CAN MODELING OF REACTIVE FLOWS DESCRIBE REALITY?

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Objectives (and an Outline)

Introduce a selection of combustion configurations that we need to be able to technically improve on during the next decade.

Engineering focus.
⇒ Predictive simulations.

Summarize the modeling used in simulating turbulent combustion.

Extremely challenging physics (case dependent)

Discuss VVUQ issues in combustion simulations.

– Grid refinement
– Sub-models, …
– IC & BC issues

Present examples of (state-of-the-art?) *engineering* combustion simulations.

Try to address/discuss the usefulness of such simulations, and if they can be trusted and/or used to improve the design and/or feed the development of new (more appropriate) models.

Gas Turbine Combustors

LM Gas Turbine Combustors

Aero Gas Turbine Combustors

Courtesy of A. Lindholm, Siemens, Finspång, Sweden

Scramjet Combustion Engines

Man always wants to travel faster

Aerospaceplanes, space launchers, r

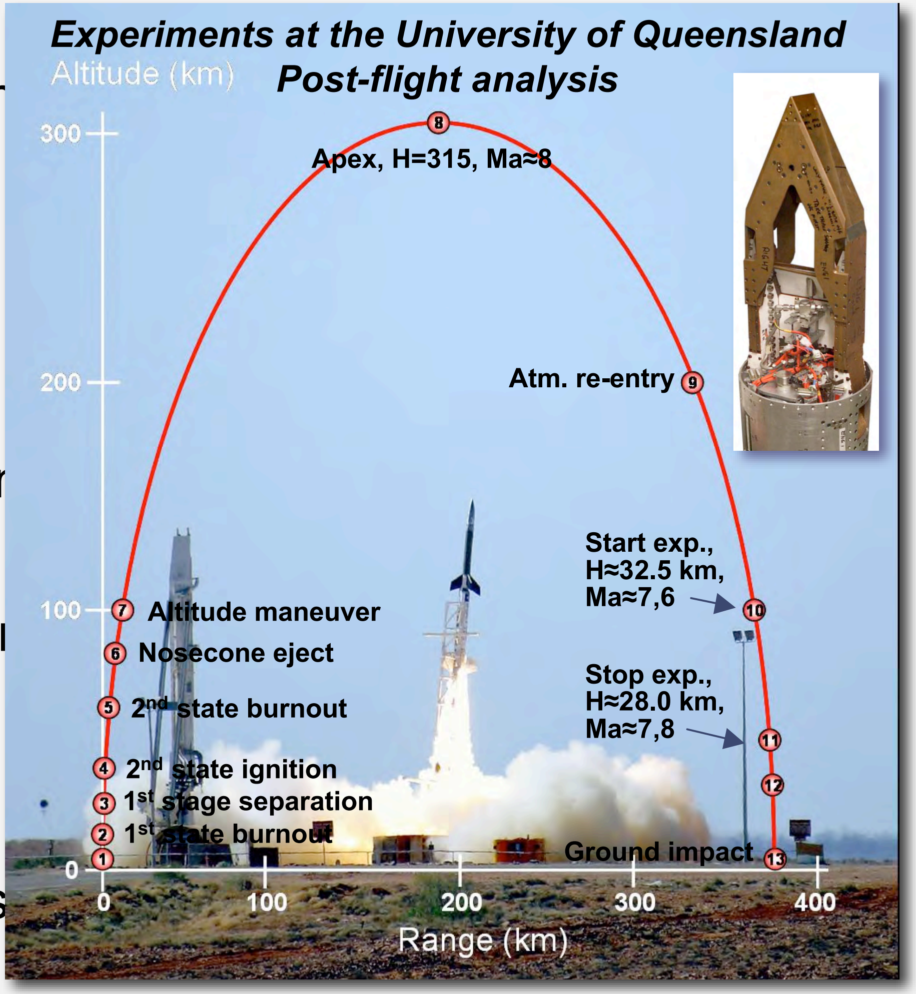
RB/TBCC
Scramjets
&
Dual-mode Scramjets

Since the mid-50's research has beer
carried out on ram-/scramjet engines

Issues with supersonic injection, mixi
self-ignition and flame stabilization, …
($s_u \approx 2$ m/s $s_t \approx 20$ m/s in a 1800 m/s flow!)

Ground based experimental facilities
not sufficient! – Run times, conditions

(High-fidelity) simulations?



Boyce *et al*, 2003, AIAA 2003-7029

Other Important Areas of Combustion

Astrophysical Combustion

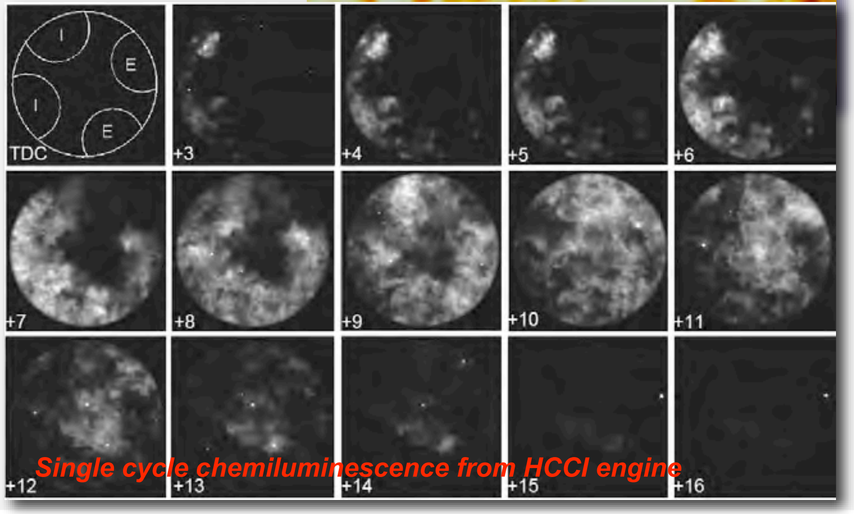
- Birth and death of the universe
- Nuclear reactions
- EOS: Completely degenerate electron gas
- It takes about 2s to blow up a White Dwarf star the size of the earth having a mass of $1.4M_{\odot}$
- Comparison: Shape of light curve – luminosity

Condensed Phase & Accidental Explosions

- Safety and weapons design as well as protection
- Often multi-phase (gas, liquid & particles)
- Comparison: Pressure-data

Internal Combustion Engines

- Transport is being more & more important to our way of life
- Reduce pollutants & increase fuel efficiency
- Spray combustion
- Comparison: Laser-based methods



Single cycle chemiluminescence from HCCI engine

Why Bother Addressing such Complex Flows?

Combustion is extremely complicated and diverse …

- Chemical kinetics,
- Mixing, self-ignition, instabilities, near wall flows, conjugate heat transfer, acoustics, …

Important to our way of life …

- Where would we have been without fire (and the IC engine)?

Survival of the earth …

- Reduce pollutants but still produce energy
- Alternatives: Wind, hydro, wave, sun, … but often with large technical problems (storage)
- Need to continue study combustion – focusing on *alternative* fuels

Other drivers

- We always want to travel faster … Economical drivers … Military drivers (spin-off)…

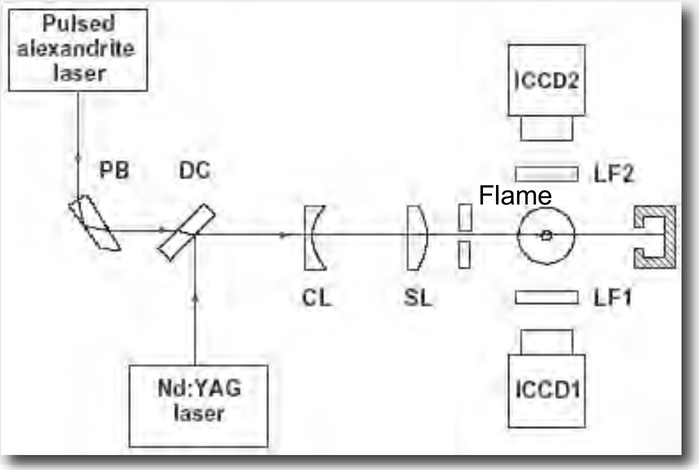
Is there any hope that we can predict combustion phenomena?

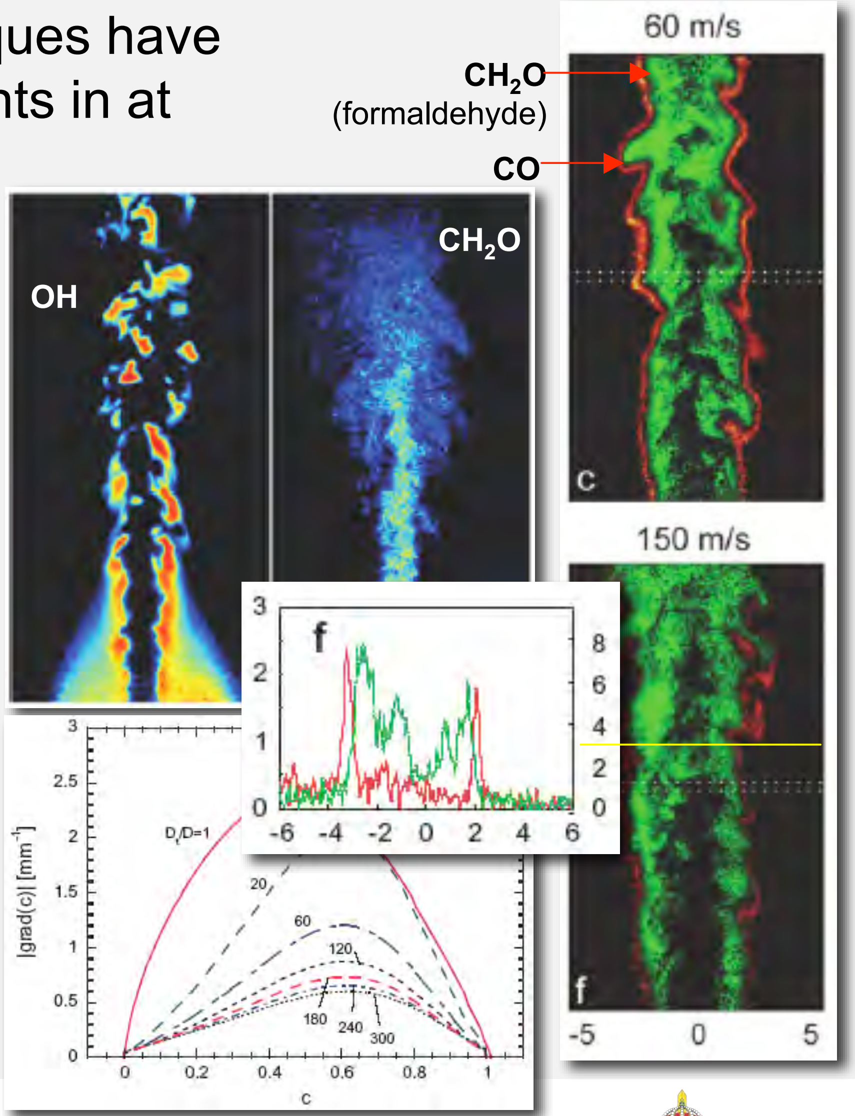
- YES! But it is not simple
- Combine experiments and simulations better – stop fight for funds
  - Non-intrusive measurement techniques
  - Supercomputing capacity available to more research groups
- Combine fundamental research with applied research
- Persistence

Experiments (vs. Simulations)

Advanced laser and optical techniques have enabled non-intrusive measurements in at least laboratory flames
(Barlow, Aldén, Wolfrum, Grisch, ..

