Numerical Modelling
And
High Performance Computing
of
CCS Derived Fuels Combustion

Eugenio Giacomazzi
TER-ENE-IMP, ENEA – C.R. Casaccia, Rome, ITALY

International School of Geophysics – 30th Course
CO$_2$ Capture and Storage: Towards a UK-Italy Common Strategy within a Global Framework
Erice [Sicily], Italy, 1-7 November 2007
Why Numerical Simulations of Combustion?

• Dealing with CO₂ sequestration implies dealing with particular fuels.

• CCS derived fuels: H₂, syngas (CO/H₂/N₂), hythane (H₂/CH₄).

• Better understanding of physics involved in combustion of these fuels to enhance energetic efficiency can be achieved by means of numerical simulation:
  • H₂, syngas, hythane “standard” combustion;
  • their MILD combustion to reduce NOx;
  • coal gasification and combustion.

In particular, since most physics is hidden in the unsteadyness, unsteady numerical simulation (LES) becomes a strategic tool to enhance control of combustion by means of new technology.

The aim of this talk is to show present capabilities of numerical simulation focusing on CCS derived fuels combustion.
Combustion Scenario

Fluid dynamics – Turbulence

Chemical kinetics

Radiant transfer of energy

Multi-phase flows
What Do We Need to Know to Simulate Combustion?

• Physics

• Modelling

• Numerics

• Super-Computing
- Turbulence and Its Modelling -
What is Turbulence?

- Spectrum of scales (eddies): from integral macroscale down to dissipative scales
- Vortices, eddies, scales
- Kinetic energy transferred “without” dissipation from average motion down to dissipative scale
- 3D unsteady flows
- Rotational flows
- High Reynolds
- Fluctuations: $1 \div 10^4$ Hz
- Intermittence: peaks larger than common fluctuations
- Increase of scalar gradients: acceleration of molecular transport
Turbulent Kinetic Energy Spectrum

\[ \frac{\partial E}{\partial t} = W(k, t) - 2\nu k^2 E \]

Anisotropic Scales

- \( U_K = (\frac{D_0}{\nu \epsilon})^{1/3} \)
- \( L_K = (\frac{D_0}{\nu \epsilon})^{2/3} \)

Dependent on conditions of formation

Isotropic Scales

- \( U_K = (\frac{\nu \epsilon}{L_0})^{1/4} \)
- \( L_K = (\frac{\nu \epsilon}{L_0})^{3/4} \)

Independent of conditions of formation

Boundary conditions effect

Dissipative subrange

Integral macroscale

\( K_e \)

Dissipative scale

\( K_d \)

Chemical reactions

Forward cascade

\( \frac{\partial E}{\partial t} \) is small

\( \frac{\partial E}{\partial t} \) is large

\( 2/3 - 5/3 \)

(Kolmogorov)

\( K^{-7} \)

(Heisenberg)

Dissipative subrange

Nonreactive

Reactive
Unsteady Spectral Characterization of Turbulent Flames

Unsteadiness of the spectra sampled in 1 s when the flame is close to extinction.

When the flame is unstable, small scales fluctuations cause large scale fluctuations (opposite when the flame is stable).

Radiant energy spectra averaged by using 60 spectra, each sampled in 1 s, when a flame is stable and when is close to extinction.

Non local (in wave numbers and not in space) scale interaction!
The Equations of Flow Motion

The flow motion is ruled by a system of equations, that for a reacting flow is

\[ \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho u) = 0 \]

\[ \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho u u) = \nabla \cdot \mathbf{S} + \rho \sum_{i=1}^{N_s} Y_i f_i \]

\[ \frac{\partial Y_i}{\partial t} + \nabla \cdot (\rho u Y_i) = - \nabla \cdot \mathbf{J}_i + \rho \dot{\omega}_i \]

Therefore, a turbulent flow can be predicted by accurately solving the Navier-Stokes equations, but ...
Why is Modelling Needed?
The Cost of Solving the Whole Spectrum of Scales

