rho(\xi, \dot{s})$$

A simple model: select a single flamelet at a specified value of $\xi = \dot{s}_R$

e.g. $T = T(\xi, \dot{s}_R) \equiv T(\xi)$ etc, where $\dot{s}_R \approx 15 s^{-1}$ (unstrained)

Turbulence-Chemistry Interactions

Probability Density Function

$$\tilde{\phi}(\mathbf{x}) = \int_0^1 \phi(\psi) P(\psi, \mathbf{x}) d\psi$$

Beta PDF

$$P(\psi; \mathbf{x}, t) = \psi^{r-1}(1-\psi)^{s-1} / \int \psi^{r-1}(1-\psi)^{s-1} d\psi$$

$$\text{where} \quad r = \tilde{\xi}\left(\frac{\tilde{\xi}(1-\tilde{\xi})}{\tilde{\xi}''^2} - 1\right) \; ; \; s = \frac{\tilde{\xi}(1-\tilde{\xi})}{\tilde{\xi}} r$$

$$\bar{\rho}\frac{\partial \tilde{\xi}''^2}{\partial t} + \bar{\rho}\tilde{u}_j \frac{\partial \tilde{\xi}''^2}{\partial x_j} = \frac{\partial}{\partial x_i}\left\{\left(\frac{\mu_{sgs}}{\sigma_{sgs}} + \frac{\mu}{\sigma}\right)\frac{\partial \tilde{\xi}''^2}{\partial x_i}\right\} - \frac{2\mu_{sgs}}{\sigma_{sgs}}\left(\frac{\partial \tilde{\xi}}{\partial x_i}\right)^2 - C_d \frac{\mu_{sgs}}{\Delta^2}\tilde{\xi}''^2$$

or

$$\tilde{\xi}''^2 = C\Delta^2\left(\frac{\partial \tilde{\xi}}{\partial x_i}\right)^2$$

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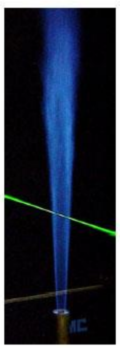
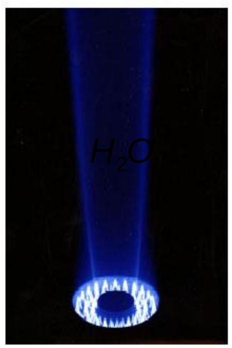
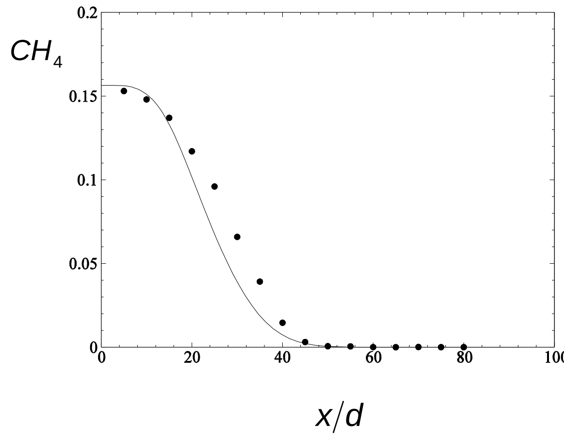
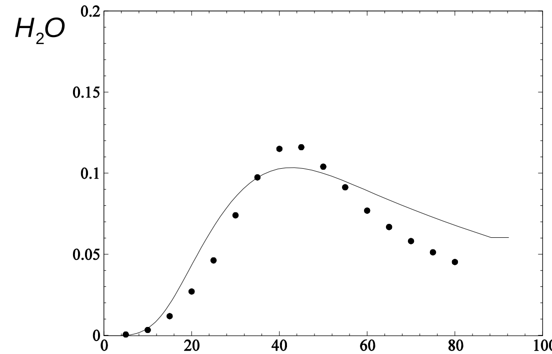
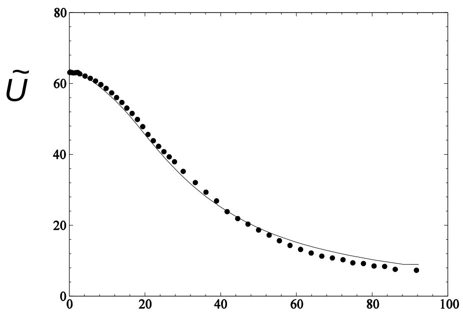
Piloted Turbulent Jet Flames

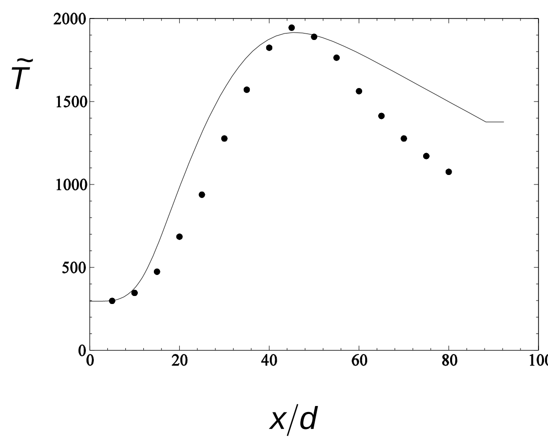


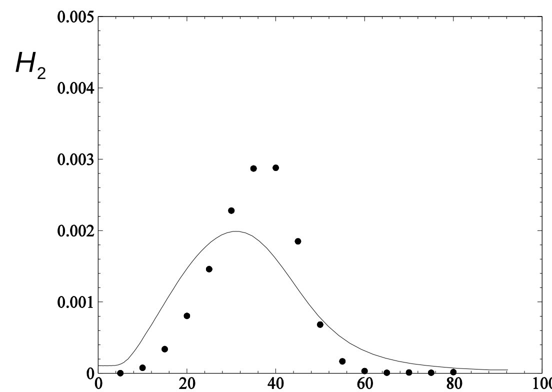


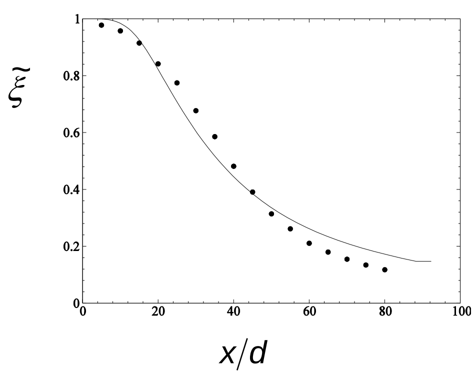






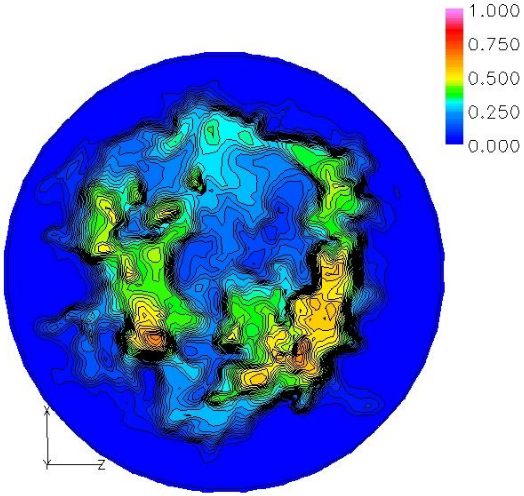




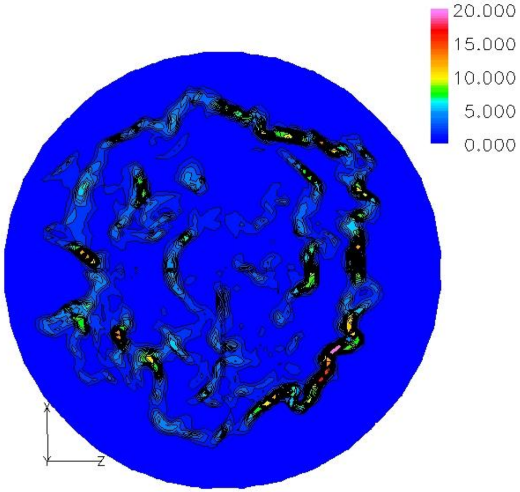


Local Extinction

- In RANs approaches the scalar dissipation,χ is often used to provide a measure of flame stretch.
- In LES the local value of χ and thus $P(\xi,\chi)$ is insufficient to describe extinction.