Gives the 'true' picture of what happens in a flame
– Difficult, expensive
– Pointwise, lines & arcs
– Tomographical reconstruction

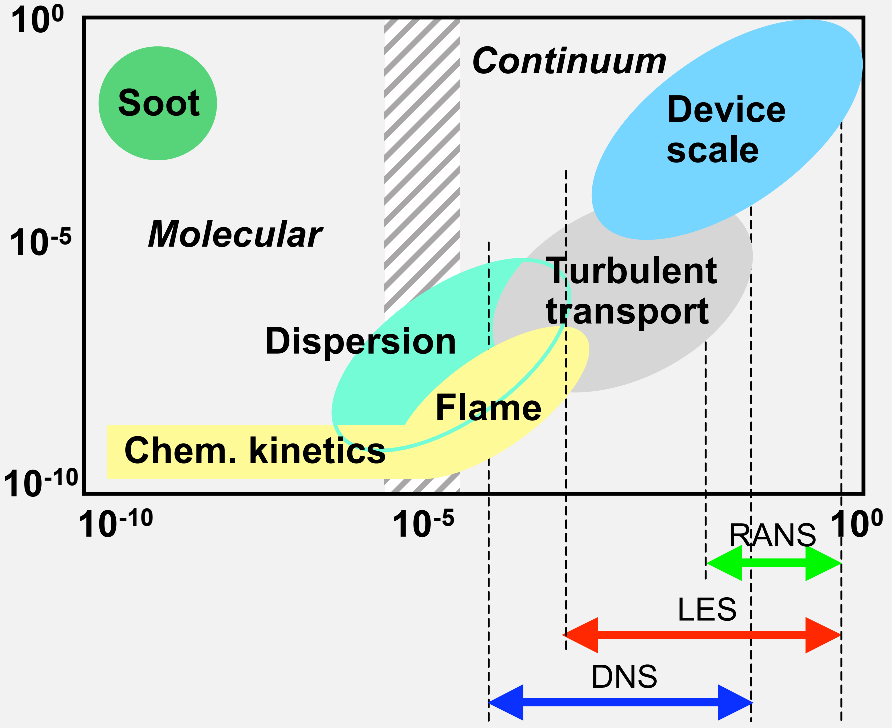




Li *et al* Comb. Flame, 2010, **157**, p 1087

Mathematical Modeling of Combustion

Multi-physics turbulent flows is a multi-scale phenomenon with key sub-processes interacting on a wide range of length and time scales

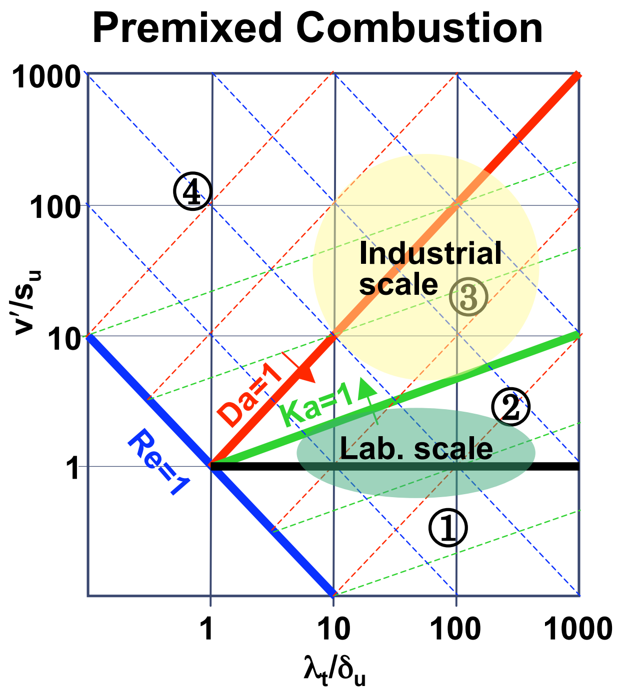


RANS = Current engineering practice

LES = The ‘to be’ engineering tool

Most suitable for combustion problems

DNS = Research tool for physics interrogation


Premixed Combustion

Reaction Regimes

① Wrinkled flamelets

② Corrugated flamelets

③ Distributed reaction zone

④ Well stirred reactor

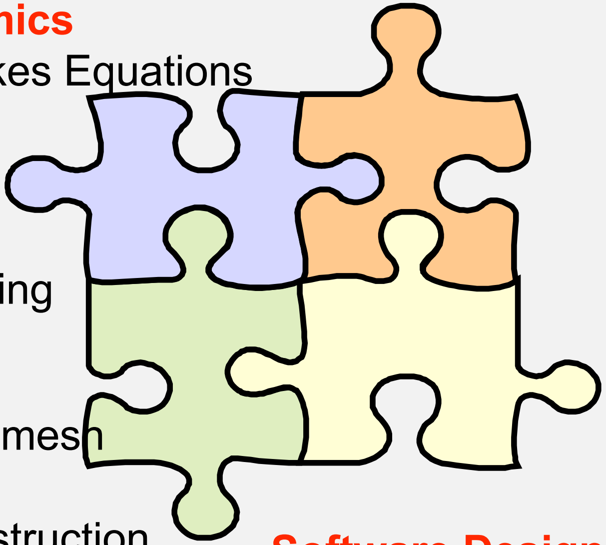
Dimensionless numbers

$Re_t = v'\lambda_t/\nu$

$Da = \tau_I/\tau_c = (\lambda_t/\delta_u)/(v'/s_u)$

$Ka = \tau_c/\tau_K = (v'/s_u)^{3/2}/(\lambda_t/\delta_u)^{1/2}$

Combustion Simulation Framework



Fluid Dynamics
- Navier Stokes Equations
- Turbulence
  - RANS
  - DES, …
  - LES, …
- Wall modeling

Numerics
- Geometry, mesh
- FVM
- Flux reconstruction
- Solvers
- Mesh motion

Software Design
- Platforms
- Parallelization
- Communication

Multi-Physics Features
- Scalar mixing
- Chemical reactions
- T/C interactions
- Multi-phase processes
- EOS
- Acoustics
- Thermal radiation
- CHT
- Component motion
- FSI

Complexity

VVUQ
- Canonical flows
- Building block flows
- Laboratory flows
- Full scale flows

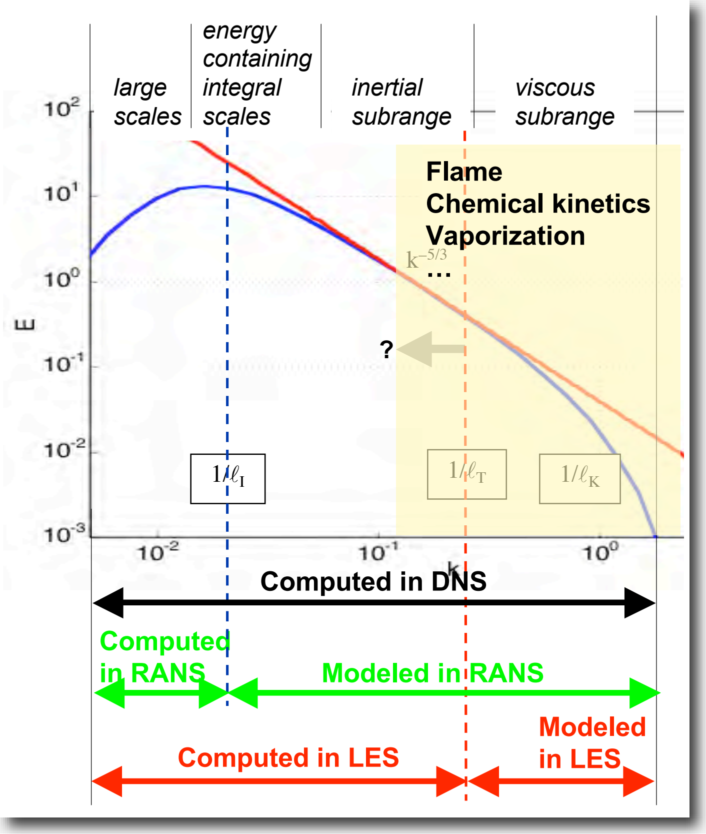
Code Requirements
- Fast, accurate, robust, flexible, parallelized, …
- Good scalability on various HPC systems
- Facilitate multi-physics modeling
- Easy implementation of complex models and methods

FOI

Simulation of Non-Reactive Flows

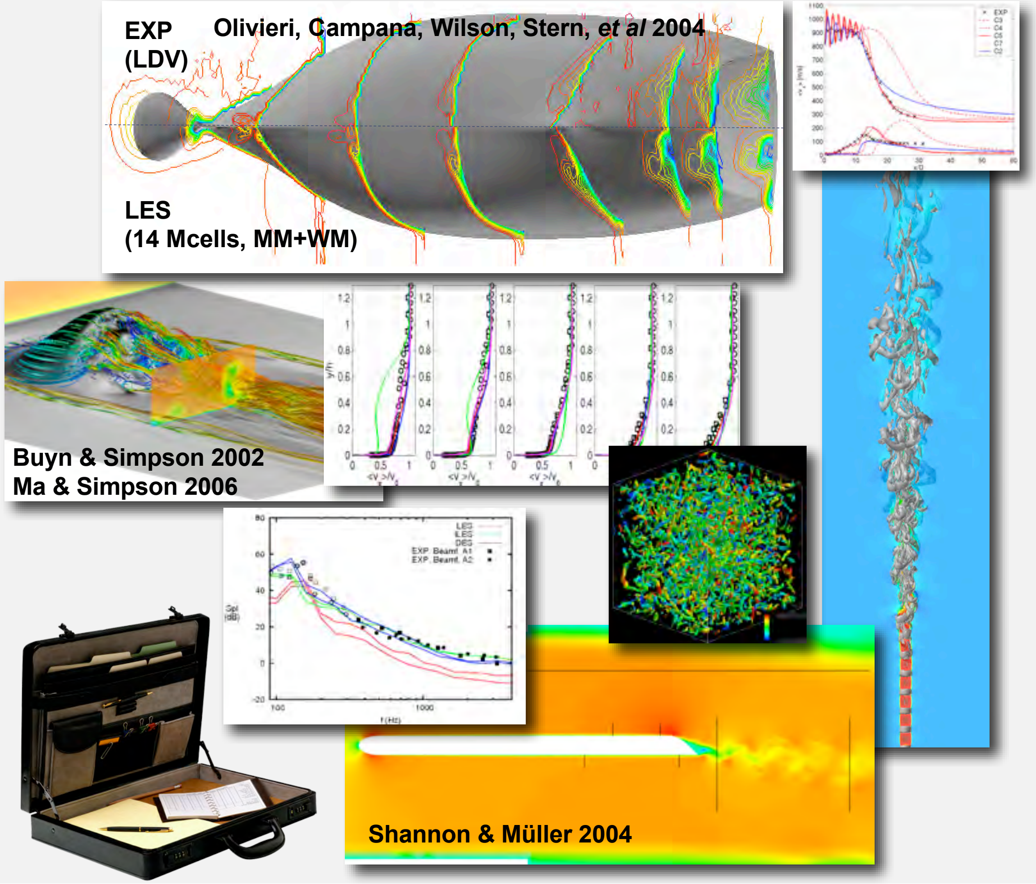
Flow Modeling

A range of flow modeling methods with different built-in features and capabilities are available