- Turbulence ⇒ spectrum of scales, from $L$ down to $\eta$

- Dissipation takes place for $0.1 < k \eta < 1$, i.e., $6 \eta < l < 60 \eta$

Therefore, to resolve the whole spectrum of scales

- **Spatial resolution** required: $(L/\eta)^3 \sim \left(Re_L^{3/4}\right)^3 = Re_L^{9/4}$

- **Time resolution** required: $\tau_L/\tau_\eta \sim Re_L^{1/2}$

- **CPU time** required: $\propto Nodes \times N_{\Delta t} \sim Re_L^{11/4}$

Note that this simple estimate is valid for a free flow. Near walls spatial resolution increases (the mixing length decreases).

Today DNS is feasible only for simple flows, even using supercomputing!
**DNS, LES and RANS**

**Direct Numerical Simulation:**
Navier-Stokes equations are solved **without modelling** (the error is only numerical).

**Large Eddy Simulation:**
Navier-Stokes equations are **spatially filtered**, hence, scales larger than the filter size $\Delta$ are resolved, while the smaller ones are modeled (thanks to their universal features).

**Reynolds Averaged Navier-Stokes:**
Navier-Stokes are **filtered in time**, hence, the spectrum of scales is reduced just to one scale, i.e., the average scale.

**LES**
- with respect to **DNS**, the description of small scales is **lost**;
- with respect to **RANS**, the dynamics of large scales is **gained**.

Is it RANS/FANS end?

**NO!** Still needed in design due to the **much lower** computational time. **LES** can be used for unsteady analysis of the **selected geometries**.
Large Eddy Simulation

- Fundamental Mathematical and Modelling Aspects -
Variable Decomposition in LES

• Field variables are decomposed into **resolved** and **subgrid-scale** (or residual) parts.

For reacting flows
  • a **Reynolds decomposition** is used for quantities per unit volume: \( \rho = \rho + \rho' \)
  • a **Favre** (density-weighted) **decomposition** is used for quantities per unit mass:
    \[
    \mathbf{u} = \bar{\mathbf{u}} + \mathbf{u}'' \quad \text{with} \quad \bar{\mathbf{u}} = \frac{\rho \mathbf{u}}{\bar{\rho}}
    \]

For nonreacting flows
  • only the **Reynolds decomposition** is used (sometimes also for reacting flows).

• The resolved, large-scale fields are related to the instantaneous full-scale fields through a **grid filtering operation** (applied to the Navier-Stokes equations) that removes scales too small to be resolved by the simulation.
Spatial Filtering in LES

A spatial filter operator $G_\Delta$ separates large resolved scales from small modelled scales.

Filtering is mathematically expressed by means of a convolution integral

$$\bar{f}(x) = \int_D f(x') G_\Delta(x-x') \, dx' \quad \text{or} \quad \bar{\rho \bar{f}}(x) = \int_D \rho f(x') G_\Delta(x-x') \, dx'$$

where $D$ is the whole domain and $G_\Delta$ is the filter of scale $\Delta$ with these properties:

$$G_\Delta(x) = G_\Delta(x')$$  \hspace{1cm} (1)

$$\int_D G_\Delta(x, x') \, dx' = 1$$ \hspace{1cm} (2)

$$G_\Delta(x) \to 0 \quad \text{for} \ x > \Delta$$ \hspace{1cm} (3)

The size of the filter has not to be necessarily uniform, i.e., $\Delta$ can vary over the grid.

Furthermore:

- $\bar{f} \neq \bar{f}$ and $\bar{f}' \neq 0$ (= only when a cut-off filter in the spectral space is used);
- commutation is assumed for derivative and filter operations, i.e., $\frac{\partial \bar{f}}{\partial t} = \frac{\partial \bar{f}}{\partial t}$, $\frac{\partial \bar{f}}{\partial x_j} = \frac{\partial \bar{f}}{\partial x_j}$.

Commutation error for symmetric filters does not depend on their shape and is $O(\Delta^2)$.

