CAN MODELING OF REACTIVE FLOWS DESCRIBE REALITY?

C. Fureby
FOI, Sweden
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.
| 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, missiles

Since the mid-50’s research has been carried out on ram-/scramjet engines

Issues with supersonic injection, mixing, self-ignition and flame stabilization, …

\( s_u \approx 2 \text{ m/s} \quad s_t \approx 20 \text{ m/s} \) 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
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

Reaction Regimes
1. Wrinkled flamelets
2. Corrugated flamelets
3. Distributed reaction zone
4. Well stirred reactor

Dimensionless numbers
- \( \text{Re}_f = \frac{\bar{v} \lambda_f}{\nu} \)
- \( \text{Da} = \frac{\tau_f}{\tau} (\frac{\lambda_f}{\delta_u}) (\frac{v}{s_u}) \)
- \( \text{Ka} = \frac{\tau_c}{\tau_K} (\frac{v}{s_u})^{3/2} (\frac{\lambda_f}{\delta_u})^{1/2} \)
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

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

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

![Diagram showing flow modeling and validation techniques]
Numerical Methods (OpenFOAM)

Unstructured Finite Volume (FV) discretization
Reynolds transport (or Gauss) theorem
\[ \bar{u} = [\bar{p}, \bar{p} \bar{Y}_i, \bar{p} \bar{v}, \bar{p} \bar{E}]^T \]
\[ \partial_t (u_p) + \frac{1}{\delta V_p} \sum_i [F_i^C(u) - F_i^D(u) + F_i^B(u)] = -(\nabla p)_p + s_p(u) \]

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
\[ T = \bar{p} ( [C(\nabla \bar{v})^T + (\nabla \bar{v}) C^T + \chi^2 (\nabla \bar{v}) d \otimes (\nabla \bar{v}) d ] + \frac{1}{2} [ \bar{v} \otimes ((\nabla^2 \bar{v})(d \otimes d)) + ((\nabla^2 \bar{v})(d \otimes d)) \otimes \bar{v} ] ) \]

Combustion Modeling using LES

Balance equations of mass, momentum and energy for a mixture
\[
\begin{aligned}
\partial_t (\rho) + \nabla \cdot (\rho \mathbf{v}) &= 0 \\
\partial_t (\rho \mathbf{v}) + \nabla \cdot (\rho \mathbf{v} \otimes \mathbf{v}) &= -\nabla p + \nabla \cdot (\mathbf{S} - \mathbf{B}) + \rho \mathbf{f} \\
\partial_t (\rho \mathbf{D}) + \nabla \cdot (\rho \mathbf{v} \mathbf{D}) &= \nabla \cdot (\rho \mathbf{v} \mathbf{D} - \rho \mathbf{f}) + \rho \mathbf{D}
\end{aligned}
\]

Filtered constitutive equations
\[
\mathbf{j}_i \approx D_i \nabla \tilde{Y}_i, \quad \mathbf{p} \approx \rho R \tilde{T} \Sigma_i (\tilde{Y}_i / M_i), \quad \mathbf{S} \approx (\lambda + \frac{\mu}{3}) (\text{tr} \mathbf{D}) \mathbf{I} + 2 \mu \mathbf{D}, \quad \mathbf{h} = k \nabla \tilde{T} \approx \kappa \nabla \tilde{T}
\]

Filtered reaction rates and chemical kinetics
\[
\begin{aligned}
\dot{w}_i &= M_i \Sigma_{j=1}^M (P''_{ij} - P'_{ij}) \quad \dot{w}_j &= M_i \Sigma_{j=1}^M (P''_{ij} - P'_{ij}) [k_{ij} \rho \Sigma_{i=1}^N Y_i^{P''} - k_{ji} \rho \Sigma_{i=1}^N Y_i^{P'}]
\end{aligned}
\]

Subgrid stress (\( \mathbf{B} \)) and flux terms (\( \mathbf{b}_E \) & \( \mathbf{b}_i \))
Definition: \( \mathbf{B} = \rho (\nabla \otimes \mathbf{v} - \mathbf{v} \otimes \nabla), \quad \mathbf{b}_E = \rho (\mathbf{v} \tilde{E} - \mathbf{v} \tilde{E}), \quad \mathbf{b}_i = \rho (\mathbf{v} \tilde{Y}_i - \mathbf{v} \tilde{Y}_i) 
\)
Model: \( \mathbf{B} = -2 \mu \kappa \mathbf{D}, \quad \mathbf{b}_E = -2 \mu_k \mathbf{D}, \quad \mathbf{b}_i = -2 \mu_k \nabla \tilde{Y}_i; \quad \mu_k = \frac{\rho c_k \Delta}{4} \frac{K^{1/2} \mathbf{D} \cdot \mathbf{D}}{4(K^{1/2} \mathbf{D} \cdot \mathbf{D})^2}
\)
OEEVM/LDKM: \( \partial_t (\rho k) + \nabla \cdot (\rho \mathbf{v} k) = -\mathbf{B} \mathbf{D} + \nabla \cdot (\mu_k \nabla k) - \rho c_k k^{3/2} / \Delta 
\)
LES Combustion Models: Overview

Flame usually thinner than the LES grid resolution ($\delta_u < \Delta$)
The filtered reaction rate $\bar{w}_j$ is highly non-linear $\Rightarrow$ 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., ...)