Validation

Very important to validate any RANS, LES, …, DNS models, methods & codes



Olivieri, Campana, Wilson, Stern, *et al* 2004

Buyn & Simpson 2002
Ma & Simpson 2006

Shannon & Müller 2004

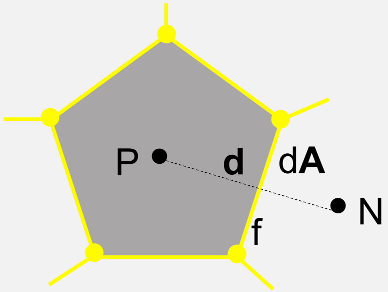
Numerical Methods (OpenFOAM)

Unstructured Finite Volume (FV) discretization

Reynolds transport (or Gauss) theorem

$\overline{\mathbf{u}}=[\overline{\rho}, \overline{\rho}\tilde{Y}_i, \overline{\rho}\tilde{\mathbf{v}}, \overline{\rho}\tilde{E}]^T$

$\partial_t(\overline{\mathbf{u}}_P)+\frac{1}{\delta V_P}\sum_f[\mathbf{F}_f^C(\overline{\mathbf{u}})-\mathbf{F}_f^D(\overline{\mathbf{u}})+\mathbf{F}_f^B(\overline{\mathbf{u}})]=-(\nabla p)_P+s_P(\overline{\mathbf{u}})$



Semi-Implicit Algorithm

Monotone or monotonicity-preserving reconstruction of convective fluxes
Central difference approximations of inner derivatives in other fluxes
Crank Nicholson time integration, Co≈0.5

Fully Explicit Algorithm

Monotone or monotonicity-preserving reconstruction of convective fluxes
Central difference approximations for inner derivatives other fluxes
RK time integration, Co≈0.5

Modified Equations Analysis (MEA)

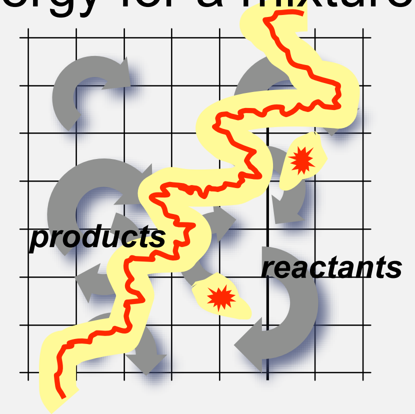
Taylor series expansion used to evaluate the leading order TE

$\mathbf{T}\approx\overline{\rho}([\mathbf{C}(\nabla\tilde{\mathbf{v}})^T+(\nabla\tilde{\mathbf{v}})\mathbf{C}^T+\chi^2(\nabla\tilde{\mathbf{v}})\mathbf{d}\otimes(\nabla\tilde{\mathbf{v}})\mathbf{d}]+\frac{1}{8}[\tilde{\mathbf{v}}\otimes((\nabla^2\tilde{\mathbf{v}})(\mathbf{d}\otimes\mathbf{d}))+((\nabla^2\tilde{\mathbf{v}})(\mathbf{d}\otimes\mathbf{d}))\otimes\tilde{\mathbf{v}}])$

*Drikakis D., Fureby C., Grinstein F.F. & Liefendahl M.; 2007, “ILES with Limiting Algorithms”,
In Implicit Large Eddy Simulation: Computing Turbulent Fluid Dynamics,
Eds. Grinstein F.F., Margolin L. & Rider B., Cambridge University Press, p 94.*

Combustion Modeling using LES

Balance equations of mass, momentum and energy for a mixture



$$G* \begin{cases} \partial_t(\bar{\rho})+\nabla\cdot(\bar{\rho}\tilde{\mathbf{v}})=0 \\ \partial_t(\bar{\rho}\tilde{\mathbf{v}})+\nabla\cdot(\bar{\rho}\tilde{\mathbf{v}}\otimes\tilde{\mathbf{v}})=-\nabla\bar{p}+\nabla\cdot(\bar{\mathbf{S}}-\boxed{\mathbf{B}})+\bar{\rho}\tilde{\mathbf{f}} \\ \partial_t(\bar{\rho}\tilde{E})+\nabla\cdot(\bar{\rho}\tilde{\mathbf{v}}\tilde{E})=\nabla\cdot(-\bar{p}\tilde{\mathbf{v}}+\tilde{\mathbf{S}}\tilde{\mathbf{v}}+\bar{\mathbf{h}}-\boxed{\mathbf{b}_E})+\bar{\rho}\tilde{\sigma} \\ \partial_t(\bar{\rho}\tilde{Y}_i)+\nabla\cdot(\bar{\rho}\tilde{\mathbf{v}}\tilde{Y}_i)=\nabla\cdot(\bar{\mathbf{j}}_i-\boxed{\mathbf{b}_i})+\boxed{\overline{\dot{w}_i}} \end{cases}$$

Filtered constitutive equations

$$\bar{\mathbf{j}}_i \approx D_i\nabla\tilde{Y}_i,\ \bar{p}\approx\bar{\rho}R\tilde{T}\Sigma_i(\tilde{Y}_i/M_i),\ \bar{\mathbf{S}}\approx(\lambda+\tfrac{2}{3}\mu)(\mathrm{tr}\tilde{\mathbf{D}})\mathbf{I}+2\mu\tilde{\mathbf{D}}_D,\ \bar{\mathbf{h}}=\overline{\kappa\nabla T}\approx\kappa\nabla\tilde{T}$$

Filtered reaction rates and chemical kinetics

$$\overline{\dot{w}_i}=M_i\Sigma_{j=1}^{M}(P''_{ij}-P'_{ij})\overline{\dot{w}_j}=M_i\Sigma_{j=1}^{M}(P''_{ij}-P'_{ij})[\overline{k_{fj}\rho^{\Sigma_i P'_{ij}}\Pi_{i=1}^{N}Y_i^{P'_{ij}}-k_{bj}\rho^{\Sigma_i P''_{ij}}\Pi_{i=1}^{N}Y_i^{P''_{ij}}}]$$

Subgrid stress ($\mathbf{B}$) and flux terms ($\mathbf{b}_E$ & $\mathbf{b}_i$)

Definition: $\mathbf{B}=\bar{\rho}(\widetilde{\mathbf{v}\otimes\mathbf{v}}-\tilde{\mathbf{v}}\otimes\tilde{\mathbf{v}}),\ \mathbf{b}_E=\bar{\rho}(\widetilde{\mathbf{v}E}-\tilde{\mathbf{v}}\tilde{E}),\ \mathbf{b}_i=\bar{\rho}(\widetilde{\mathbf{v}Y_i}-\tilde{\mathbf{v}}\tilde{Y}_i)$

Model: $\mathbf{B}=-2\mu_k\tilde{\mathbf{D}},\ \mathbf{b}_E=-2\frac{\mu_k}{Pr_t}\nabla E_i,\ \mathbf{b}_i=-2\frac{\mu_k}{Sc_i}\nabla\tilde{Y}_i;\ \mu_k=\tilde{\rho}\boxed{c_k\Delta}k^{1/2} \longrightarrow \boxed{c_k\Delta=-\frac{\mathbf{L}_D\cdot(K^{1/2}\overline{\overline{\mathbf{D}}}_D)}{4(K^{1/2}\overline{\overline{\mathbf{D}}}_D)^2}}$

OEEVM/LDKM: $\partial_t(\bar{\rho}k)+\nabla\cdot(\bar{\rho}\tilde{\mathbf{v}}k)=-\mathbf{B}\cdot\tilde{\mathbf{D}}+\nabla\cdot(\mu_k\nabla k)-\bar{\rho}c_\varepsilon k^{3/2}/\Delta$

LES Combustion Models: Overview

Flame usually thinner than the LES grid resolution ($\delta_u < \Delta$)

The filtered reaction rate $\overline{\dot{w}_j}$ is highly non-linear ⇒ large local variations

Turbulence chemistry interactions (TCI) very important

Specific modeling (of either equation set and/or terms) required

c/z equation flamelet models

Propagation based or filtering based (e.g. Veynante *et al*, Weller *et al*., …)

Ξ, Σ, s_u

G/z equation flamelet models

Interface tracking of the flame front (e.g., Pitch *et al*)

Thickened Flame Model (TFM) + reduced chemistry

Artificially thicken the flame to fit on the grid (e.g., O'Rourke & Bracco, Collin *et al*)

EDC or PaSR models + reduced chemistry

Eddy Dissipation Concept or Partially Stirred Reactor subgrid TCI models (e.g., Fureby *et al*)

Transported & presumed PDF models + reduced chemistry

Probabilistic approach using subgrid PDF (e.g., Pope, Givi *et al*)

Linear Eddy Models (LEM) + reduced chemistry

1D sub-models for reaction-mixing in each LES cell (Menon *et al*, Kerstein *et al*)

LES Combustion Models: EDC/PaSR

Multi-scale model based on the assumption that reactions take place on the smallest *fine structures* (*) embedded in the *surroundings* (^{0})

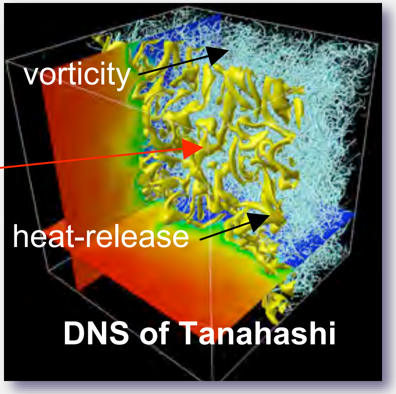
Subgrid balance equations

$$\begin{cases}\bar{\rho}(Y_i^* - \tilde{Y}_i) = (1-\gamma^*)\tau^* \dot{w}_i(\bar{\rho}, Y_i^*, T^*) \\ \bar{\rho}\Sigma_{i=1}^N (Y_i^* h_i^* - \tilde{Y}_i \tilde{h}_i) = (1-\gamma^*)\tau^* \Sigma_{i=1}^N h_{i,f}^\theta \dot{w}_i(\bar{\rho}, Y_i^*, T^*)\end{cases}$$