Some filters are not affected by this error. However, it is generally neglected and assumed to be incorporated in the SGS model.
Spatial Filters in LES

- **Sharp (spectral) Cut-Off** (in the spectral space):
  \[ \tilde{G}(k) = \begin{cases} 
  1 & \text{if } k \leq \pi / \Delta \\
  0 & \text{otherwise}
\end{cases} \]
  where \( k \) is the spatial wave number (cut-off length scale = 2\( \Delta \))
  corresponding to \( G(|x|, \Delta) = 1 / \Delta \sin \left[ \pi |x| / \Delta \right] / (\pi |x| / \Delta) \).

- **Top-hat or box** (in the physical space, corresponding to averaging over a box of size \( \Delta \)):
  \[ G(x) = \begin{cases} 
  1 / \Delta & \text{if } |x_i| \leq \Delta / 2, i = 1, 2, 3 \\
  0 & \text{otherwise}
\end{cases} \]
  corresponding to \( \tilde{G}(k) = \sin \left[ k \Delta / 2 \right] / (k \Delta / 2) \) that filter scales with \(|k| \leq \pi / \Delta\).

- **Gaussian** (in the physical space):
  \[ G(x) = \left( \frac{6}{\pi \Delta \gamma} \right)^{1/2} \exp \left[ -\frac{6}{\Delta \gamma} |x|^2 \right] \]
  corresponding to \( \tilde{G}(k) = e^{-k^2 \Delta^2 / 24} \).

- **Implicitly defined** by the computational grid and directly used in the SGS model (corresponds to top-hat or grid filtering):
  \[ \Delta = \sqrt[3]{Vol_{cell}} \]
LES Filtered Navier-Stokes Equations

LES equations for the resolved fields are formally derived by substituting the field variables decomposition into the governing equations, and then subjecting the equations to the grid filter.

\[
\frac{\partial \bar{\rho}}{\partial t} + \frac{\partial \bar{\rho} \bar{u}_i}{\partial x_i} = 0
\]

\[
\frac{\partial \bar{\rho} \bar{u}_i}{\partial t} + \frac{\partial}{\partial x_j} \left[ \bar{\rho} \bar{u}_i \bar{u}_j + \bar{\rho} \delta_{ij} - \bar{\tau}_{ij} + \tau_{i,j}^{SGS} \right] = 0
\]

\[
\frac{\partial \bar{\rho} \bar{E}}{\partial t} + \frac{\partial}{\partial x_i} \left[ (\bar{\rho} \bar{E} + p) \bar{u}_i + \bar{q}_i + \sum_{k=1}^{N_S} q_{i,k}^{SGS} - \bar{\tau}_{ij} \bar{u}_i + H_i^{SGS} + \sigma_i^{SGS} \right] = 0
\]

\[
\frac{\partial \bar{\rho} \bar{Y}_k}{\partial t} + \frac{\partial}{\partial x_i} \left[ \bar{\rho} \bar{Y}_k \bar{u}_i - \bar{\rho} \bar{Y}_k \bar{V}_{i,k} + Y_{i,k}^{SGS} + \Theta_{i,k}^{SGS} \right] = -\bar{\rho} \bar{\omega}_k
\]

\[
p = \bar{\rho} R_g T
\]

Statistical effects of the instantaneous small-scale fluctuations are in unclosed terms representing the influence of the subgrid scales on the resolved scales:

\[
\tau_{i,j}^{SGS} = \bar{\rho} \bar{u}_i \bar{u}_j - \bar{\rho} \bar{u}_i \bar{u}_j \\
H_i^{SGS} = \bar{\rho} \bar{H}_i \bar{u}_i - \bar{\rho} \bar{H}_i \bar{u}_i \\
\sigma_i^{SGS} = \bar{\tau}_{i,j} \bar{u}_i - \bar{\tau}_{i,j} \bar{u}_i \\
q_{i,k}^{SGS} = h_k D_k \partial Y_k / \partial x_i - \bar{h}_k \bar{D}_k \partial \bar{Y}_k / \partial x_i
\]

\[
Y_{i,k}^{SGS} = \bar{\rho} u_i \bar{Y}_k - \bar{\rho} u_i \bar{Y}_k \\
\Theta_{i,k}^{SGS} = \bar{\rho} V_{i,k} \bar{Y}_k - \bar{\rho} V_{i,k} \bar{Y}_k
\]