Instantaneous mixture fraction contours 20mm



Instantaneous mixture fraction dissipation rate 20mm

Premixed Flames: Parameters

	Length	Time
Energy containing motions:	ℓ	$\tau_t = \ell / U$
Kolmogorov scales:	$\tau_k = \left(\nu / \varepsilon \right)^{1/2}$	$\eta = \left(\nu^3 / \varepsilon \right)^{1/4}$
Chemical reaction scales:	$\ell_L^\circ = \nu / S_L^\circ$	$\tau_L^\circ = \ell_L^\circ / S_L^\circ$

where S_L° is the burning velocity of an unstrained laminar flame

Reynolds number: $$\mathrm{Re} = U\ell / \nu$$

Damköhler Number: $$D_A = \frac{\tau_t}{\tau_L^\circ} = \frac{\ell S_L^\circ}{U \ell_L^\circ}$$

Karlovitz Number: $$K_A = \frac{\tau_L^\circ}{\tau_k} = \mathrm{Re}^{1/2} / D_A$$

Premixed Flames

Define a reaction progress variable, e.g. $c = \dfrac{Y_{H_2O}(\mathbf{x},t)}{Y_{H_2O,burnt}}$

unburnt gas $c = 0$

burnt gas $c = 1$

$$\bar{\rho}\frac{\partial \tilde{c}}{\partial t} + \bar{\rho}\tilde{U}_i \frac{\partial \tilde{c}}{\partial x_i} = \frac{\partial}{\partial x_i}\left\{\left(\frac{\mu_t}{\sigma_t} + \frac{\mu}{\sigma}\right)\frac{\partial \tilde{c}}{\partial x_i}\right\} + \bar{\omega}(\mathbf{x},t)$$

View Flame as a propagating material surface – propagating at a speed equal to the local burning velocity, (Bray, Peters, Candel et al, Bradley et al and others)

$\bar{\omega}(\mathbf{x},t)$ *is obtained from either FSD, G-equation, Scalar Dissipation for which an additional equation is solved.*

Partially Premixed and Stratified Flames

At a minimum both the mixture fraction and reaction progress variable is required.

Reaction Progress Variable becomes:

$$c = \frac{Y(\mathbf{x},t)}{Y_b(\mathbf{x},t)} \text{ with } Y_b(\mathbf{x},t) = Y_b(\xi(\mathbf{x},t))$$

and $$\frac{\mathrm{d}c}{\mathrm{dt}} = \frac{\partial c}{\partial Y}\frac{\mathrm{d}Y}{\mathrm{dt}} + \frac{\partial c}{\partial \xi}\frac{\mathrm{d}\xi}{\mathrm{dt}}$$

Resulting equation complex; additional terms sometimes neglected.

A solution: solve equations for Y and $\xi \Rightarrow c(\mathbf{x},t)$

Reaction rate obtained as for premixed flames with additional assumptions, e.g. $P(c,\xi) = P(c)P(\xi)$

Finite Rate Chemistry Effects

- Fully coupled flow and chemical reaction required
- Detailed but reduced chemical mechanism required
- Currently available approaches:
  - Thickened Flame Model
  - CMC – with at least double conditioning
  - PDF transport equation methods
    - Lagrangian stochastic particles
    - Eulerian Stochastic fields

Combustion: Sub-Grid Pdf Equation Method

Fine grained pdf
$$F\left(\underline{\psi};\mathbf{x},t\right)=\prod_{\alpha=1}^{N_s}\delta\left(\psi_\alpha-\phi_\alpha\left(\mathbf{x},t\right)\right)$$

Sub-grid Pdf
$$\bar{\rho}\tilde{P}_{sgs}\left(\underline{\psi};\mathbf{x},t\right)=\int_\Omega \rho\left(\mathbf{x}',t\right)\mathrm{F}\left(\underline{\psi};\mathbf{x}',t\right)G(\mathbf{x}-\mathbf{x}';\Delta)\,dx'$$

The modelled sub-grid Pdf Equation

$$\bar{\rho}\frac{\partial\tilde{P}_{sgs}\left(\underline{\psi}\right)}{\partial t}+\bar{\rho}\tilde{u}_j\frac{\partial\tilde{P}_{sgs}\left(\underline{\psi}\right)}{\partial x_j}-\frac{\partial}{\partial x_j}\left(\frac{\mu}{\sigma}\frac{\partial\bar{P}_{sgs}\left(\underline{\psi}\right)}{\partial x_j}\right)+\sum_{\alpha=1}^{N}\frac{\partial\bar{\rho}\dot{\omega}_\alpha\left(\underline{\psi}\right)\tilde{P}_{sgs}\left(\underline{\psi}\right)}{\partial\psi_\alpha}$$
$$-\frac{\mu}{\sigma}\sum_{\alpha=1}^{N}\sum_{\beta=1}^{N}\frac{\partial\tilde{\varphi}_\alpha}{\partial x_i}\frac{\partial\tilde{\varphi}_\beta}{\partial x_i}\frac{\partial^2 P\left(\underline{\psi}\right)}{\partial\psi_\alpha\partial\psi_\beta}=\frac{\partial}{\partial x_i}\left(\frac{\mu_{sgs}}{\sigma_{sgs}}\frac{\partial\tilde{P}_{sgs}\left(\underline{\psi}\right)}{\partial x_i}\right)$$
$$-\frac{C_d}{\tau_{sgs}}\sum_{\alpha=1}^{N}\frac{\partial}{\partial\psi_\alpha}\left[\left(\psi_\alpha-\tilde{\phi}_\alpha\left(\mathbf{x},t\right)\right)\bar{\rho}\tilde{P}\left(\underline{\psi}\right)\right]$$

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Stochastic Field Solution Method

Represent *PDF* by *N* stochastic fields

Configuration field methods, M. Laso and H.C. Öttinger (1993); Stochastic Fields, Valino (1998), Sabel'nikov (2005)

Ito formulation

$\xi_\alpha^n(\mathbf{x},t)$ is advanced from t to $t+dt$ according to:

$$\bar{\rho}\, d\xi_\alpha^n = -\bar{\rho}\tilde{u}_i \frac{\partial \xi_\alpha^n}{\partial x_i} dt + \frac{\partial}{\partial x_i}\left[\left(\frac{\mu}{\sigma}+\frac{\mu_{sgs}}{\sigma_{sgs}}\right)\frac{\partial \xi_\alpha^n}{\partial x_i}\right] dt$$

$$+\left(2\bar{\rho}\frac{\mu_{sgs}}{\sigma_{sgs}}\right)^{1/2}\frac{\partial \xi_\alpha^n}{\partial x_i} dW_i^n(t) - 0.5 C_d \bar{\rho}\tau_{sgs}^{-1}\left(\xi_\alpha^n - \tilde{\phi}_\alpha^n\right)dt + \bar{\rho}\dot{\omega}_\alpha^n\left(\underline{\xi}^n\right)dt$$

where $1 \le n \le N$, $dW_i^n \approx \eta_i^n \sqrt{dt}$

and η_i^n is a $[-1,+1]$ dichotomic vector

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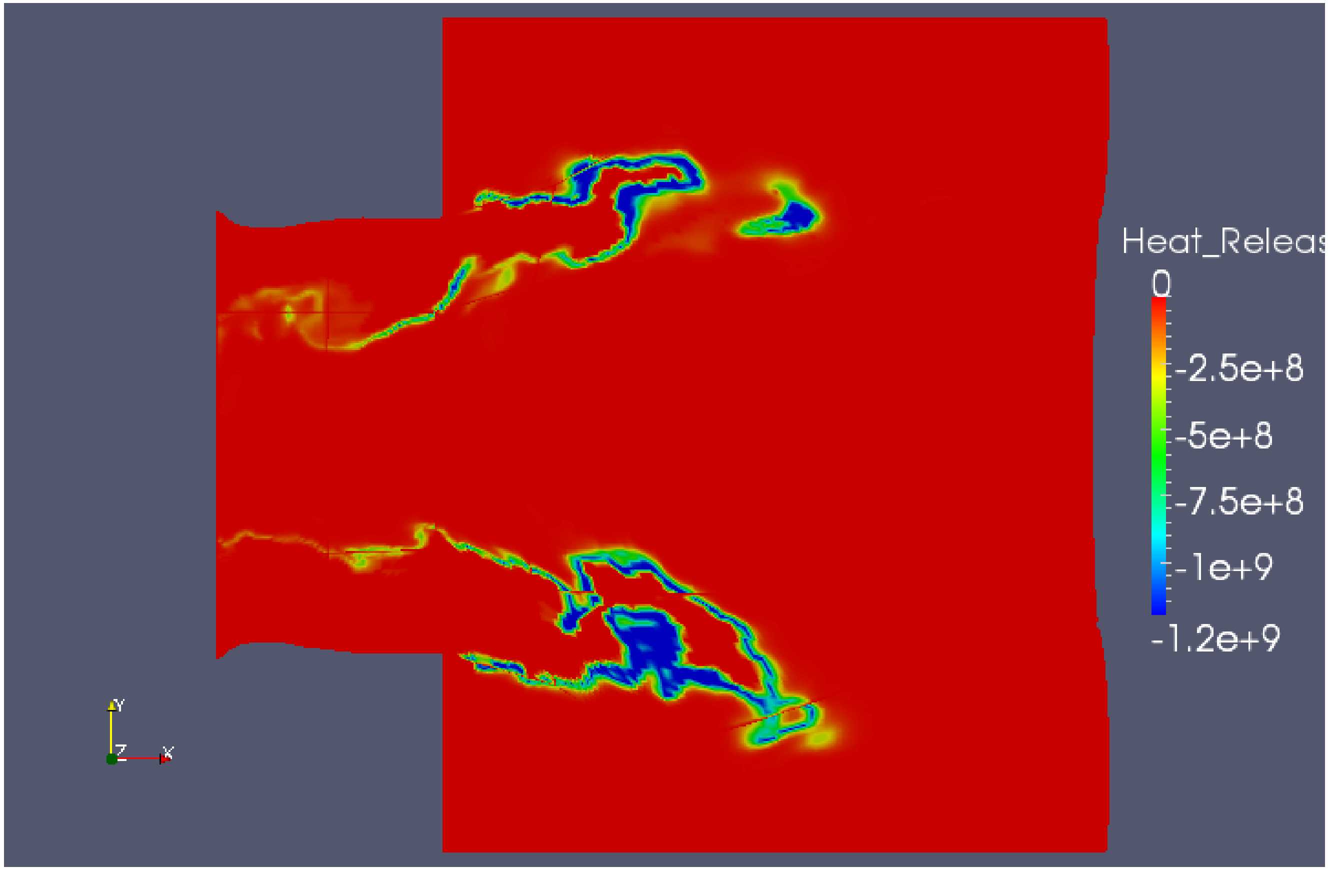
Pdf Equation/Stochastic Fields: Applications