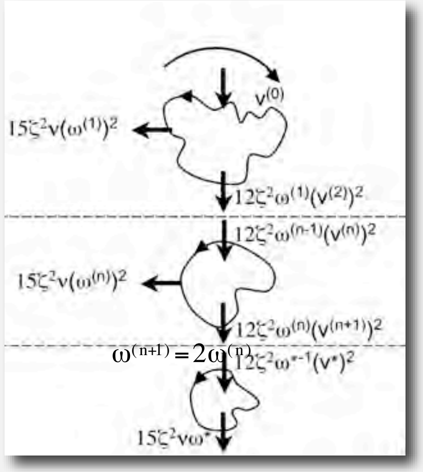
Need to determine τ^* and γ^*

γ^*

τ^*



DNS of Tanahashi



EDC model

- Cascade process (v^*, τ^*)
- K41 consistent
- $v^* \approx v_K$, $\ell^* \approx 2\ell_K$, $\tau^* \approx 2\tau_K$
- Reaction space: tubes/sheets at high T
- $\gamma^* \approx \chi(v^*/v')^2 \approx \chi(\mu/\mu_k)^{3/4}$

PaSR model

- K41 hypothesis
- τ^* based on $[\tau_K, \tau']$ $\tau^* \approx (\tau_K \tau')^{1/2}$, $\tau' = \Delta/v'$
- Reaction space: tubes/sheets at high T
- $\gamma^* \approx \tau_c/(\tau_c + \tau^*)$

$$\boxed{\partial_t(\bar{\rho}\tilde{Y}_i) + \nabla\cdot(\bar{\rho}\tilde{\mathbf{v}}\tilde{Y}_i) = \nabla\cdot((D_i + \mu_k/Sc_k)\nabla Y_i) + \gamma^* M_i P_{ij} \dot{w}_j(Y_i^*, T^*)}$$

Chemical Kinetics

Describing chemical kinetics (with sufficient accuracy and degree of detail) is very difficult due to the complexity of the reaction mechanisms

Hydrogen: H_2-air; 8 species, 38 reactions (O'Conaire *et al* 2004)

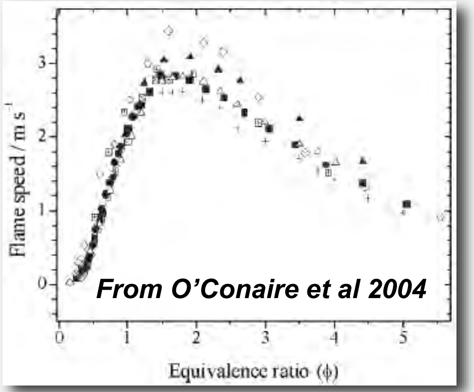
Methane: CH_4-air; 53 species, 325 reactions (GRI3.0)

N-Heptane: C_7H_{16}-air; 561 species, 2539 reactions (Lu & Law 2008)

Jet-A: $C_{12}H_{23}$-air; 18 species, 46 reactions (Yungster & Breisacher 2005)

Design of 'detailed reaction mechanisms'

- Identify all possible reactions ⇒ Reaction mechanism
- Collision theory $\dot{w} = \sigma A \left(\frac{8 k_B T}{\pi \mu_{AB}}\right)^{1/2} c_\alpha c_\beta e^{-E_A/RT}$
- Experimental data fits
  - Flame speed measurements
  - Ignition delay measurements Laser
  - Flow reaction measurements
- Simulations of measurements



From O'Conaire et al 2004

How much chemistry do we need? and for which purpose?

Chemical Kinetics cont’d

http://www.me.berkeley.edu/gri_mech/version30/files30/grimech3...

```
! GRI-Mech Version 3.0 7/30/99  CHEMKIN-II format
! See README30 file at anonymous FTP site unix.sri.com, directory gri;
! WorldWideWeb home page http://www.me.berkeley.edu/gri_mech/ or
! through http://www.gri.org , under 'Basic  Research',
! for additional information, contacts, and disclaimer
ELEMENTS
O  H  C  N  AR
END
SPECIES
H2        H         O         O2        OH        H2O       HO2       H2O2
C         CH        CH2       CH2(S)    CH3       CH4       CO        CO2
HCO       CH2O      CH2OH     CH3O      CH3OH     C2H       C2H2      C2H3
C2H4      C2H5      C2H6      HCCO      CH2CO     HCCOH     N         NH
NH2       NH3       NNH       NO        NO2       N2O       HNO       CN
HCN       H2CN      HCNN      HCNO      HOCN      HNCO      NCO       N2
AR        C3H7      C3H8      CH2CHO    CH3CHO
END
!THERMO
! Insert GRI-Mech thermodynamics here or use in default file
!END
REACTIONS
2O+M<=>O2+M                              1.200E+17   -1.000        .00
H2/ 2.40/ H2O/15.40/ CH4/ 2.00/ CO/ 1.75/ CO2/ 3.60/ C2H6/ 3.00/ AR/  .8
O+H+M<=>OH+M                             5.000E+17   -1.000        .00
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/
O+H2<=>H+OH                              3.870E+04    2.700    6260.00
O+HO2<=>OH+O2                            2.000E+13     .000        .00
O+H2O2<=>OH+HO2                          9.630E+06    2.000    4000.00
O+CH<=>H+CO                              5.700E+13     .000        .00
O+CH2<=>H+HCO                            8.000E+13     .000        .00
O+CH2(S)<=>H2+CO                         1.500E+13     .000        .00
O+CH2(S)<=>H+HCO                         1.500E+13     .000        .00
O+CH3<=>H+CH2O                           5.060E+13     .000        .00
O+CH4<=>OH+CH3                           1.020E+09    1.500    8600.00
O+CO(+M)<=>CO2(+M)                       1.800E+10     .000    2385.00
   LOW/ 6.020E+14     .000    3000.00/
H2/2.00/ O2/6.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/3.50/ C2H6/3.00/ AR/
O+HCO<=>OH+CO                            3.000E+13     .000        .00
O+HCO<=>H+CO2                            3.000E+13     .000        .00
O+CH2O<=>OH+HCO                          3.900E+13     .000    3540.00
O+CH2OH<=>OH+CH2O                        1.000E+13     .000        .00
O+CH3O<=>OH+CH2O                         1.000E+13     .000        .00
O+CH3OH<=>OH+CH2OH                       3.880E+05    2.500    3100.00
O+CH3OH<=>OH+CH3O                        1.300E+05    2.500    5000.00
O+C2H<=>CH+CO                            5.000E+13     .000        .00
O+C2H2<=>H+HCCO                          1.350E+07    2.000    1900.00
O+C2H2<=>OH+C2H                          4.600E+19   -1.410   28950.00
O+C2H2<=>CO+CH2                          6.940E+06    2.000    1900.00
O+C2H3<=>H+CH2CO                         3.000E+13     .000        .00
O+C2H4<=>CH3+HCO                         1.250E+07    1.830     220.00
O+C2H5<=>CH3+CH2O                        2.240E+13     .000        .00
O+C2H6<=>OH+C2H5                         8.980E+07    1.920    5690.00
O+HCCO<=>H+2CO                           1.000E+14     .000        .00
O+CH2CO<=>OH+HCCO                        1.000E+13     .000    8000.00
O+CH2CO<=>CH2+CO2                        1.750E+12     .000    1350.00
O2+CO<=>O+CO2                            2.500E+12     .000   47800.00
O2+CH2O<=>HO2+HCO                        1.000E+14     .000   40000.00
H+O2+M<=>HO2+M                           2.800E+18    -.860        .00
O2/ .00/ H2O/ .00/ CO/ .75/ CO2/1.50/ C2H6/1.50/ N2/ .00/ AR/ .00/
H+2O2<=>HO2+O2                           2.080E+19   -1.240        .00
H+O2+H2O<=>HO2+H2O                       11.26E+18    -.760        .00
H+O2+N2<=>HO2+N2                         2.600E+19   -1.240        .00
H+O2+AR<=>HO2+AR                         7.000E+17    -.800        .00
H+O2<=>O+OH                              2.650E+16   -.6707   17041.00
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http://www.me.berkeley.edu/gri_mech/version30/files30/grimech3...

```
2H+M<=>H2+M                              1.000E+18   -1.000        .00
H2/ .00/ H2O/ .00/ CH4/2.00/ CO2/ .00/ C2H6/3.00/ AR/ .63/
2H+H2<=>2H2                              9.000E+16    -.600        .00
2H+H2O<=>H2+H2O                          6.000E+19   -1.250        .00
2H+CO2<=>H2+CO2                          5.500E+20   -2.000        .00
H+OH+M<=>H2O+M                           2.200E+22   -2.000        .00
H2/ .73/ H2O/3.65/ CH4/2.00/ C2H6/3.00/ AR/ .38/
H+HO2<=>O+H2O                            3.970E+12     .000     671.00
H+HO2<=>O2+H2                            4.480E+13     .000    1068.00
H+HO2<=>2OH                              0.840E+14     .000     635.00
H+H2O2<=>HO2+H2                          1.210E+07    2.000    5200.00
H+H2O2<=>OH+H2O                          1.000E+13     .000    3600.00
H+CH<=>C+H2                              1.650E+14     .000        .00
H+CH2(+M)<=>CH3(+M)                      6.000E+14     .000        .00
     LOW  /  1.040E+26   -2.760   1600.00/
     TROE/   .5620  91.00  5836.00  8552.00/
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/
H+CH2(S)<=>CH+H2                         3.000E+13     .000        .00
H+CH3(+M)<=>CH4(+M)                      13.90E+15    -.534     536.00
     LOW  /  2.620E+33   -4.760   2440.00/
     TROE/   .7830   74.00  2941.00  6964.00 /
H2/2.00/ H2O/6.00/ CH4/3.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/
H+CH4<=>CH3+H2                           6.600E+08    1.620   10840.00
H+HCO(+M)<=>CH2O(+M)                     1.090E+12     .480    -260.00
     LOW  /  2.470E+24   -2.570    425.00/
     TROE/   .7824  271.00  2755.00  6570.00 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/
H+HCO<=>H2+CO                            7.340E+13     .000        .00
H+CH2O(+M)<=>CH2OH(+M)                   5.400E+11     .454    3600.00
     LOW  /  1.270E+32   -4.820   6530.00/
     TROE/   .7187  103.00  1291.00  4160.00 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/
H+CH2O(+M)<=>CH3O(+M)                    5.400E+11     .454    2600.00
     LOW  /  2.200E+30   -4.800   5560.00/
     TROE/   .7580   94.00  1555.00  4200.00 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/
H+CH2O<=>HCO+H2                          5.740E+07    1.900    2742.00
H+CH2OH(+M)<=>CH3OH(+M)                  1.055E+12     .500      86.00
     LOW  /  4.360E+31   -4.650   5080.00/
     TROE/   .600  100.00  90000.0  10000.0 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/
H+CH2OH<=>H2+CH2O                        2.000E+13     .000        .00
H+CH2OH<=>OH+CH3                         1.650E+11     .650    -284.00
H+CH2OH<=>CH2(S)+H2O                     3.280E+13    -.090     610.00
H+CH3O(+M)<=>CH3OH(+M)                   2.430E+12     .515      50.00
     LOW  /  4.660E+41   -7.440   14080.0/
     TROE/   .700  100.00  90000.0 10000.00 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/
H+CH3O<=>H+CH2OH                         4.150E+07    1.630    1924.00
H+CH3O<=>H2+CH2O                         2.000E+13     .000        .00
H+CH3O<=>OH+CH3                          1.500E+12     .500    -110.00
H+CH3O<=>CH2(S)+H2O                      2.620E+14    -.230    1070.00
H+CH3OH<=>CH2OH+H2                       1.700E+07    2.100    4870.00
H+CH3OH<=>CH3O+H2                        4.200E+06    2.100    4870.00
H+C2H(+M)<=>C2H2(+M)                     1.000E+17   -1.000        .00
     LOW  /  3.750E+33   -4.800   1900.00/
     TROE/   .6464  132.00  1315.00  5566.00 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/
H+C2H2(+M)<=>C2H3(+M)                    5.600E+12     .000    2400.00
     LOW  /  3.800E+40   -7.270   7220.00/
     TROE/   .7507   98.50  1302.00  4167.00 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/
H+C2H3(+M)<=>C2H4(+M)                    6.080E+12     .270     280.00
     LOW  /  1.400E+30   -3.860   3320.00/
```

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http://www.me.berkeley.edu/gri_mech/version30/files30/grimech3...