These unclosed terms contain SubGrid Scale (SGS) effects and have to be modeled.
The Eddy Viscosity in LES and RANS/FANS Modelling

- Eddy Viscosity (viscous stress analogy) models link subgrid stresses $\tau_{ij}^{SGS}$ to strain rate $\bar{\epsilon}_{ij}$

$$\tau_{ij}^{SGS} - \frac{\delta_{ij}}{3} \tau_{kk}^{SGS} = -2\nu_t \bar{\epsilon}_{ij}$$

- Usually the subgrid eddy viscosity is defined by means of algebraic models.
  - Easy and low cost.
  - A simple algebraic model can describe physics of small scales, that are more homogeneous and isotropic than large scales.
  - Subgrid stresses are a small fraction of the total, thus errors of the SGS model should not decrease global accuracy of the results.

Eddy viscosity is distributed differently in RANS and LES and it has different order of magnitudes.

Example: eddy viscosity distribution in the recirculation zone downstream of a bluff-body.
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**Correa and Gulati Test Case**

<table>
<thead>
<tr>
<th>$X_{\text{Fuel}}$</th>
<th>CO</th>
<th>$H_2$</th>
<th>$N_2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>%</td>
<td>27.5</td>
<td>32.3</td>
<td>40.2</td>
</tr>
</tbody>
</table>

1 atm: validation with experiments

10 atm: only numerical solution

<table>
<thead>
<tr>
<th>$p$</th>
<th>1 atm</th>
<th>10 atm</th>
</tr>
</thead>
<tbody>
<tr>
<td>Thermal Power</td>
<td>4.2 kW</td>
<td>42 kW</td>
</tr>
<tr>
<td>$Re_{\text{Air}}$</td>
<td>37000</td>
<td>370000</td>
</tr>
<tr>
<td>$Re_{\text{Fuel}}$</td>
<td>25500</td>
<td>255000</td>
</tr>
<tr>
<td>$\eta_{\text{Air}}$</td>
<td>21 $\mu$m</td>
<td>4 $\mu$m</td>
</tr>
<tr>
<td>$\eta_{\text{Fuel}}$</td>
<td>1.5 $\mu$m</td>
<td>0.3 $\mu$m</td>
</tr>
<tr>
<td>$\Phi_{\text{global}}$</td>
<td>0.017</td>
<td>0.017</td>
</tr>
<tr>
<td>$Ma_{\text{Fuel}}$</td>
<td>0.32</td>
<td>0.32</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th></th>
<th>Air</th>
<th>Fuel</th>
</tr>
</thead>
<tbody>
<tr>
<td>$U$</td>
<td>6.5 m/s</td>
<td>80 m/s</td>
</tr>
<tr>
<td>$T$</td>
<td>300 K</td>
<td>300 K</td>
</tr>
</tbody>
</table>
The flame oscillates due to periodic vortex shedding from the inner edge of the bluff-body.

1 atm
Hot spots are periodically released downstream.

Hot spots could still burn at the exit going through turbine blades.

Zoomed-in view of the recirculation zone downstream of the bluff-body.
Strategy: **auxiliary pulsed air jet** to prevent "opening" of inner vortex

- located in the bluff-body
- $U_{JET} = 30 m/s \sim 1.5 \text{times}$ translational velocity of inner vortex

**no – JET Case**

**JET Case**
Effect of The Control Strategy

GE Burner with Active Control by Air Jet - $p = 10$ atm

Temperature Scale ($T [K]$):
- 332
- 429
- 526
- 622
- 719
- 816
- 913
- 1009
- 1106
- 1203
- 1299
- 1396
- 1493
- 1590
- 1686
- 1783
- 1880
Effect of the Control Strategy

GE Burner with Active Control by Air Jet - $p = 10$ atm

Zoomed-in view of the recirculation zone downstream of the bluff-body (burner operated with active control)
Effect of The Control Strategy