Simulated Flames

- Auto-ignition – Hydrogen and n-heptane
- Lifted flames : Cabre - Hydrogen & methane
- Forced ignition: methane,
- Local extinction – Sandia Flames D, E & F
- Premixed swirl burner (Darmstadt)
- Darmstadt stratified flame
- Lean burn (natural gas) industrial combustor
- Premixed baffle stabilised flame
- Cambridge/Sandia stratified flames
- Methanol Spray flames
- Axisymmetric swirl combustor
- FAUGA Combustor,
- Sector combustor
- Genrig combustor

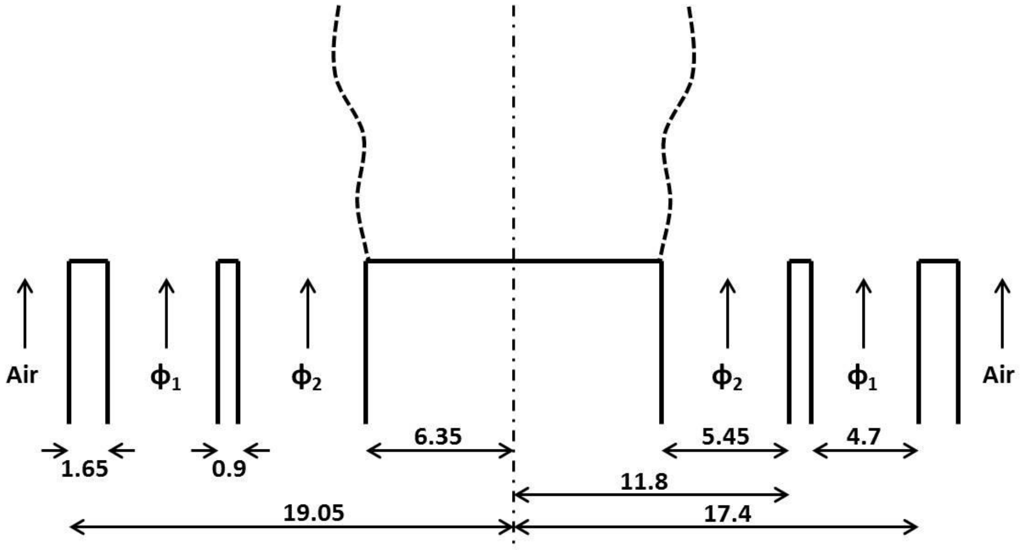
Kerosene spray

SGT100 Combustor: Snapshot of Heat Release Rate

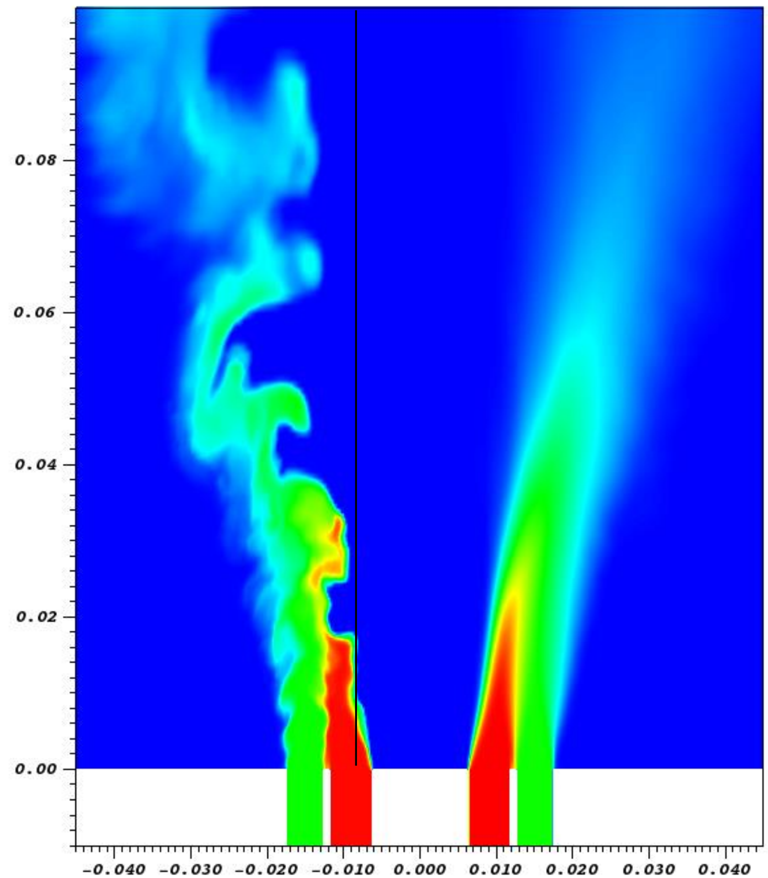


Stratified Premixed Turbulent Flames

- The Cambridge Stratified Swirl Burner



Ui (m/s)	Uo (m/s)	Uco (m/s)	Λ (mm)	Re_i	Re_o	ϕ_g
8.7	18.7	0.4	1.9	6000	11500	0.75



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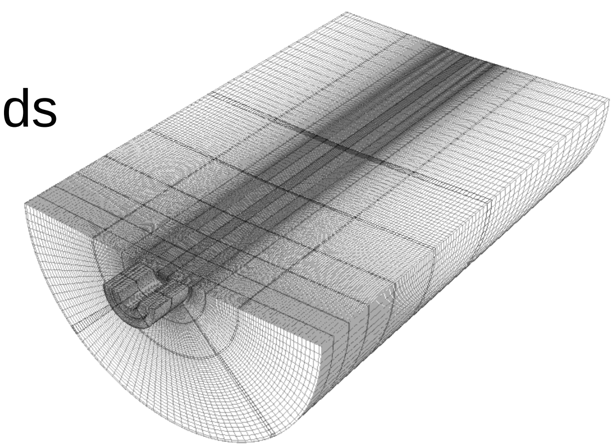
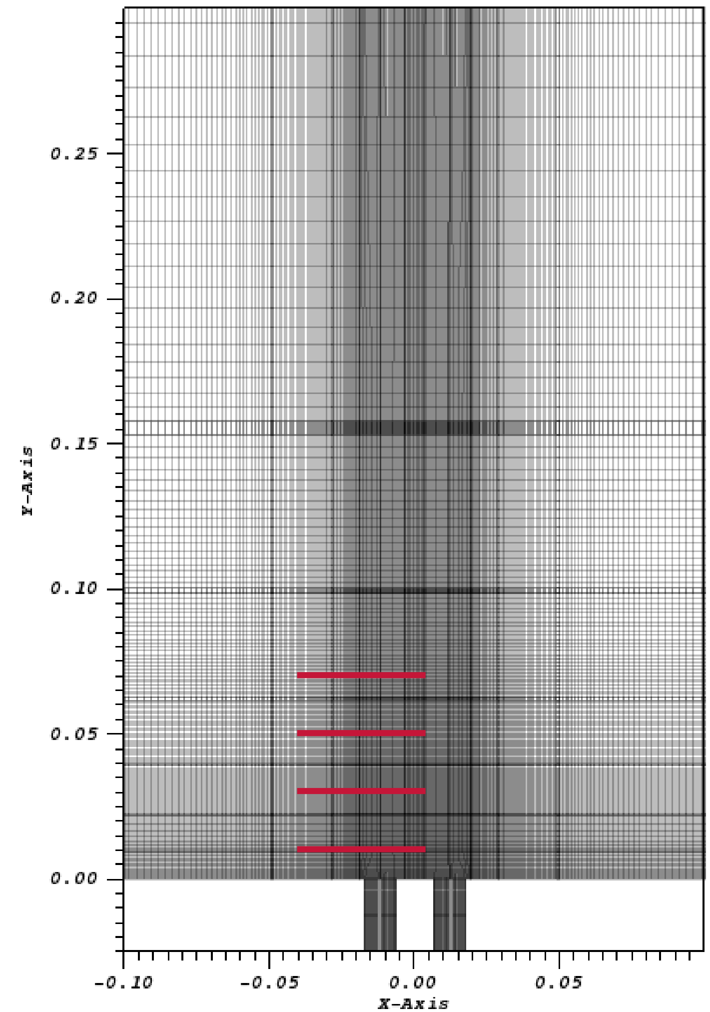
Computational Setup