```
     TROE/   .7820  207.50  2663.00  6095.00 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/
H+C2H3<=>H2+C2H2                         3.000E+13     .000
H+C2H4(+M)<=>C2H5(+M)                    0.540E+12     .454
     LOW  /  0.600E+42   -7.620   6970.00/
     TROE/   .9753  210.00   984.00  4374.00 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/
H+C2H4<=>C2H3+H2                         1.325E+06    2.530
H+C2H5(+M)<=>C2H6(+M)                    5.210E+17    -.990
     LOW  /  1.990E+41   -7.080   6685.00/
     TROE/   .8422  125.00  2219.00  6882.00 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/
H+C2H5<=>H2+C2H4                         2.000E+12     .000
H+C2H6<=>C2H5+H2                         1.150E+08    1.900
H+HCCO<=>CH2(S)+CO                       1.000E+14     .000
H+CH2CO<=>HCCO+H2                        5.000E+13     .000
H+CH2CO<=>CH3+CO                         1.130E+13     .000
H+HCCOH<=>H+CH2CO                        1.000E+13     .000
H2+CO(+M)<=>CH2O(+M)                     4.300E+07    1.500
     LOW  /  5.070E+27   -3.420  84350.00/
     TROE/   .9320  197.00  1540.00 10300.00 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/
OH+H2<=>H+H2O                            2.160E+08    1.510
2OH(+M)<=>H2O2(+M)                       7.400E+13    -.370
     LOW  /  2.300E+18    -.900  -1700.00/
     TROE/   .7346   94.00  1756.00  5182.00 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/
2OH<=>O+H2O                              3.570E+04    2.400
OH+HO2<=>O2+H2O                          1.450E+13     .000
 DUPLICATE
OH+H2O2<=>HO2+H2O                        2.000E+12     .000
 DUPLICATE
OH+H2O2<=>HO2+H2O                        1.700E+18     .000
 DUPLICATE
OH+C<=>H+CO                              5.000E+13     .000
OH+CH<=>H+HCO                            3.000E+13     .000
OH+CH2<=>H+CH2O                          2.000E+13     .000
OH+CH2<=>CH+H2O                          1.130E+07    2.000
OH+CH2(S)<=>H+CH2O                       3.000E+13     .000
OH+CH3(+M)<=>CH3OH(+M)                   2.790E+18   -1.430
     LOW  /  4.000E+36   -5.920   3140.00/
     TROE/   .4120  195.0  5900.00  6394.00/
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/
OH+CH3<=>CH2+H2O                         5.600E+07    1.600
OH+CH3<=>CH2(S)+H2O                      6.440E+17   -1.340
OH+CH4<=>CH3+H2O                         1.000E+08    1.600
OH+CO<=>H+CO2                            4.760E+07    1.228
OH+HCO<=>H2O+CO                          5.000E+13     .000
OH+CH2O<=>HCO+H2O                        3.430E+09    1.180
OH+CH2OH<=>H2O+CH2O                      5.000E+12     .000
OH+CH3O<=>H2O+CH2O                       5.000E+12     .000
OH+CH3OH<=>CH2OH+H2O                     1.440E+06    2.000
OH+CH3OH<=>CH3O+H2O                      6.300E+06    2.000
OH+C2H<=>H+HCCO                          2.000E+13     .000
OH+C2H2<=>H+CH2CO                        2.180E-04    4.500
OH+C2H2<=>H+HCCOH                        5.040E+05    2.300
OH+C2H2<=>C2H+H2O                        3.370E+07    2.000
OH+C2H2<=>CH3+CO                         4.830E-04    4.000
OH+C2H3<=>H2O+C2H2                       5.000E+12     .000
OH+C2H4<=>C2H3+H2O                       3.600E+06    2.000
OH+C2H6<=>C2H5+H2O                       3.540E+06    2.120
OH+CH2CO<=>HCCO+H2O                      7.500E+12     .000
2HO2<=>O2+H2O2                           1.300E+11     .000
 DUPLICATE
```

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http://www.me.berkeley.edu/gri_mech/version30/files30/grimech3...