- No hot spots released!
- Flame **shortens**: lower average $T$ at exit section.
- Combustion **efficiency** in terms of unburnt fuel at the exit.
  $$\zeta_F = \frac{m_F^{\text{exit}}}{m_F^{\text{inlet}}}$$
  Pulsed air jet increases efficiency by $\sim 60\%$ ($\zeta_{CO}$). In both cases $\zeta_{H_2} = 0$.
- **Thermal NO** very low in both cases (short convective time and low average $T$).
- Efficiency increased
- More $CO_2$ to capture (post-combustion treatment)
Active control strategy, based on the activation of surrounding air jets, is derived from numerical LES simulation

[Giacomazzi E. and Bruno C., ISABE 2001].
At present, LES cannot be applied to large scale combustors since computationally expensive. In these cases, the **whole combustor** can be analyzed by means of RANS techniques to capture macroscopic features.

- **LES** features better than RANS in predicting **turbulence related phenomena**.

  E.g., only the first part of the sketched combustor really needs LES analysis.

  The effects to take into account may be:
  - three- or two-phase flow;
  - liquid break-up;
  - turbulence in liquid and gas;
  - effects of coal particles on turbulence and vice versa;
  - radiant transfer of energy;
  - coal drying, devolatilization, oxidation, and gasification.

**NOTES**

- Present multi-phase scenario:
  - **LES** of multi-phase flows is at an **early stage** (**Many European projects**)
  - **DNS** is **simpler**, but limited to **very small volumes**!

- **Radiant** transfer of energy is typically neglected in LES to reduce computational cost, but it is **mandATORY** in some applications (MILD, coal combustion, …).
- Commonly Simplified Physics in Turbulent Combustion -
Commonly Simplified Physics in Turbulent Combustion

- **Chemical kinetics**: consider not only the main products but also some radicals. ⇒ Some level of “detail” is important to capture ignition and extinctions.

- **Compressibility**: acoustic-thermo-fluid-dynamic coupling is critical in instabilities. ⇒ The “low Mach number” approximation must be avoided even though $M << 1$. This increases computational time in unsteady simulations.

Coal Mach 1.92 supersonic jet

[Image: Mach 1.92 supersonic jet
[J. Freund, 2001 – APS Gallery of Fluid Motion]
• **Preferential diffusion**: close to injection, turbulent stirring is not so strong to make the effective individual diffusivities nearly equal. This results into thermo-diffusive mechanisms and thus **additional wrinkling** in turbulent flames.

- **Le_R < 1**: diffusion of reactants ("R") towards flame front is favoured, thus increasing flame surface area and **enhancing flame wrinkling**.

- **Le_R > 1**: heat ("H") diffusion towards reactants is favoured, thus decreasing flame surface up to a planar flame front.
In multicomponent gaseous diffusion, at least the zeroth-order model of Hirschfelder and Curtiss should be applied:

\[ D_{ij}^{[0]} = D_i = \frac{1 - Y_i}{\sum_{j=1, j \neq i}^{N_s} X_j / D_{ii}} \]

This model still involves the calculation of binary mass diffusion coefficients from kinetic theory expressions. This is still expensive in a CFD computation.

A very simple and economic way to obtain individual species diffusion coefficients consists in deriving them from assumed Lewis or Schmidt numbers [Smooke and Giovangigli, 1991]:

\[ L_e_i = \alpha / D_i = S_c_i / Pr \quad \Rightarrow \quad D_i = \alpha / L_e_i \]

\[ S_c_i = \nu / D_i \quad \Rightarrow \quad D_i = \nu / S_c_i \]

where \( \alpha = k / (\rho C_p) \) is the mixture thermal diffusivity, and \( Pr = \mu C_p / k \) is the Prandtl number.

As a matter of fact, the constant Lewis and Schmidt number assumptions have never been justified nor verified in practical flames.
Nonpremixed flames experience more thermochemical states than premixed ones. Thus, Lewis or Schmidt numbers against temperature distributions are expected to be broader.

