



### Pierre Q Gauthier PhD Visiting Professor of Low Emissions Combustion Modelling

# The Role of CFD in Combustor Design and Development (Part I)

### **Challenge:** Several decades of relevant scales

#### • Typical range of spatial scales

- Scale of combustor: 10 100 cm
- Energy containing eddies: 1 10 cm
- Small-scale mixing of eddies: 0.1 10 mm
- Diffusive-scales, flame thickness: 10 100 μm
- Molecular interactions, chemical reactions: 1 10 nm
- Spatial and temporal dynamics <u>inherently coupled</u>
- <u>All scales are relevant</u> and must be resolved or modeled



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O(4) Range

**O(4)** 

### **CFD-based Modelling Techniques**

• RANS (Reynolds Averaged Navier-Stokes) Average the governing equations - model all scales Modelling generally well developed Inexpensive (relatively!) - remains standard for industrial problems

#### • LES (Large Eddy Simulation)

Filter the governing equations - modelling required at the sub-gridscaleCombustion physics and chemistry tends to happen on sub-grid scalesNow becoming applicable to industrial problems

#### • DNS (Direct Numerical Simulation)

Solve the governing equations directly - no modelling of the physics Resolution of all scales required - high accuracy numerical methods Computationally very expensive Feeds modelling data to LES and RANS

### Turbulence

"Big whirls have little whirls, That feed on their velocity; And little whirls have lesser whirls, And so on to viscosity." Lewis Fry Richardson



### LES





Eddies in turbulent flows contain Energy resulting in a level of turbulent mixing and shear forces. Kolmogorov's Energy cascade Theory: Energy is passed from eddies with larger wave numbers, to eddies with smaller wave numbers.

(1941 paper 'The local Structure of Turbulence at High Reynolds Number', in which he sites T. Von Karman and G.I. Taylor)

Sub-Grid Scale Turbulence Models are still required

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Page 4 20XX-XX-XX

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**<u>Global Reactions</u>** → One or more 'reactions' tuned to reproduce Thermo-Chemical effects



<u>Detailed Chemistry</u> → Chain-Initiating, Chain-Carrying, Chain-Branching...Chain-Terminating



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Page 5 20XX-XX-XX

**<u>Reduced Chemistry</u>** → Keep Important Pathways...even add a little NOx!

$(R_1)$	$H_2 \leftrightarrow 2H$
$(R_2)$	$\mathrm{H_2} + \mathrm{O_2} \leftrightarrow \mathrm{2OH}$
$(R_3)$	$2H_2 + O_2 \leftrightarrow 2H_2O$
$(R_4)$	$2CO + O_2 \leftrightarrow 2CO_2$
$(R_5)$	$2CH_4 + O_2 \leftrightarrow 2CO + 4H_2$
$(R_6)$	$\rm 2CH_4 \leftrightarrow \rm 2CH_3 + H_2$
$(R_7)$	$2CH_4 + 3O_2 \leftrightarrow C_2H_2 + 6OH$
$(R_{8})$	$2\text{HCN} + \text{O}_2 \leftrightarrow 2\text{CO} + \text{H}_2 + \text{N}_2$
$(R_{9})$	$O_2 + N_2 \leftrightarrow 2NO$
$(R_{10})$	$O_2 + 2N_2 \leftrightarrow 2N_2O$

### **Turbulence Chemistry Interactions**

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9.6 oxetane + H

14.4 cyclopropanol + H

2.1 cis- and trans-1-propenol + H 3 ethene + CH,OH

-9.0 vinyl alcohol + CH.

7.9 allyl alcohol + H

-11.6 ethyl + CH,O



**Old School** – Uses information from Turbulence Models Where we need to be - More Detailed Chemistry  $\tau = \frac{\varepsilon}{k}$  Turb. Time Scale + OH 30  $\boldsymbol{\varpi}_{f} = -C_{EBU} \overline{\rho} \overline{Y}_{f} \mathscr{V}_{k}$ 20  $\varpi_{ox} = -C_{EBU}\overline{\rho} \overline{Y}_{Ox} / \varepsilon_k$ 13.1 12 (kcal mol<sup>-1</sup>)  $\varpi_{\rm Pr} = -C_{EBU}\overline{\rho} \,\overline{\bar{Y}}_{\rm Pr} / \frac{\varepsilon}{\varepsilon + 1} \,\varepsilon / \varepsilon$ u -10 **Newer School** – Flamelets -20 -24.9 CH,CH,CH,OH -27.2 CH<sub>3</sub>CHCH<sub>2</sub>OH CH,CH,CHOH  $y_1' = -0.04y_1 + 10^4 y_2 y_3$ 

 $y_2' = 0.04y_1 - 10^4 y_2 y_3 - 3 \cdot 10^7 y_2^2$  $y'_3 = 3 \cdot 10^7 y_2^2$ 

CH,CH,CH,O

Page 6

20XX-XX-XX



### **Combustion Regimes**







### **Combustion Models** (The Usual Suspects)

**Global Chemistry** 

• Westbrook-Dryer 2-step with Finite-Rate EBU

**Detailed Chemistry** 

- Reduced Reaction Mechanisms
  - Species Transport with EDC/ISAT Chemistry Model
- Full Reaction Mechanisms
  - PDF/Flamelet Model

### Equilibrium Chemistry PDFs

### **T60 WLE**

#### SIFMFNS



- 1/12 Sector model: to include 2 fuel injectors and mounting pin
- •Full Combustion System from OGV to NGV
- •Inlet Profile includes wake effects from OGVs
- •Combustor Liner Thickness included  $\rightarrow$  Conjugate Heat Transfer Modeled
- •Full details of Injector air passages modeled
- •Fuel supply passage not modeled
- •Liner Effusion Cooling Implicitly modeled
- •All Chute Flows and Film Cooling Flows Explicitly modeled
- •Steady-State Reacting Flow and Unsteady Reacting Flow

### **CFD Bocos**



Combustor exit plane: RTDF, Temperatures



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### Flow colored by Stoichiometric Fuel Mass Fraction

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### **Combustor Gas Temperatures** (Injector Plane)

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### Liner Effusion Cooling Model

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### **Combustor Liner Wall Temperatures Thermal Paint Validation**







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Methods Development and Validation...

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### **Simplified Representative Test-Case**



Fluid And Solid Meshed

Mesh ~500k cells

Similar Mesh Density as Combustor

Boundary Layers Used for Gas-Solid Boundaries

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### **Test-Case Temperature Field**







#### Heat Transfer Coefficient (HTC)

Experimental evidence of HTC enhancement due to cooling flow



Colours in a complex fluid flow - Giovanni Maria Carlomagno



A turbulent jet in crossflow analysed with proper orthogonal decomposition KNUD ERIK MEYER1, JAKOB M. PEDERSEN1 AND OKTAY O ZCAN2

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#### Hot-side HTC



$$HTC = \frac{q}{\left(T_{f} - T_{m}\right)}$$

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#### Conjugate CFD .Vs. Thermal Code + CFD









### Conjugate CFD



Restricted © Siemens AG 20XX Page 20  **Combustor Noise:** 

**Thermo Acoustic Instabilities** 

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## **DLE** in its simplest form



Page 22 20XX-XX-XX



### **Dominant Mechanism behind Combustion Noise**



These originate from the presence of **mixing ducts**. Can they be eliminated by passive design?



### **Combustion Instability Study & Modeling**



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#### Development of a new fuel-air mixing approach



B) NEW APPROACH

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#### Implementation of **Damping Technologies**



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#### **Questions?**



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