```
2HO2<=>O2+H2O2                           4.200E+14     .000   12000.00
 DUPLICATE
HO2+CH2<=>OH+CH2O                        2.000E+13     .000        .00
HO2+CH3<=>O2+CH4                         1.000E+12     .000        .00
HO2+CH3<=>OH+CH3O                        3.780E+13     .000        .00
HO2+CO<=>OH+CO2                          1.500E+14     .000   23600.00
HO2+CH2O<=>HCO+H2O2                      5.600E+06    2.000   12000.00
C+O2<=>O+CO                              5.800E+13     .000     576.00
C+CH2<=>H+C2H                            5.000E+13     .000        .00
C+CH3<=>H+C2H2                           5.000E+13     .000        .00
CH+O2<=>O+HCO                            6.710E+13     .000        .00
CH+H2<=>H+CH2                            1.080E+14     .000    3110.00
CH+H2O<=>H+CH2O                          5.710E+12     .000    -755.00
CH+CH2<=>H+C2H2                          4.000E+13     .000        .00
CH+CH3<=>H+C2H3                          3.000E+13     .000        .00
CH+CH4<=>H+C2H4                          6.000E+13     .000        .00
CH+CO(+M)<=>HCCO(+M)                     5.000E+13     .000        .00
     LOW  /  2.690E+28   -3.740   1936.00/
     TROE/   .5757  237.00  1652.00  5069.00 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/
CH+CO2<=>HCO+CO                          1.900E+14     .000   15792.00
CH+CH2O<=>H+CH2CO                        9.460E+13     .000    -515.00
CH+HCCO<=>CO+C2H2                        5.000E+13     .000        .00
CH2+O2=>OH+H+CO                          5.000E+12     .000    1500.00
CH2+H2<=>H+CH3                           5.000E+05    2.000    7230.00
2CH2<=>H2+C2H2                           1.600E+15     .000   11944.00
CH2+CH3<=>H+C2H4                         4.000E+13     .000        .00
CH2+CH4<=>2CH3                           2.460E+06    2.000    8270.00
CH2+CO(+M)<=>CH2CO(+M)                   8.100E+11     .500    4510.00
     LOW  /  2.690E+33   -5.110   7095.00/
     TROE/   .5907  275.00  1226.00  5185.00 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/
CH2+HCCO<=>C2H3+CO                       3.000E+13     .000        .00
CH2(S)+N2<=>CH2+N2                       1.500E+13     .000     600.00
CH2(S)+AR<=>CH2+AR                       9.000E+12     .000     600.00
CH2(S)+O2<=>H+OH+CO                      2.800E+13     .000        .00
CH2(S)+O2<=>CO+H2O                       1.200E+13     .000        .00
CH2(S)+H2<=>CH3+H                        7.000E+13     .000        .00
CH2(S)+H2O(+M)<=>CH3OH(+M)               4.820E+17   -1.160    1145.00
     LOW  /  1.880E+38   -6.360   5040.00/
     TROE/   .6027  208.00  3922.00  10180.0 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/
CH2(S)+H2O<=>CH2+H2O                     3.000E+13     .000        .00
CH2(S)+CH3<=>H+C2H4                      1.200E+13     .000    -570.00
CH2(S)+CH4<=>2CH3                        1.600E+13     .000    -570.00
CH2(S)+CO<=>CH2+CO                       9.000E+12     .000        .00
CH2(S)+CO2<=>CH2+CO2                     7.000E+12     .000        .00
CH2(S)+CO2<=>CO+CH2O                     1.400E+13     .000        .00
CH2(S)+C2H6<=>CH3+C2H5                   4.000E+13     .000    -550.00
CH3+O2<=>O+CH3O                          3.560E+13     .000   30480.00