- BOFFIN-LES
- 13.5M cells & 610 blocks
  3.7M cells & 163 blocks
  0.8M cells &   27 blocks
- Synthetic turbulence generation
- Dynamic Smagorinsky model
- Constant Prandtl/Schmidt number = 0.7
- Reduced GRI 3.0 with 19 species and 15 reactions
- 8 stochastic fields

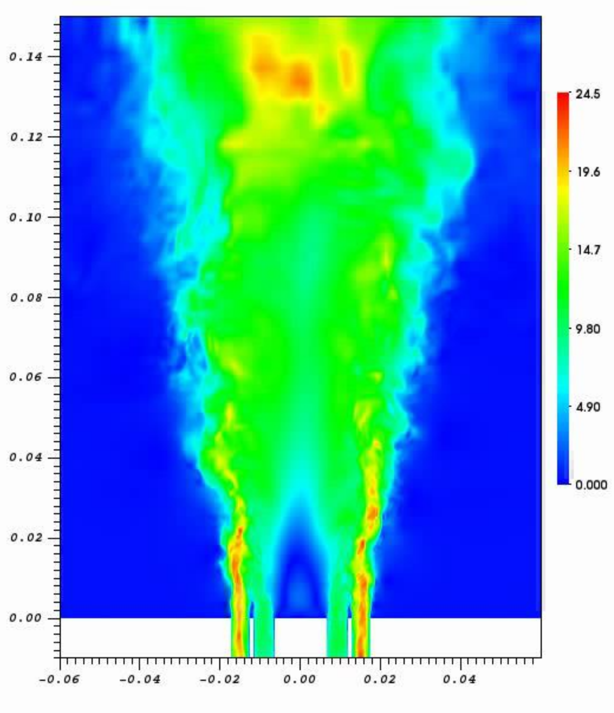




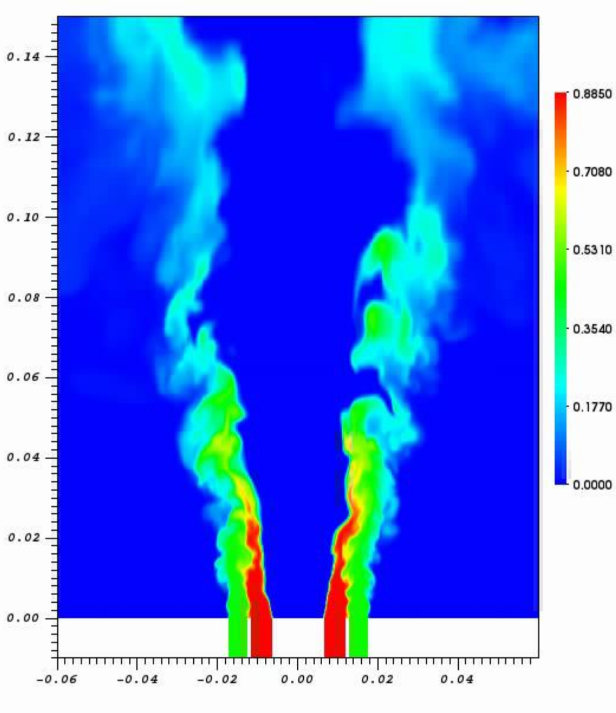
~ measurement locations

Results – SwB5