- The Schmidt number distributions are tighter than the Lewis distributions.
Mass Diffusivities via Individual Lewis or Schmidt Numbers?

Final Receipt

• Since Schmidt number against temperature distributions for individual species are less broad than those of Lewis number, in both premixed and non-premixed flames, the constant Schmidt number assumption seems more correct.
• Since non-premixed flames, and in particular those experiencing localized extinctions, involve many thermo-chemical states, distributions derived from non-premixed flames are more meaningful than those of premixed ones.
• Since these distributions are generally skewed or unbalanced, the median describes their central tendency better than the mean.
• Thus,

\[ D_{i,\text{mix}} = \frac{\alpha}{Le_i} \]

where \( Sc_i \) is the median of the non-premixed flame \( Sc_i \) against T distributions.

Commonly Simplified Physics in Turbulent Combustion

- **Mixture transport properties**: most simplifications strongly affect flame dynamics.

  E.g., the nonpremixed syngas-air SANDIA “Flame A” is **stably anchored** in experiments.

  In **numerical simulations**, the **anchoring changes** depending on the modelling of the mixture thermal conductivity, $K_{\text{mix}}$:
  - if $K_{\text{mix}}$ is modeled with the more accurate Mathur’s empirical law, the flame is **stably anchored**.
  - if $K_{\text{mix}}$ is modeled as $\sum_{i=1}^{N_s} Y_i K_i$, the flame shows **localized extinctions**.
Commonly Simplified Physics in Turbulent Combustion

- **Thermal radiation**: cannot be neglected in sooting flames, or when there is a strong dilution due to CO\textsubscript{2} and H\textsubscript{2}O (as in MILD combustion).

- **Small scale phenomena**:
  - **Dilatation** due to heat release
    - non-equilibrium of small scales
    - nonnegligible reverse energy cascade expected
    - intermittency
  - **Interaction** between eddies and flame structures → effects on turbulent spectra
  - **Pressure and temperature gradient diffusion** (Soret effect): important in mixing
  - **Viscous heating**
  - **Bulk viscosity**: cannot be neglected when flows experience “rapid” compressions, such as across shock waves, or expansions, as in supersonic expansion from holes in vacuo
  - **Dufour effect**: commonly negligible even though Soret effect is not

These effects should be included in SGS modelling of turbulent combustion.
Turbulent combustion is a multi-physics and multi-scale phenomenon.

Modelling this physics and the multi-scale interaction is the key to capture the complex dynamics of turbulent flames, in terms of localized extinctions and reignitions, flame pulsations, lift-off and blowout, and to test active and/or passive control strategies.
Multi-Scale Structure of Turbulent Flows

Sections: Y = 0 and Z = 41 mm

Cross-Section Z = 41 mm
The Test Case HM1 (SANDIA)

- **Nominal conditions**
  - **nonpremixed** flame
  - **axial jet: CH$_4$/H$_2$** (Hythane) mixture (50% in volume)
    - $U_z = 118$ m/s, $T = 300$ K, $Re = 13500$, $d_{JET}=3.6$ mm
    - $Re_{z=0} = 18000$
  - **coaxial jet: Air**
    - $U_z = 40$ m/s, $T = 300$ K, $Re = 300000$

- **Characteristics**
The actual flame is strongly **three-dimensional** and has three characteristic zones:

  - a stabilizing **recirculation** zone, extending up to $\sim 80$ mm downstream of the bluff-body;
  - a **neck** zone, where intense stretching produces local extinctions;
  - a **burnout** region further downstream, where the flame propagates in a jet-like manner.
$T = 9.1 \text{ ms}$

$\Delta f = 110 \text{ Hz}$
Recirculation Zone Dynamics

- Flow experiences
  - **symmetric vortex shedding** of large coherent structures from the **outer edge** of the bluff-body at \( \sim 100 \text{ Hz} \) ⇒ **intense flame stretching**, particularly close to the flame neck;
  - shedding of **irregular eddies** from the **inner edge** of the bluff-body spread over a wide range of frequencies \((790 \div 1600 \text{ Hz})\) ⇒ **intense mixing** inside the recirculation zone.
Effects of dilatation due to combustion