CH3+O2<=>OH+CH2O                         2.310E+12     .000   20315.00
CH3+H2O2<=>HO2+CH4                       2.450E+04    2.470    5180.00
2CH3(+M)<=>C2H6(+M)                      6.770E+16   -1.180     654.00
     LOW  /  3.400E+41   -7.030   2762.00/
     TROE/   .6190  73.20  1180.00  9999.00 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/
2CH3<=>H+C2H5                            6.840E+12     .100   10600.00
CH3+HCO<=>CH4+CO                         2.648E+13     .000        .00
CH3+CH2O<=>HCO+CH4                       3.320E+03    2.810    5860.00
CH3+CH3OH<=>CH2OH+CH4                    3.000E+07    1.500    9940.00
CH3+CH3OH<=>CH3O+CH4                     1.000E+07    1.500    9940.00
CH3+C2H4<=>C2H3+CH4                      2.270E+05    2.000    9200.00
CH3+C2H6<=>C2H5+CH4                      6.140E+06    1.740   10450.00
HCO+H2O<=>H+CO+H2O                       1.500E+18   -1.000   17000.00
```

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11-01-30 23.08

http://www.me.berkeley.edu/gri_mech/version30/text30.html

Reduced Chemical Kinetics

Example: Jet A is a kersone grade fuel with a carbon number distribution between 8 and 16.

Jet A can be assumed to consist of C_8H_{18}, $C_{10}H_{22}$, $C_{12}H_{22}$, $C_{12}H_{24}$, $C_{14}H_{26}$ and $C_{16}H_{28}$ with the average molecular formula $C_{12}H_{23.}$

Jet-A: $C_{12}H_{23}$-air; 18 species, 46 reactions (Yungster & Breisacher 2005)

Reduction technique of Meredith & Black based on SQP to simulate a set of continuously stirred tank reactors.

⇒ 5 species and 2 reactions

⇒ Acceptable agreement for $0.3<\varphi<1.3$

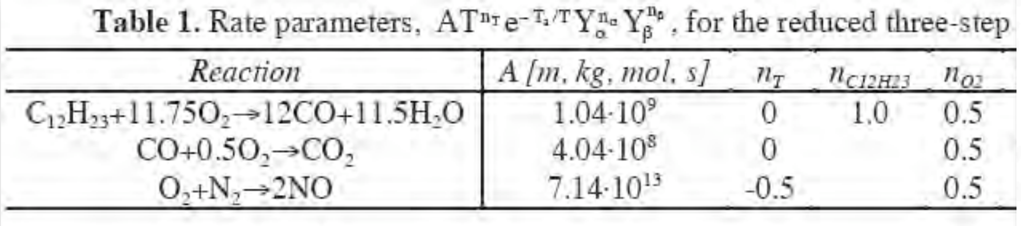


Table 1. Rate parameters, $AT^{n_T}e^{-T_a/T}Y_\alpha^{n_\alpha}Y_\beta^{n_\beta}$, for the reduced three-step

Reaction	*A [m, kg, mol, s]*	n_T	n_{C12H23}	n_{O2}
$C_{12}H_{23}+11.75O_2 \rightarrow 12CO+11.5H_2O$	$1.04\cdot10^9$	0	1.0	0.5
$CO+0.5O_2 \rightarrow CO_2$	$4.04\cdot10^8$	0		0.5
$O_2+N_2 \rightarrow 2NO$	$7.14\cdot10^{13}$	-0.5		0.5

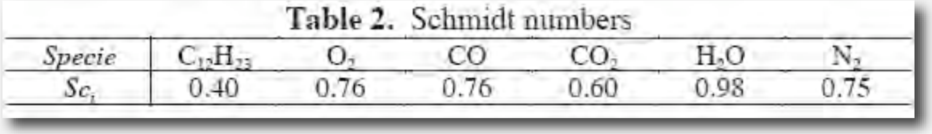
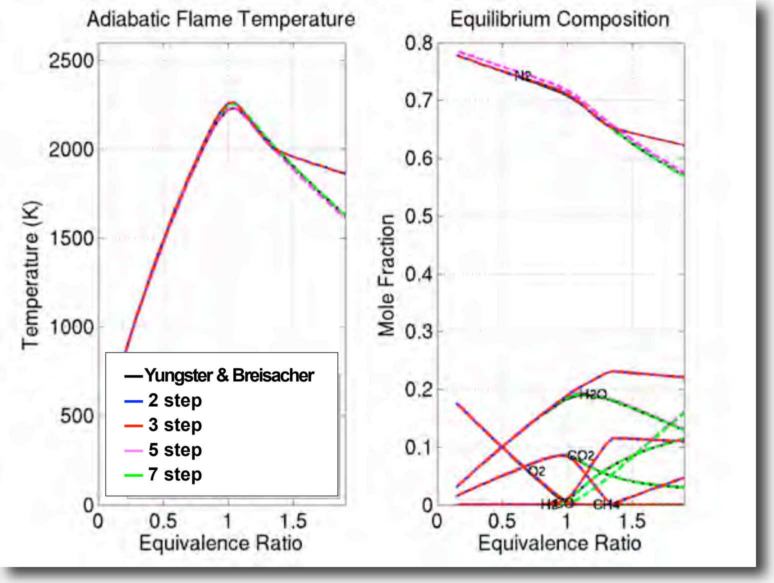


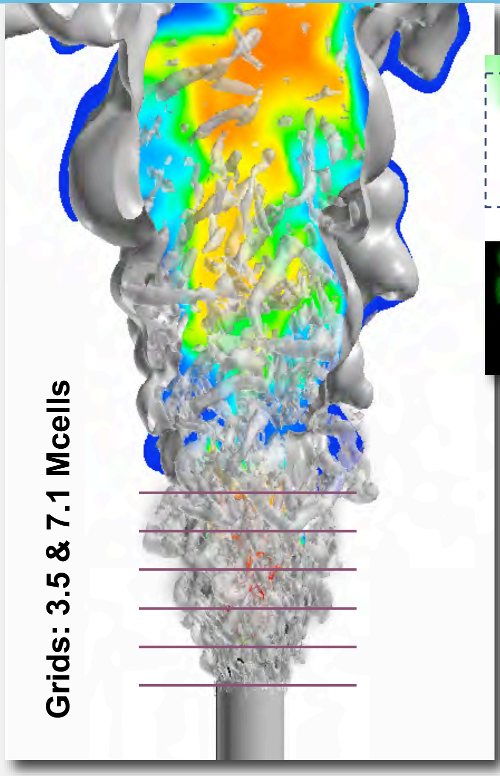
Table 2. Schmidt numbers

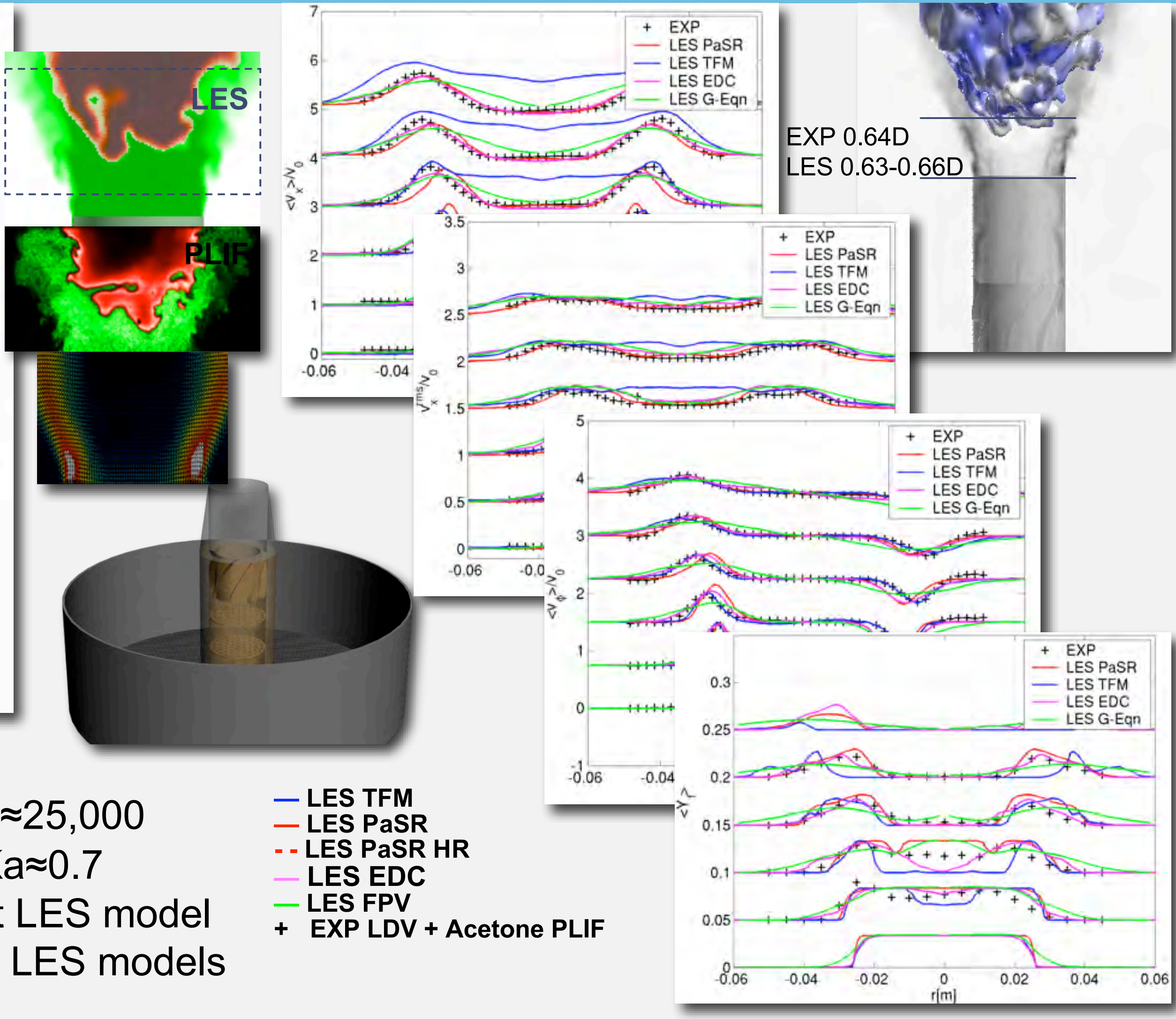
Specie	$C_{12}H_{23}$	O_2	CO	CO_2	H_2O	N_2
Sc_i	0.40	0.76	0.76	0.60	0.98	0.75



Yungster & Breisacher AIAA 2005-4210
Meredith & Black AIAA 2006-1168

Validation: Low Swirl Burner





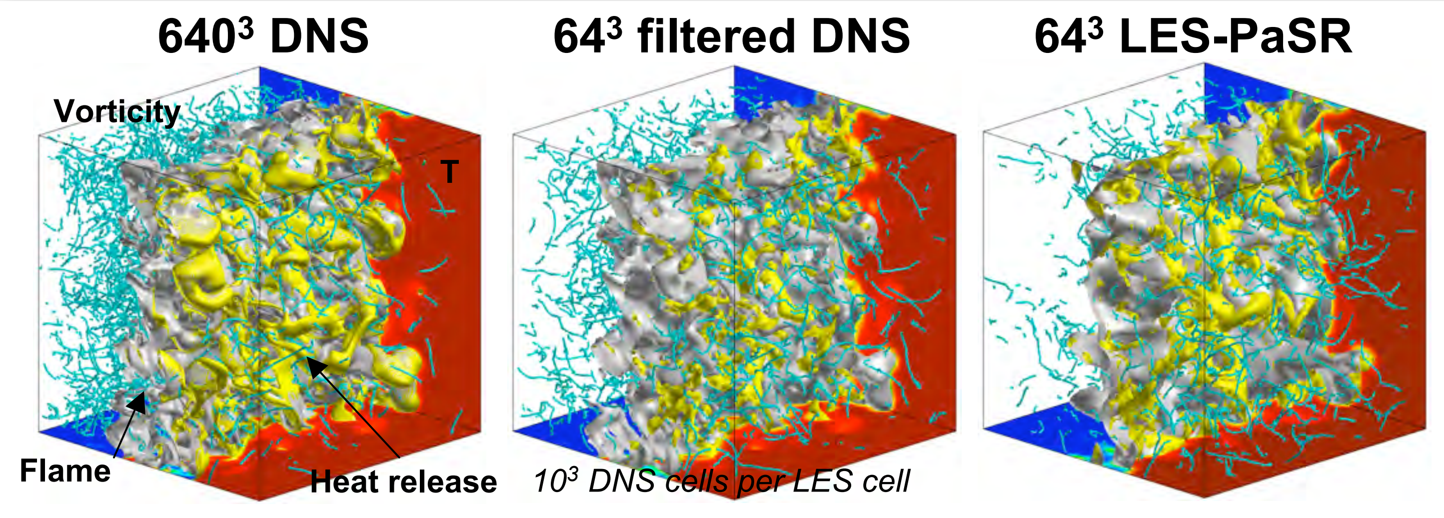
— LES TFM
— LES PaSR
- - LES PaSR HR
— LES EDC
— LES FPV
+ EXP LDV + Acetone PLIF

EXP: Pettersson *et al*
CH_4/air, $\Phi\approx0.5$, Re≈25,000
$Re_t\approx218$, Da≈20, Ka≈0.7
LTH: G equation flamelet LES model
FOI: EDC, PaSR & TFM LES models

Nogenmyr et al.; 2008, AIAA 2008-0513
Nogenmyr et al.; 2009, Comb. Flame. ***156****, p 25*

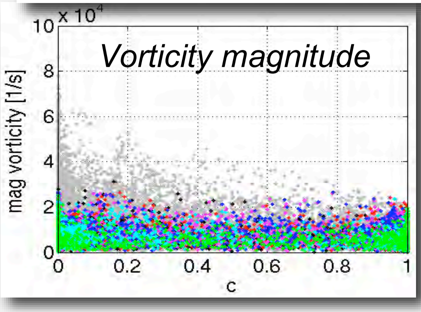
Detailed Physics: Planar Flame in HIT

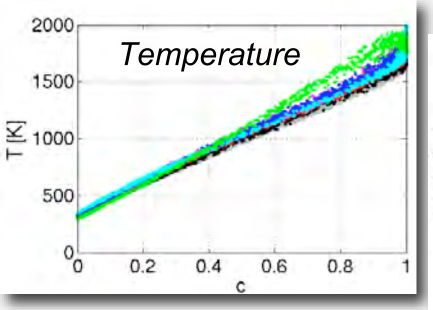
Need to understand how different LES combustion models capture the at least a canonical flame. DNS & LES of a box of size 18 mm.

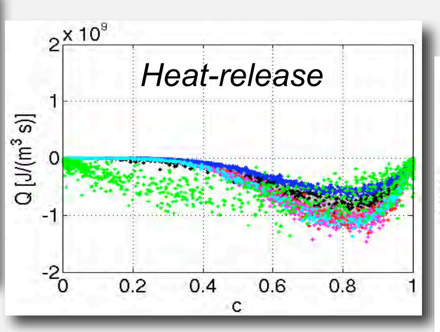


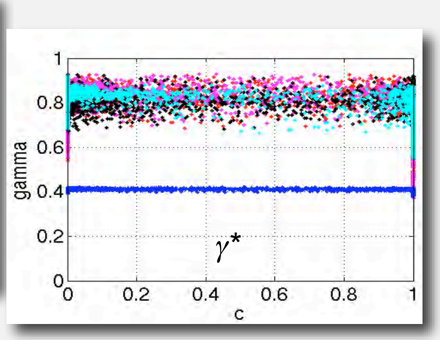
$Re_l \approx 374$
$Re_T \approx 44$
$Ka \approx 3.4$
$Da = 5.5.$

DNS
Filtered DNS
LES-FPV
LES-PaSR
LES-EDC
LES-TFM
LES new model