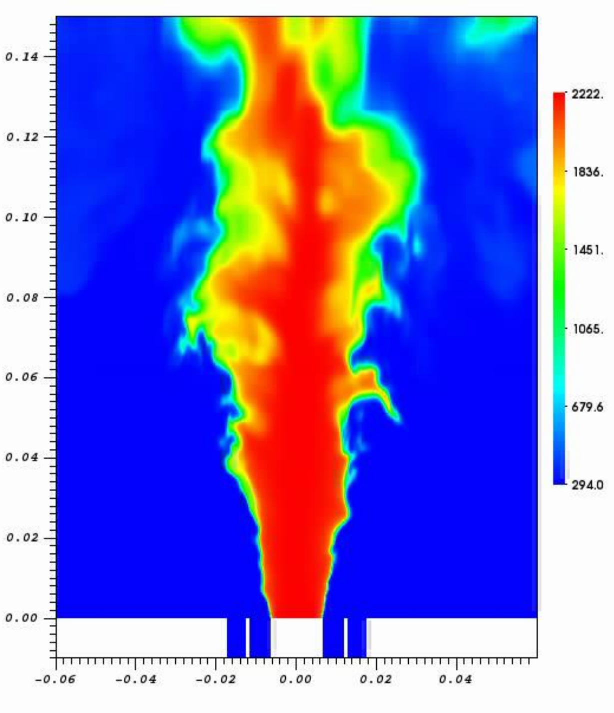
Velocity Magnitude



Methane

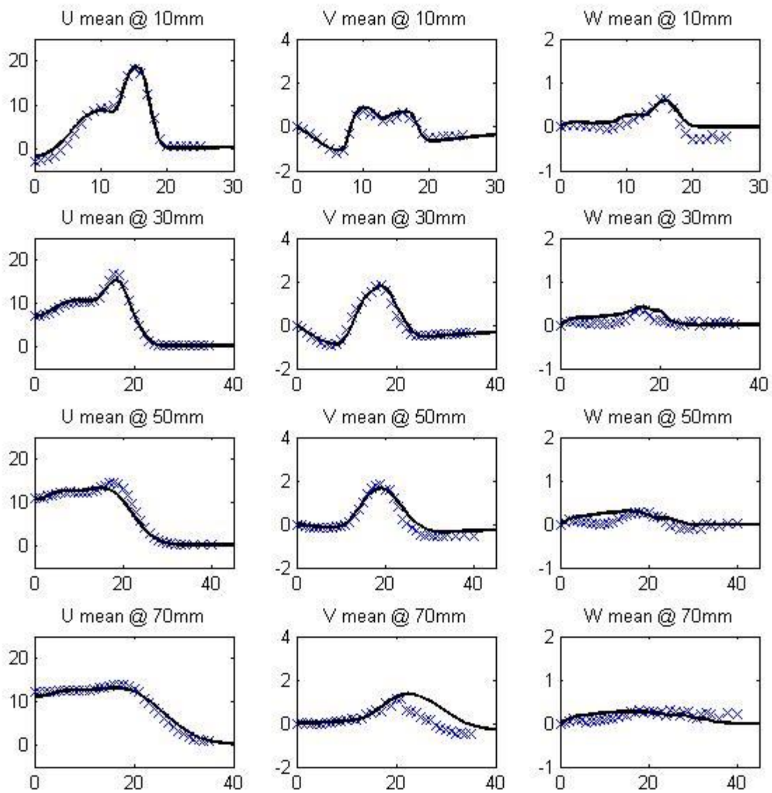


Temperature

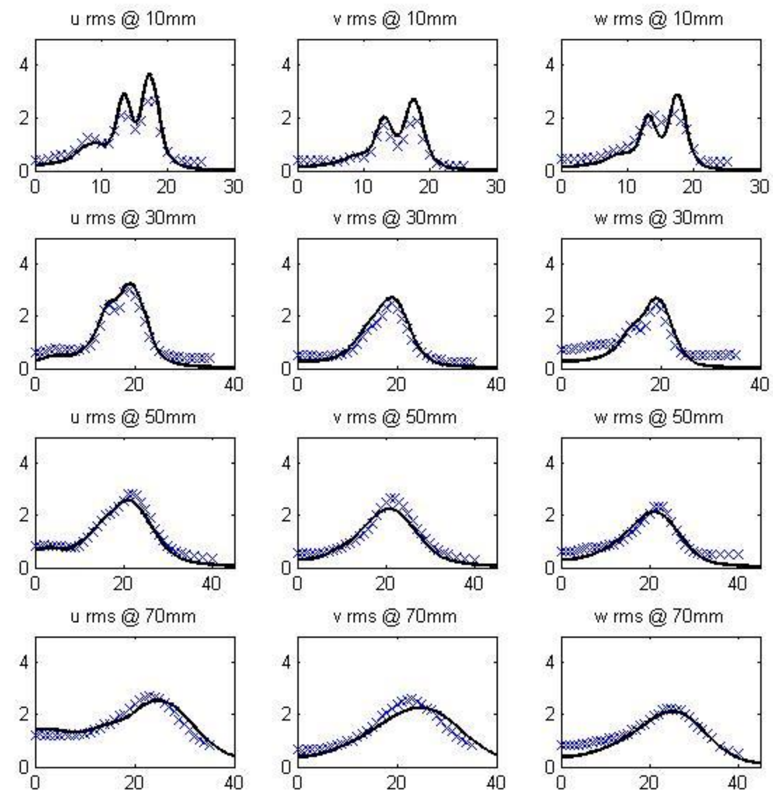


Results – SwB5 Velocities

Mean Velocities



RMS Velocities



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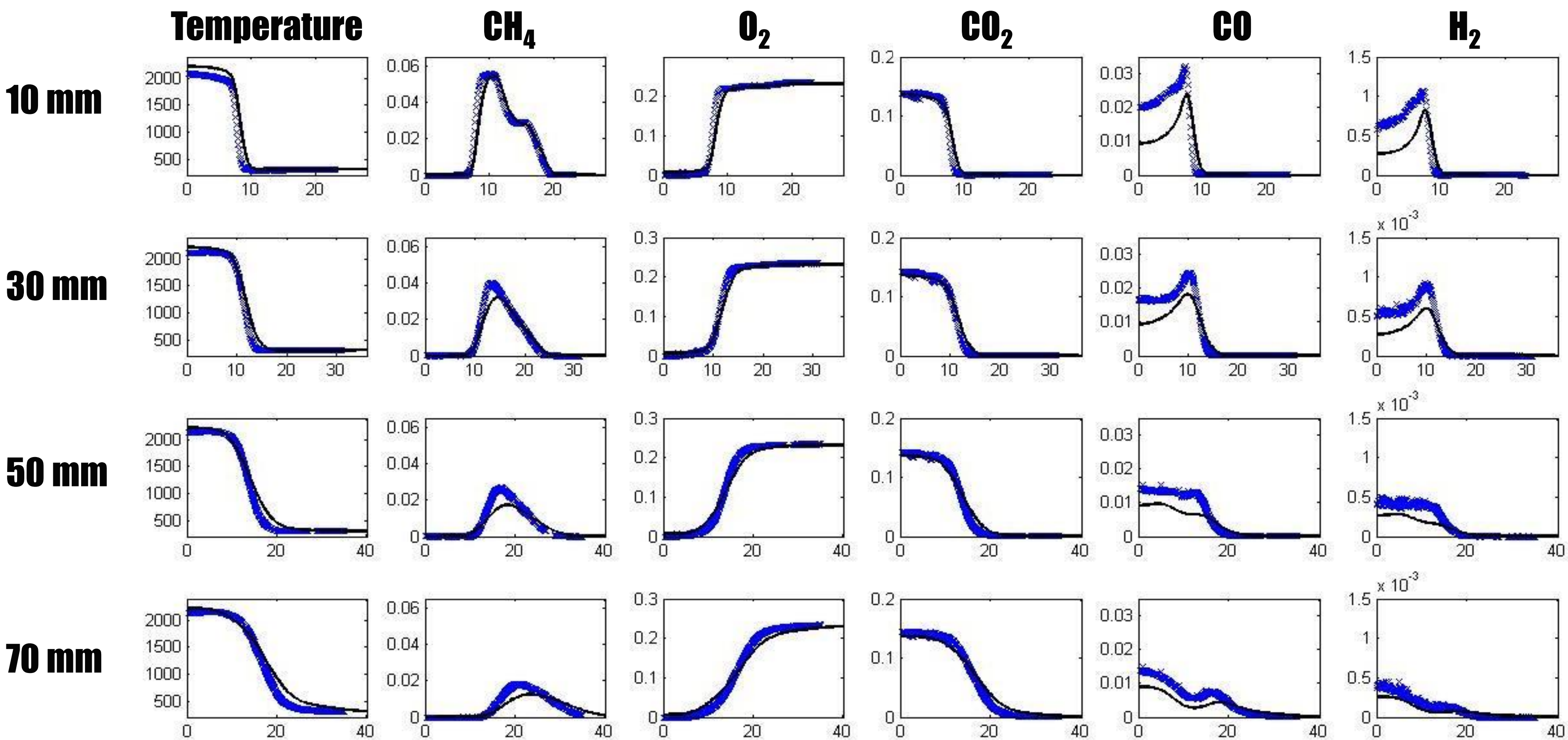
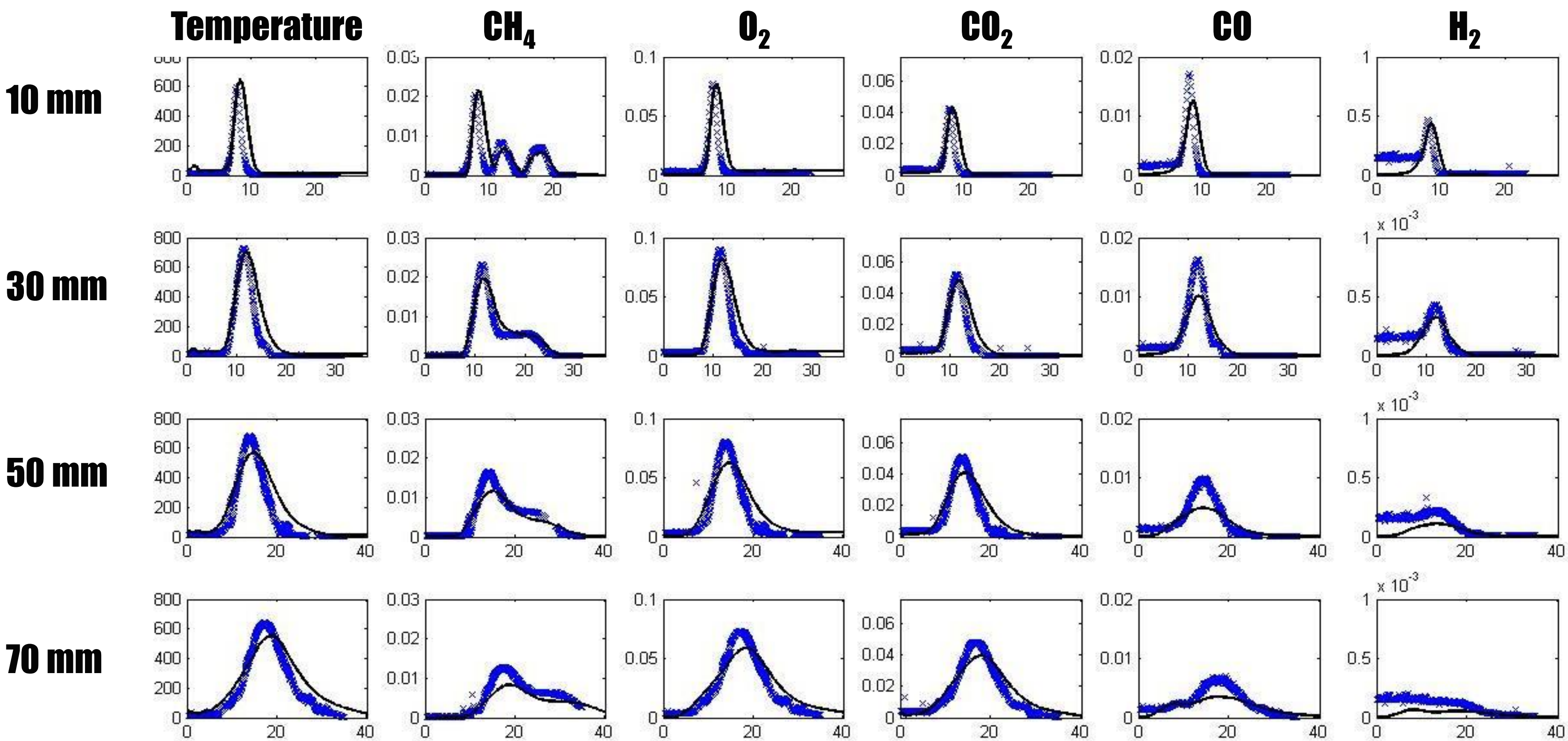
Results – SwB5 Scalars - Mean