- Local density changes due to combustion expand products, locally accelerating the flow (via $\nabla \cdot \mathbf{u}$ term)
- High heat release frequencies
- Non-equilibrium reactive fine structures
- Reverse energy cascade: heat released inside fine structures $\Rightarrow$ local intermittent dilatation pumping energy into lower frequencies

Capturing these intermittent dilatational phenomena may reveal itself crucial to study certain type of combustion instabilities.
The “CO/H₂/N₂ Jet Flame A” of Sandia/ETH-Zurich

Unconfined turbulent jet flame in low-velocity coflow

- **Geometry**
  - nozzle inner diameter: \( d = 4.58 \text{ mm} \) (outer = 6.34 mm);
  - thickness of nozzle tubing: 0.88 mm \( \Rightarrow \text{very tight bluff-body} \);
  - coaxial channel (up to burner’s base): 300 mm \( \times \) 300 mm.

- **Reactants**
  - axial jet: CO/H₂/N₂ (Syngas, 40/30/30 in volume)
    - \( U_z = 76 \text{ m/s}, \ T = 292 \text{ K}, \ Re = 16700 \)
  - coaxial jet: Wet Air
    - \( U_z = 0.75 \text{ m/s}, \ T = 290 \text{ K}, \ X_{H₂O} = 0.012 \).

- **Flame characteristics**
  - flame length: \( L_{stoich} \sim 47 \text{ d} \);
  - stoichiometric mixture fraction: \( F_{stoich} = 0.295 \);
  - squared-off nozzle provides stabilization of the flame;
  - no lift off or localized extinction observed (z/d = 20, first exp. section).

- **Why choosing this test case for simulations**
  - simple geometry and many measurements;
  - syngas has a modest chemical kinetics complexity;
  - ... but the tubing wall that anchors the flame is too tight \( \Rightarrow \) computational inconvenience (high resolution required).
Chemical Kinetics

- **Simplified kinetics** ⇒ **FAST case**
  
  Fast Chemistry for **Hydrogen** oxidation → Hydrogen kinetics controlled by turbulence (EDC):

  \[
  H_2 + \frac{1}{2} O_2 \rightarrow H_2O \quad \Rightarrow \quad \dot{\omega}^* = \frac{\rho^*}{\tau^*(1 - \gamma^*)} \min \left[ Y_{H_2}, \frac{Y_{O_2}}{8} \right] \frac{kg_{H_2}}{m^3 \cdot s}
  \]

  Modified [Adams et al., 2000] Dryer and Glassman [1973] **single step** for **CO** oxidation:

  \[
  CO + \frac{1}{2} O_2 \leftrightarrow CO_2
  \]

  The flame is obviously **anchored also on a coarse computational grid** with poor spatial resolution in the tight (0.88 mm) region downstream of the nozzle tubing.

- **Finite rate kinetics** ⇒ **RED cases**

  **Reduced mechanism of Chen** [Sandia/TNF Website]
  
  (6 steps, 10 species, 70 reactions skeletal mechanism, 5 species in partial equilibrium).

  \[
  O_2 + H \leftrightarrow OH + O \quad \text{The flame does not anchor on computational grids that are coarse close to the nozzle tubing.}
  \]

  \[
  H_2 + O \leftrightarrow H + OH
  \]

  \[
  H_2 + OH \leftrightarrow H + H_2O
  \]

  \[
  H_2 \leftrightarrow 2H
  \]

  \[
  CO + OH \leftrightarrow H + CO_2
  \]

  \[
  N_2 + O_2 \leftrightarrow 2NO
  \]

  - **Investigation of the anchoring** mechanism by simulating the fuel injection region on a very fine grid (spatial resolution of 10^{-5} m).
  - Development of an **artificial stabilization mechanism** that works on coarser grids to simulate the whole flame.
Investigation of Flame Anchoring

The flame is anchored on the inner edge of the injection nozzle.