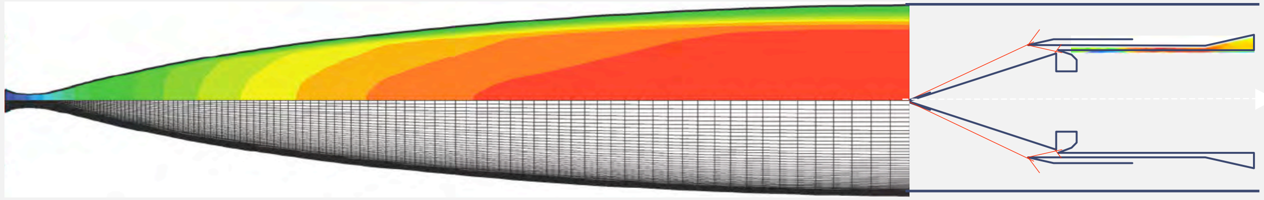
CESAR Aero GT Engine Combustor

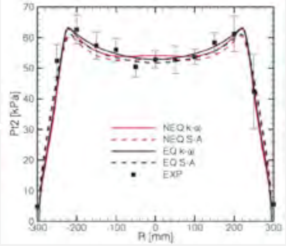
Fedina *et al* AIAA 2011-0785

The HYSHOT Combustor

A detailed CFD study of the flight experiments must incorporate also the HEG nozzle and test section. **Combine RANS and LES.**

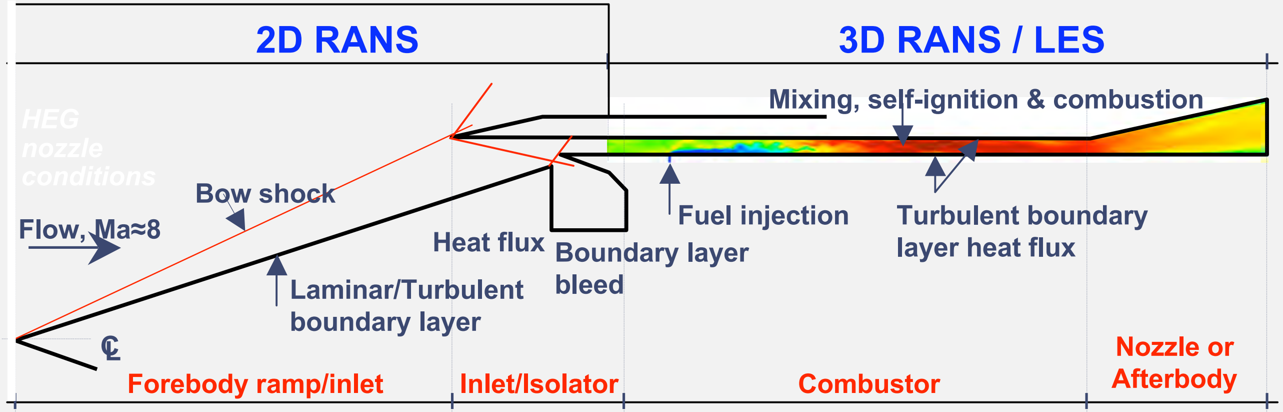
Stand alone RANS in HEG nozzle (DLR)

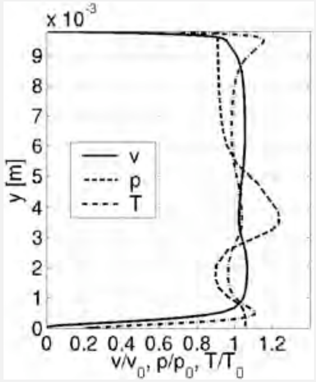




Axisymmetric RANS model with 20,000 cells

RANS in HEG test section + RANS/LES in combustor



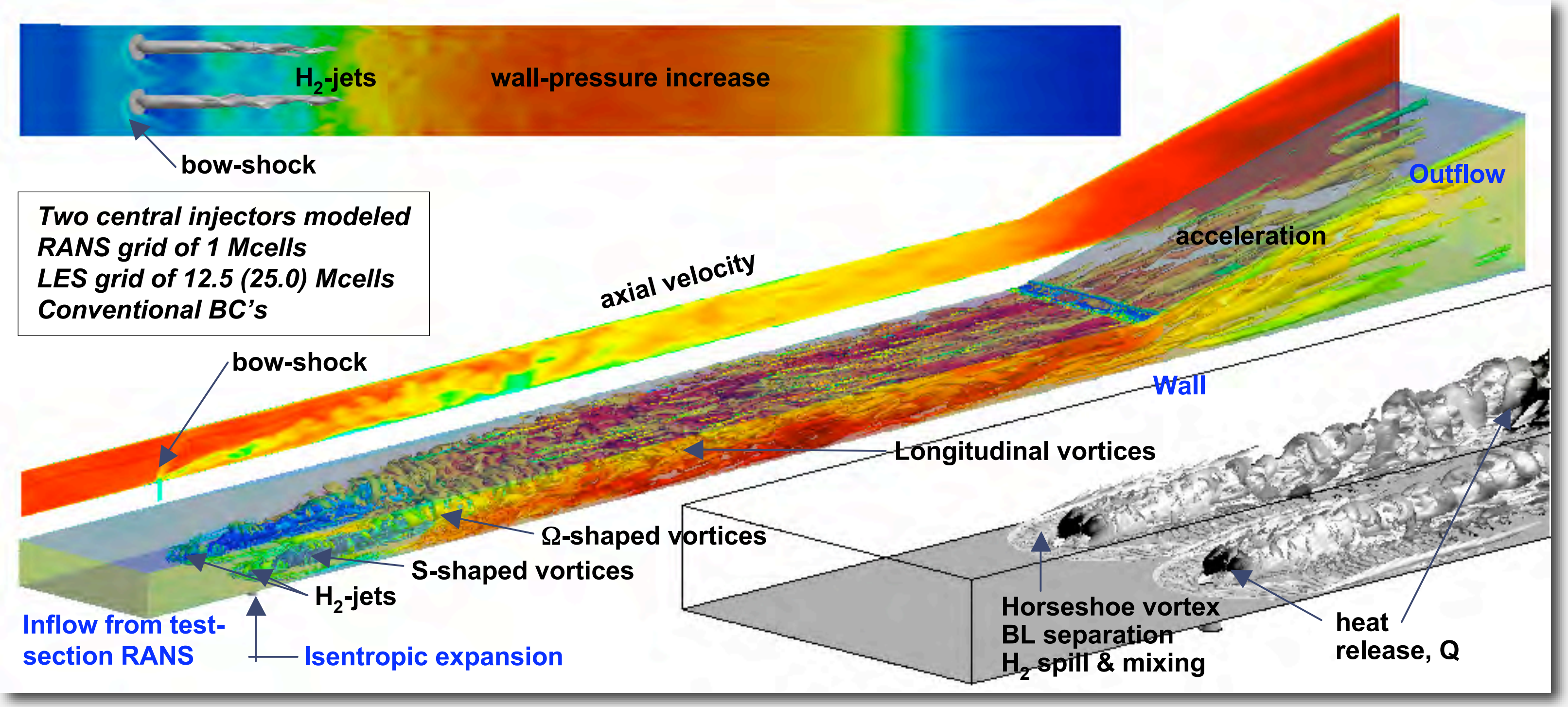


v_0=1800 m/s, T_0=1459 K, p_0=53.0 kPa.

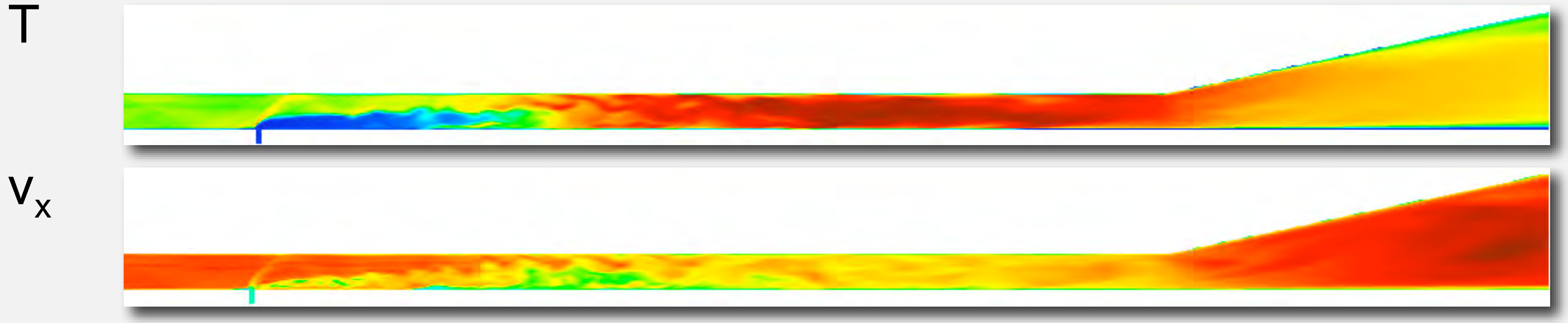
2D planar RANS (15,000 cells) of the flow in the entire HEG test section
3D RANS (1 Mcells) and 3D LES (12.5/25.0 Mcells) of the flow in the combustor

Karl *et al*, 2006, AIAA 2006-8041
Fureby *et al*, 2010, Proc. Comb. Inst.

Large Scale Global Flow Features

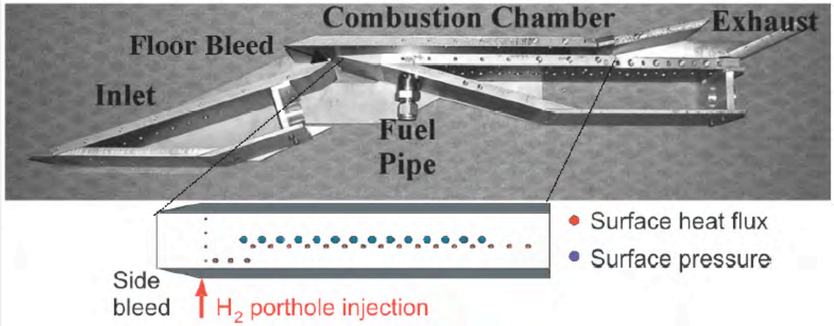


Two central injectors modeled
RANS grid of 1 Mcells
LES grid of 12.5 (25.0) Mcells
Conventional BC's



Fureby *et al*, 2010, Proc. Comb. Inst.

Validation & Combustion Dynamics



Significant unsteadiness and coherent structure dynamics

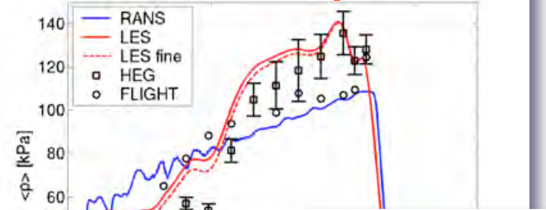
- Acoustic energy balance

$$\partial_t(\mathcal{E})+\nabla\cdot\mathcal{F}\approx\frac{\gamma-1}{\gamma p_0}p'\dot{Q}$$

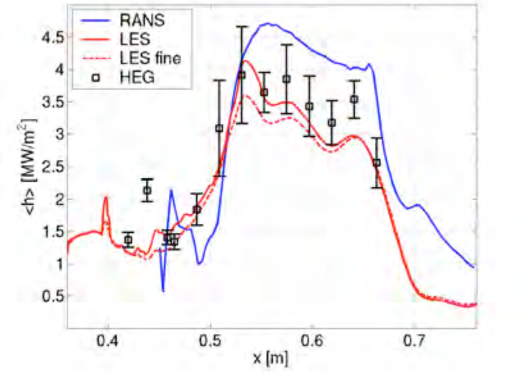
- FFT Analysis

  P1: Jet-shear layer, P3: Longitudinal

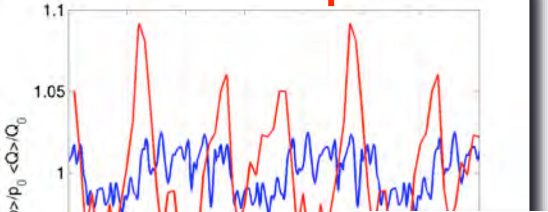
Centerline wall pressure



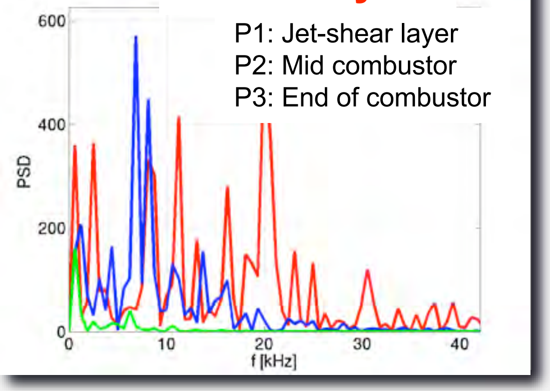
Off-centerline heat-flux



Heat-release & pressure

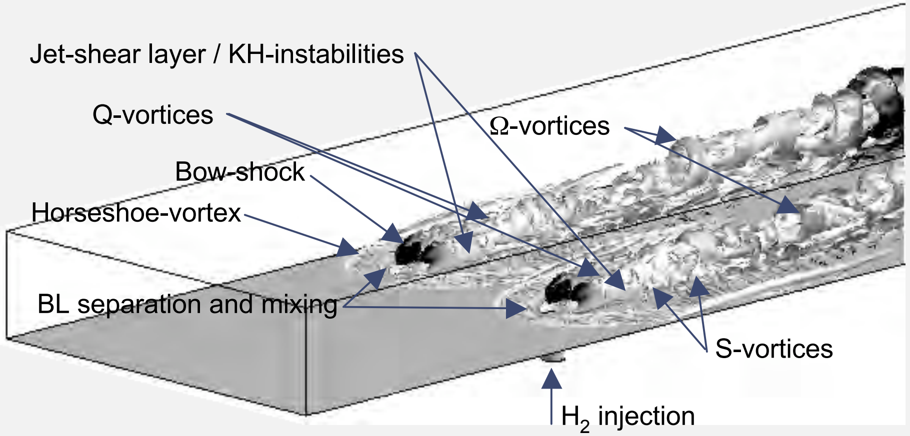


FFT analysis



Fureby *et al*, 2010, Proc. Comb. Inst.

Mixing, Flameholding, Self-ignition, …



Jet-shear layer / KH-instabilities

Q-vortices

Ω-vortices

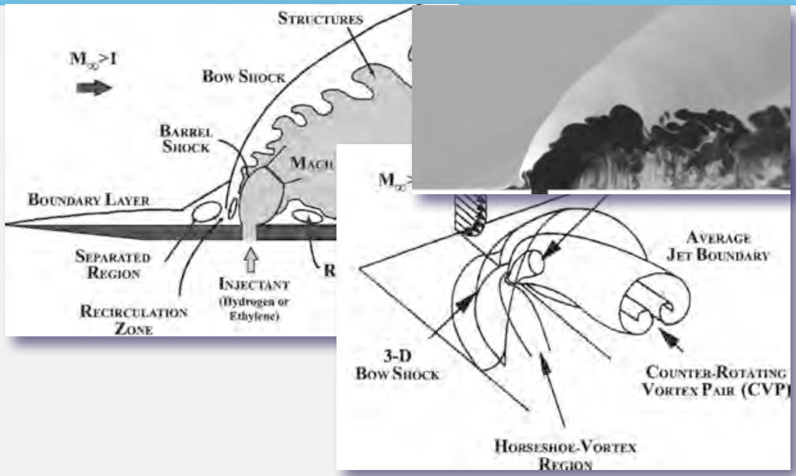
Bow-shock

Horseshoe-vortex

BL separation and mixing

S-vortices

H_2 injection

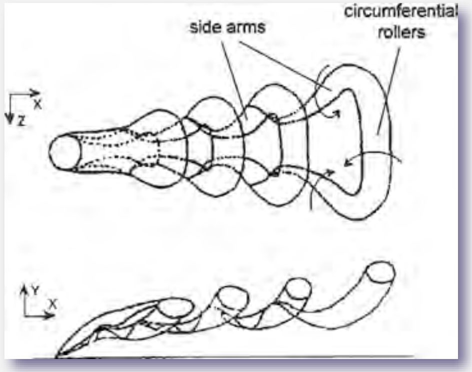


Bow shock causes BL to separate and H_2 to leak into downstream BL region

H_2 rich jet shear layer undergoes KH instabilities

H_2 rich side arms (S-vortices) and spanwise rollers (Q-vortices) are formed

The H_2 rich S and Q-vortices are transported downstream under intense shear during which H_2 mix macroscopically with hot air. S and Q vortices merge to Ω-vortices.



Stretching increases the interfacial area and steepens the concentration gradients whilst enhancing the diffusive micromixing.

Self-ignition takes place after micromixing is complete.

Fureby *et al*, 2010, Proc. Comb. Inst.

Can Modeling of Reactive Flows Describe Reality?

YES and NO.

The computational framework (models, methods and codes) is now available. The computational infrastructure is somewhat limited but is rapidly becoming available.

Need to develop a better understanding of the chemistry and how to model certain processes (TCI, …) (sub-models). Importance?

How does turbulence influence … and vice versa.

- Scalar mixing
- Combustion chemistry
- Conjugate heat transfer
- Acoustics

Need to better work with the experimentalists.

Need to use our skills to demonstrate to companies, funding agencies, etc. that engineering problems can be computed.

Things evolve … Plasma assisted combustion …