Results – SwB5 Scalars - RMS



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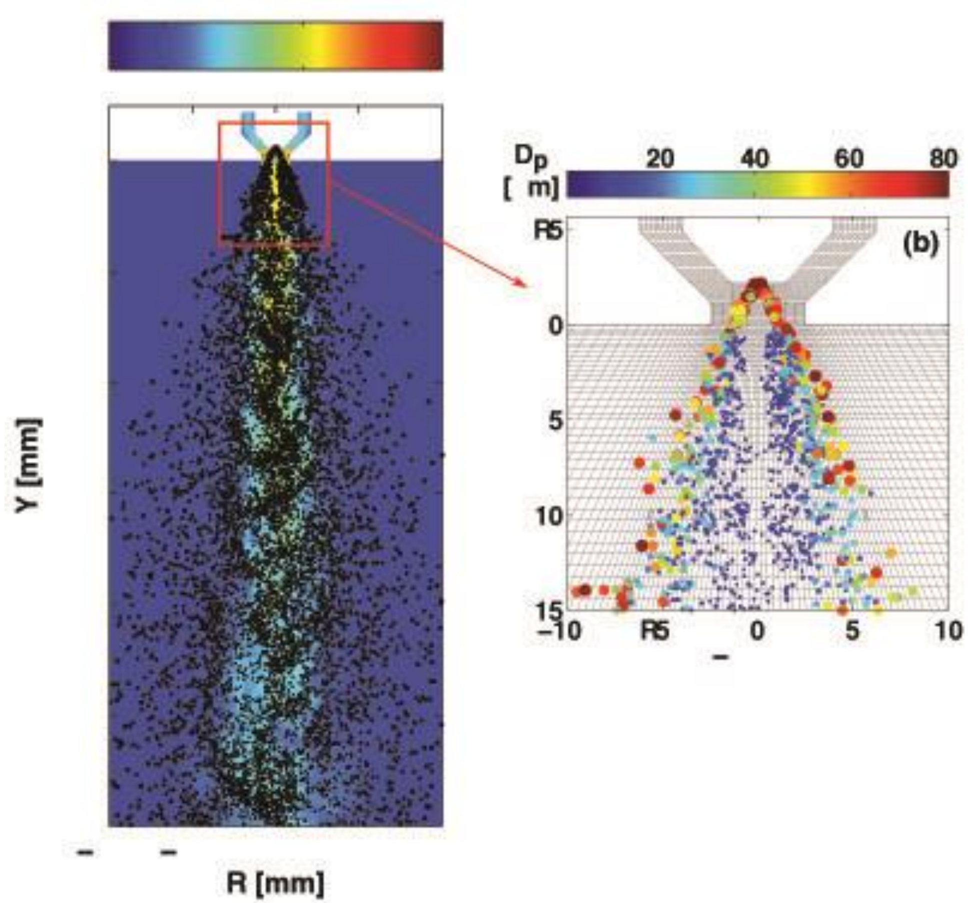
Methanol Spray Flame

<u>Gas Phase</u>

- Stochastic Fields
  - ➢ 18 species-84 reaction steps for methanol-air combustion

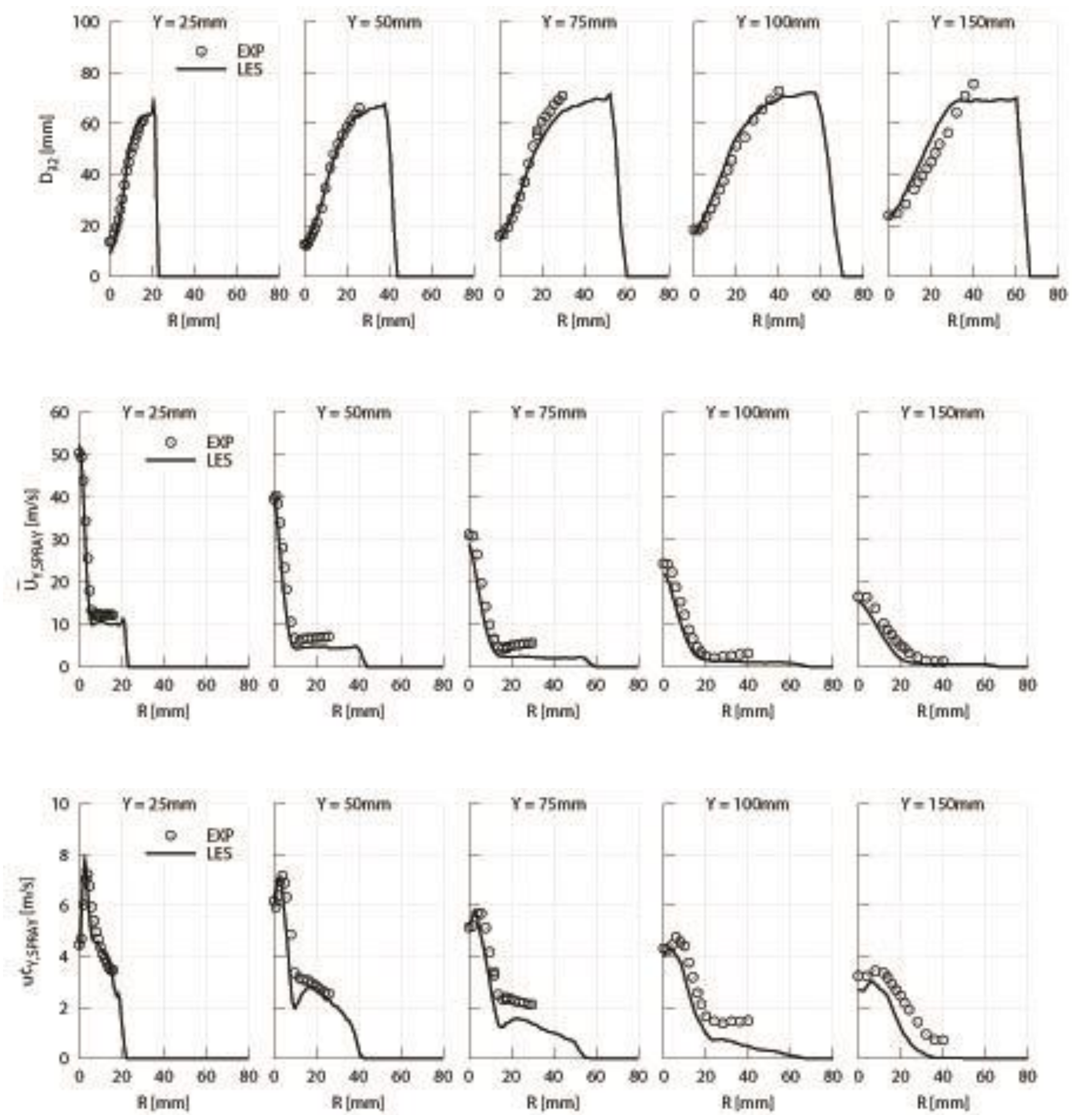
<u>Dispersed Phase</u>

- Lagrangian stochastic particles (droplets) with models for:
  - ➢ Sub-grid dispersion
  - ➢ Abramson-Sirignano evaporation
  - ➢ Stochastic breakup model



The instantaneous gas-phase velocity field with droplet motions and (b) a detailed view of breakup processes near the atomiser. Note that the appearance of droplets is scaled according to their size.

Methanol Spray: Profiles of SMD and mean and rms droplet axial velocity



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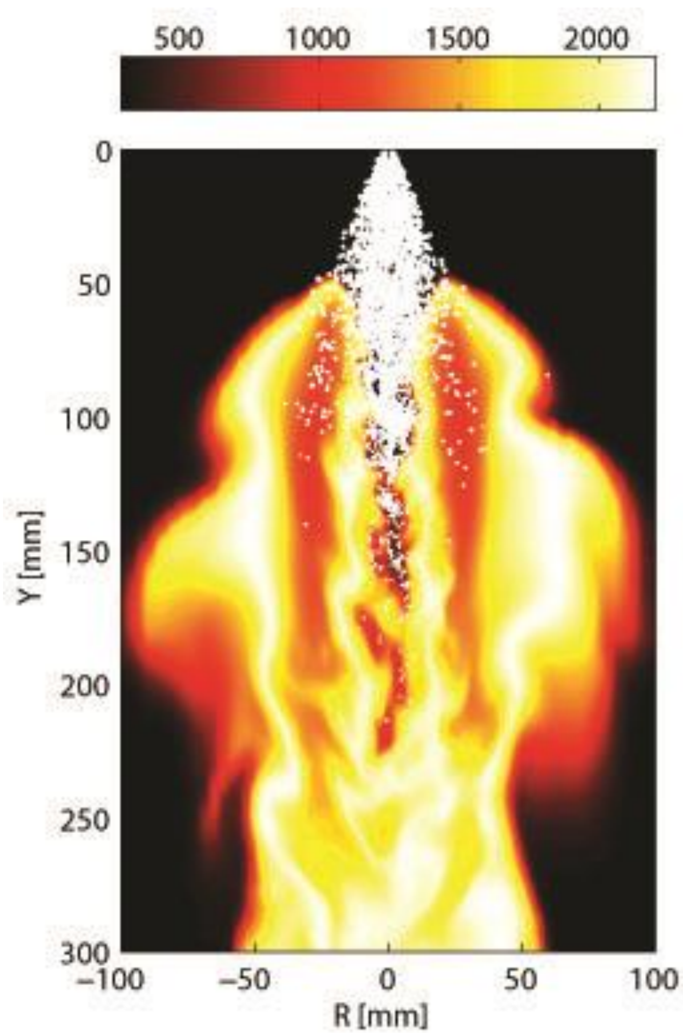
Reacting Spray: Instantaneous gas-phase temperature