Syngas flames anchor easily. Attention should be payed when converting old plants!

Anchoring conditions in terms of mixing and sufficiently long residence time are due to small vortices alternatively shed from the squared-off inner and outer edges of the nozzle tubing.

Some positive effects for flame stabilization are also expected to be due to preferential diffusion, that can accelerate the mixing of hydrogen and air.
 Flame Dynamics

- **Starting** from the anchored and continuous flame of the FAST case, the flame initially lifts off.
- The flame is **anchored** on the outer edge of the nozzle; instead, in the RED\_ZOOM case, it was anchored on the inner edge.
- From the anchored flame front (~5 mm long) **hot pockets** of products accelerate **driven by buoyancy**.
- These hot pockets **ignite unburnt mixture** downstream thus producing a flame front that accelerates and reaches the main propagating flame at ~10 cm (close to z / d = 20, 1\textsuperscript{st} exp. sect.).
- Thus the “numerical” flame experiences periodic reignitions and extinctions close to the nozzle.
Large Eddy Simulation
- Numerical Aspects -
Motions with **scales comparable to the grid-spacing** may have **significant energy** at high Re.

- **Coarse meshes** cause **aliasing errors**: the energy of high wavenumbers not represented on the grid is aliased onto the resolved wavenumbers.
- The resulting **grid-to-grid oscillations** (wiggles) can become locally dominant and cause numerical instability when using high-order central difference schemes.
- These spurious oscillations are an indication of **poor resolution** of relevant lengthscale and must be **avoided** or **reduced**, e.g., by explicit **filtering** of field variables.
Effects of Reflecting and Non-Reflecting Boundary Conditions

3-D axisymmetric jet

- Downstream outflow is purely non-reflecting.
- Lateral outflow is partially non-reflecting.
- Inlet is reflecting and forces shedding at $f = U_b/L$ ($U_b = \text{bulk velocity}; L = \text{injector length}$)

$\Rightarrow$ Expansion waves moving upstream are reflected at the inlet, resulting in a phenomenon that seems physical, but in fact it is numerical.
- Super-Computing -
Domain Decomposition

- Execution of code is split into $N_p$ processes.

- The calculation domain is also split into $N_p$ sub-domains (optimal decomposition).

- Each processor of the parallel machine executes just one of the $N_p$ processes.

- The calculation sub-domains have boundary nodes (ghost frame) used to exchange data between processors of adjacent sub-domains or used for physical boundary conditions.
The relative speed-up $S$ is the ratio between the time needed with one processor, $T_1$, and the time needed with $N$ processors, $T_N$.

The **linear (ideal) speed-up** is a straight line: $S = T_1 / T_N = T_1 / (T_1/N) = N$
Domain decomposition based on the number of computational nodes and communications between processors.

Dynamic Domain Decomposition

Instantaneous computational cost for the chemical mechanism in a CH$_4$/H$_2$/Air flame.

Details of computational grid.

CH$_4$-H$_2$ finite chemistry with 19 species and 15 global steps.

Dynamic decomposition:
Load balancing between CPUs during computation.
Dynamic Domain Decomposition

Numerical simulation with **20 CPUs**: 10 (z) x 1 (r) x 2(θ).

Average time per time-step:

- dynamic decomposition **OFF**: 17.5 s
- dynamic decomposition **ON**: 12 s

Gain: **30%**

(communication time included)

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Gain in computational time per time-step

Imposed tolerance: 10% of average time per time-step.
General Conclusions

- LES results are **promising** ⇒ LES closer to industrial applications.
  Problem: **Time-to-solution** is still too large! ⇒ **Clusters** with more CPUs!

- **SGS model** in combustion should be “enriched” of relevant physics.

- **Boundary conditions** are critical to capture the correct dynamics of the flow.

- To **check** model and numerics **accuracy** we must look at moments, correlations, spectra but usually we have only **averaged** quantities from experiments (sometimes also fluctuations and characteristic frequencies).
Thanks for your attention

... And

Join LES!!!

Subgrid kinetic energy iso-surfaces