**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

\[
\begin{align*}
\bar{p}(Y_i^* - \bar{Y}_i) &= (1 - \gamma^*) \tau^* \dot{\bar{w}}_i (\bar{p}, Y_i^*, T^*) \\
\bar{p} \sum_{i=1}^N (Y_i^* h_i^* - \bar{Y}_i \bar{h}_i) &= (1 - \gamma^*) \tau^* \sum_{i=1}^N h_i^0 \dot{\bar{w}}_i (\bar{p}, Y_i^*, T^*)
\end{align*}
\]

Need to determine \( \tau^* \) and \( \gamma^* \)

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

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

\[
\begin{align*}
\partial_t (\bar{p} \tilde{Y}_i) + \nabla \cdot (\bar{p} \tilde{v} \tilde{Y}_i) &= \nabla \cdot ((D_i + \mu_k/Sc_k) \nabla Y_i) + \gamma^* M_i P_{ij} \dot{w}_j (Y_i^*, T^*)
\end{align*}
\]
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$_7$H$_{16}$-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 $\dot{w} = \sigma A \left( \frac{8k_B T}{\pi \mu_{AB}} \right)^{1/2} c_\alpha c_\beta e^{-E_A/RT}$
• Experimental data fits
  – Flame speed measurements
  – Ignition delay measurements
  – Flow reaction measurements
• Simulations of measurements

How much chemistry do we need? and for which purpose?
Chemical Kinetics cont’d

http://www.me.berkeley.edu/gri_mech/version30/text30.html
**Example:** Jet A is a kerosene grade fuel with a carbon number distribution between 8 and 16.

Jet A can be assumed to consist of $\text{C}_8\text{H}_{18}$, $\text{C}_{10}\text{H}_{22}$, $\text{C}_{12}\text{H}_{22}$, $\text{C}_{12}\text{H}_{24}$, $\text{C}_{14}\text{H}_{26}$ and $\text{C}_{16}\text{H}_{28}$ with the average molecular formula $\text{C}_{12}\text{H}_{23}$.

Jet-A: $\text{C}_{12}\text{H}_{23}$-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.*

$\Rightarrow$ 5 species and 2 reactions  
$\Rightarrow$ Acceptable agreement for $0.3<\phi<1.3$

<table>
<thead>
<tr>
<th>Reaction</th>
<th>$A \ (m, \ kg, \ mol, \ s)$</th>
<th>$\eta_T \eta_{\text{H}_2}$</th>
<th>$\eta_{\text{O}_2}$</th>
<th>$\eta_{\text{N}_2}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\text{C}<em>{12}\text{H}</em>{23} + 11.75\text{O}_2 \rightarrow 12\text{CO} + 11.5\text{H}_2\text{O}$</td>
<td>1.04$\times$10$^9$</td>
<td>0</td>
<td>1.0</td>
<td>0.5</td>
</tr>
<tr>
<td>$\text{CO} + 0.5\text{O}_2 \rightarrow \text{CO}_2$</td>
<td>4.04$\times$10$^8$</td>
<td>0</td>
<td>0.5</td>
<td></td>
</tr>
<tr>
<td>$\text{O}_2 + \text{N}_2 \rightarrow 2\text{NO}$</td>
<td>7.14$\times$10$^{13}$</td>
<td>-0.5</td>
<td>0.5</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Species</th>
<th>$S_{\text{C}_2}$</th>
<th>$\text{C}<em>{12}\text{H}</em>{23}$</th>
<th>$\text{O}_2$</th>
<th>CO</th>
<th>CO$_2$</th>
<th>H$_2$O</th>
<th>N$_2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$S_{\text{C}_2}$</td>
<td>0.40</td>
<td>0.76</td>
<td>0.76</td>
<td>0.60</td>
<td>0.98</td>
<td>0.75</td>
<td></td>
</tr>
</tbody>
</table>

---

Yungster & Breisacher AIAA 2005-4210  
Meredith & Black AIAA 2006-1168
EXP: Pettersson et al  
CH$_4$/air, $\Phi$≈0.5, Re≈25,000  
Re$_f$≈218, Da≈20, Ka≈0.7

LTH: G equation flamelet LES model

FOI: EDC, PaSR & TFM LES models

Validation: Low Swirl Burner

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.

\[ \begin{align*}
\text{640}^3 \text{ DNS} & \quad \text{64}^3 \text{ filtered DNS} & \quad \text{64}^3 \text{ LES-PaSR} \\
\text{Vorticity} & \quad \text{T} & \quad \text{Heat release} \\
\text{Flame} & \quad 10^3 \text{ DNS cells per LES cell} & \\
\end{align*} \]

Re\text{f}=374
Re\text{T}=44
Ka=3.4
Da=5.5.
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**

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
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

Inflow from test-section RANS
H₂-jets
bow-shock
Isentropic expansion
H₂-jets
S-shaped vortices
Ω-shaped vortices
Longitudinal vortices
Horseshoe vortex
BL separation
H₂ spill & mixing
Heat release, Q

wall-pressure increase
axial velocity
acceleration
Outflow
Wall

T
Vₓ

Validation & Combustion Dynamics

Significant unsteadiness and coherent structure dynamics
- Acoustic energy balance
  \[ \partial_t (E) + \nabla \cdot F \approx \frac{1}{\gamma p_0} p' Q \]
- FFT Analysis
  P1: Jet-shear layer, P3: Longitudinal

Centerline wall pressure

Flight data at lower \( \varphi \)

Off-centerline heat-flux

Heat-release & pressure

fft analysis

P1: Jet-shear layer
P2: Mid combustor
P3: End of combustor

Bow shock causes BL to separate and H\textsubscript{2} to leak into downstream BL region.

H\textsubscript{2} rich jet shear layer undergoes KH instabilities.

H\textsubscript{2} rich side arms (S-vortices) and spanwise rollers (Q-vortices) are formed.

The H\textsubscript{2} rich S and Q-vortices are transported downstream under intense shear during which H\textsubscript{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.

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 …