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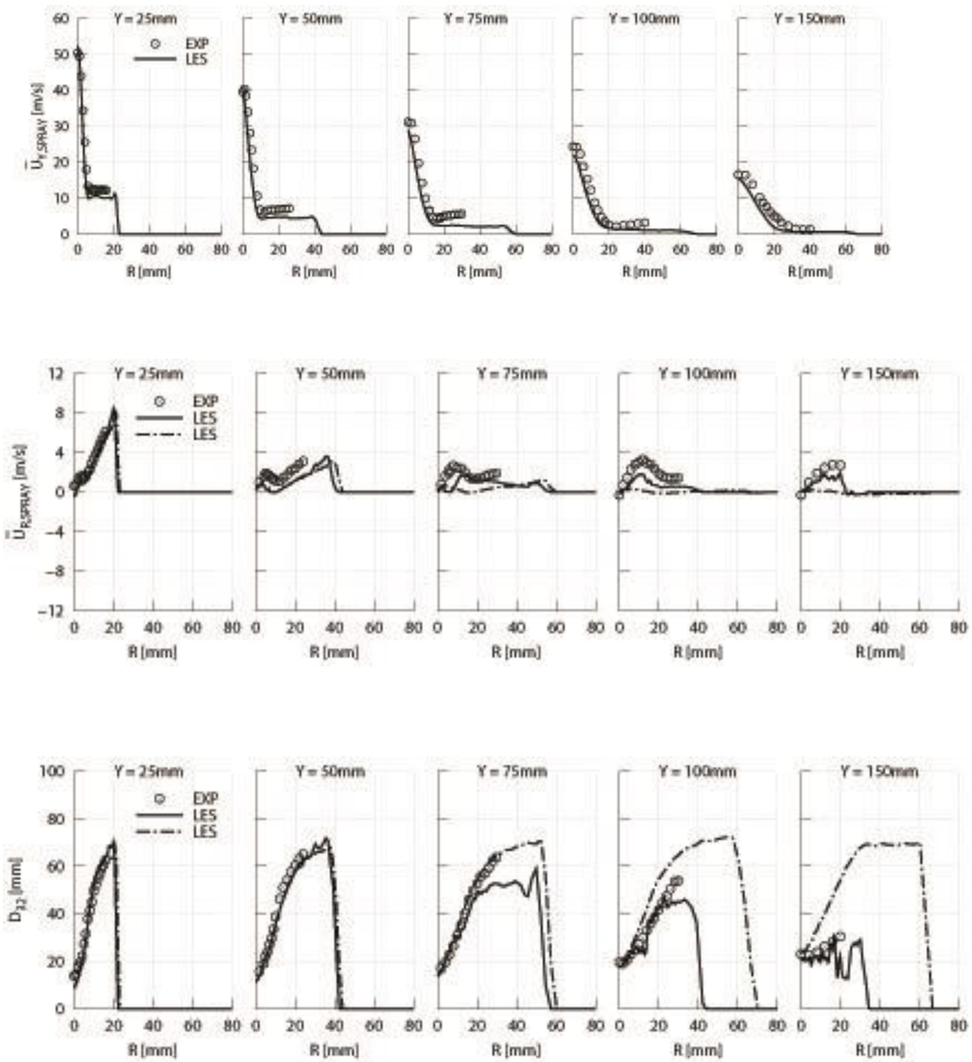
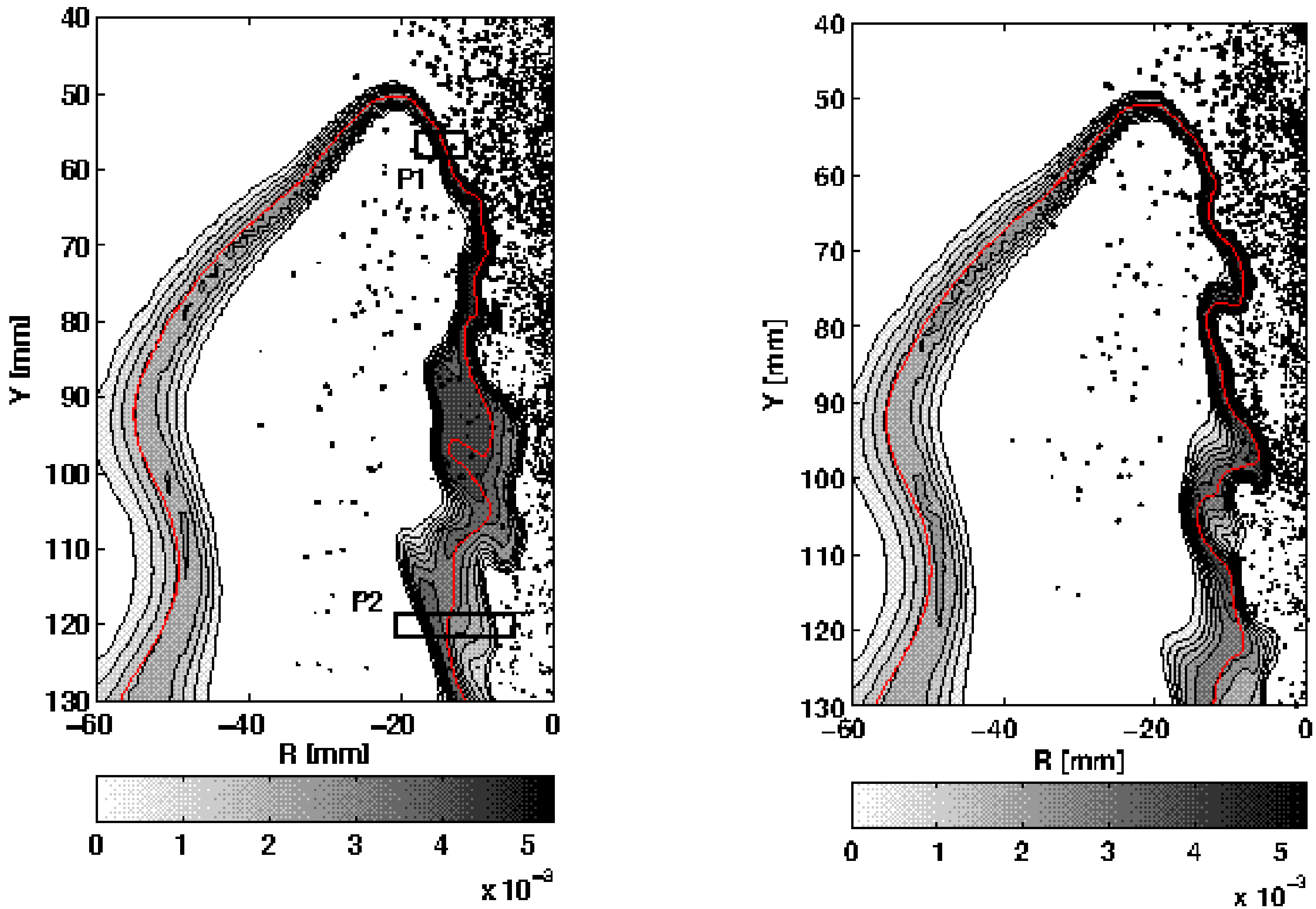
Reacting Spray: Profiles of mean and radial Droplet velocity snd SMD



Instantaneous OH mass fraction and droplets



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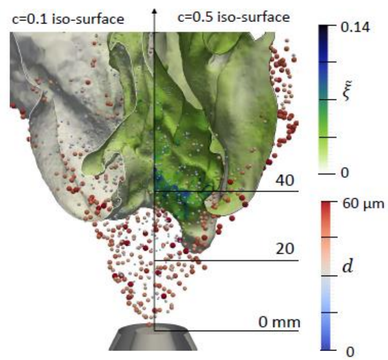
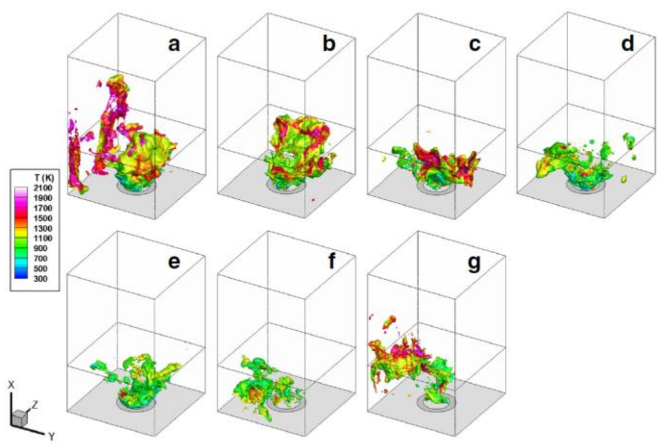
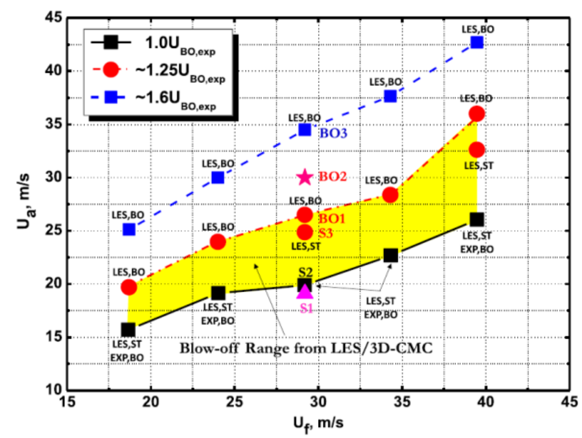
LES with Conditional Moment Closure: ignition, blow-off, emissions







Mastorakos, Cambridge

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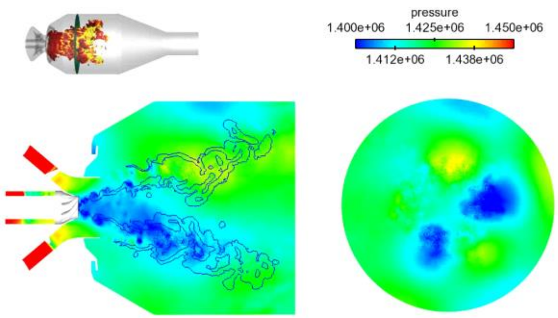
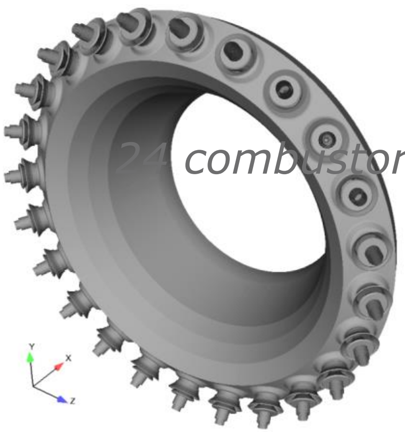
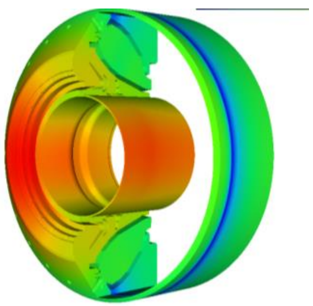
Large Eddy Simulation of Swirl Stabilized Combustor

1 combustor



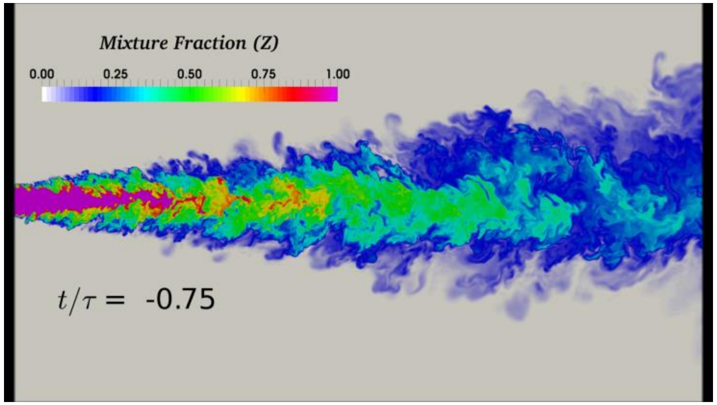


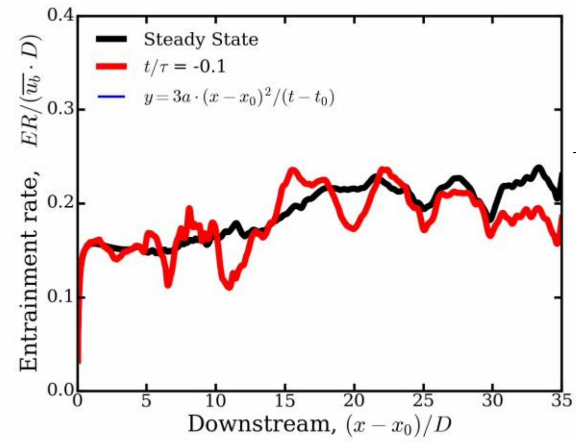
24 combustors



24 combustors
+ outer casing

Modelling of fuel injection (DNS)





$$E = \frac{3a\left(x - x_0\right)^2}{\left(t - t_0\right)}$$

Dong-hyuk Shin, Edinburgh University

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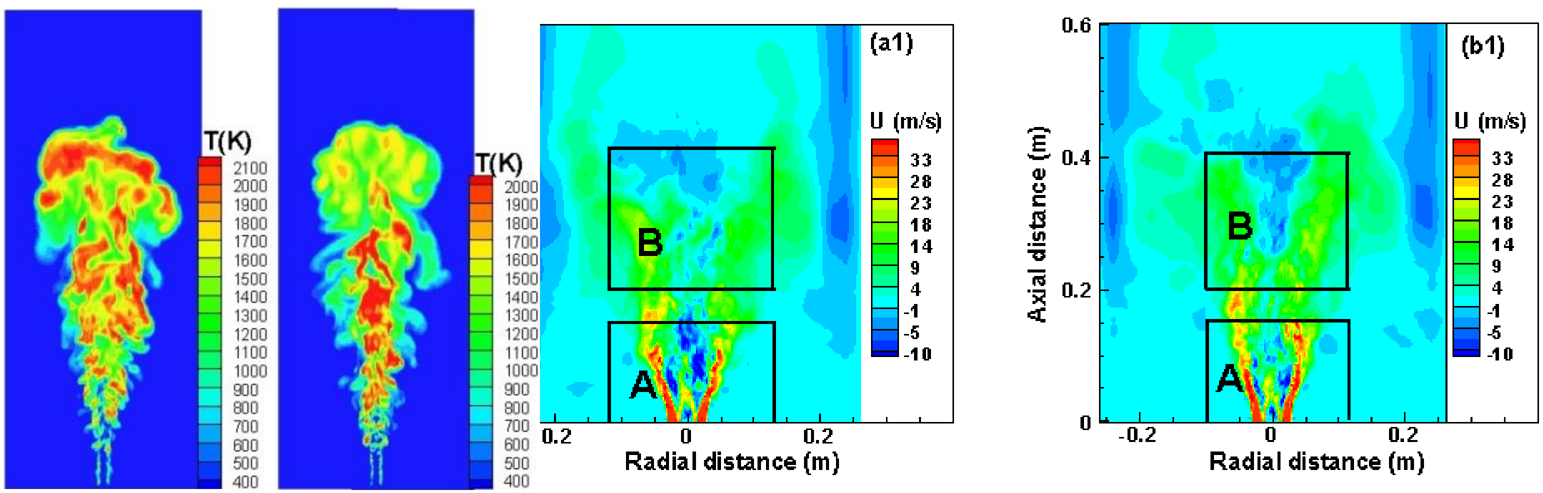
High-Hydrogen Content Alternative Fuel Blends for Stationary and Motive Combustion Engines



Large eddy simulations of non-premixed syngas jet flames and swirling flames

1. ***Ranga Dinesh***, *Jiang, van Oijen et al. Proc. Combust. Inst. , 2013*
2. ***Ranga Dinesh***, *Jiang, van Oijen et al. Int. J. Hydrogen Energy, 2013*
3. ***Ranga Dinesh***, *Luo et al. Int. J. Hydrogen Energy 2013*
4. ***Ranga Dinesh***, *van Oijen et al. Int. J. Hydrogen Energy 2015*

Conclusions

Velocity

Large Eddy Simulation is capable of reproducing the velocity field in the majority of inert and combusting flows.

Providing that the Reynolds number, $\mathrm{Re} = u'L/\nu_{sgs}$ is large and the flow is adequately resolved then results are relatively insensitive to the sub-grid stress and scalar-flux models.

Near Wall Flows and the Viscous sublayer

- models needed if DNS like requirements are to be avoided.
- no accurate and reliable wall models currently exist.

Combustion

Thin flame LES combustion models give good results when applied appropriately.

The LES Stochastic field pdf method together with detailed but reduced chemistry has been applied to a wide range of flames – non-premixed, partially premixed, premixed and spray flames - to good effect.

Practical liquid fuel systems limited by chemical reaction mechanisms.