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

Typical Gas Turbine Serial Staging



Secondary Reactants can mix with Primary Products prior to combustion.

NOx & CO predictions require separate transport



Length, Velocity and Time Scales of Gas Turbine Flames



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Eddy Dissipation Concept (EDC) over the Years

The EDC is a cell-reactor type of model. In CFD, the computational cell is split into a reactor part and a mixing part. Fluctuations are ignored in the reacting part.

- 1. RANS-based EDC: Magnussen, 1989, 2000.
- 2. LES formulation: Panjwani et. al., 2010
- 3. Reactor Volume fraction defined to be a ratio of time-scales: Sabelnikov and Fureby, 2013; Moule et. al., 2013
- 4. Reactor defined as PSR, PaSR, Unsteady-PaSR Fureby
- 5. Applications to:
 - 1. MILD combustion (RANS) De et. al., 2011
 - 2. Supersonic combustion (LES) Moule et. al. 2013
 - 3. DLE Gas turbine combustion (LES) Fureby 2012, Bulat et. al., 2015



Flame Interactions With Turbulent Eddies



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The EDC Model for Turbulence-Chemistry Interaction

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Fine Structure Surrounding Fluid

$$\widetilde{Y_k} = \gamma^* Y_k^* + (1 - \gamma^*) Y_k^0$$

$$\gamma^* = C_{\xi} \left(\frac{\nu}{\omega k^2}\right)^{\frac{1}{4}} \approx \frac{L^*}{L} \propto (Re_{\lambda})^{-\frac{3}{2}}$$

Time spent in these fine-structures:

$$\tau^* = C_\tau \sqrt{\nu \ \omega}$$

A skeletal chemistry mechanism can be integrated over this time to obtain the fine structure reaction rate.

Magnussen, 1989

Turbulent Reaction Rate

$$\widetilde{\dot{\omega}_i} = \frac{\rho \xi^2}{\left(1 - \xi^3\right) \tau^*} \left(Y_i^* - Y_i^0\right)$$

Reactor residence time is limited by turbulent mixing primarily and determines whether sufficient time of contact between reactants and products is available for sustained combustion.

The residence time determines whether reactions proceed to full completion or not.

Issues:

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- Small scale fluctuations are ignored (no pdf). 1.
- Constants are derived assuming the energy spectrum is unaffected by heat release. 2.
- 3. Mixing time-scale is based on kinetic energy dissipation, not scalar dissipation.

DES-SST-EDC Loop



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Application to the PSI Combustor



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Pressurized ~ 5 bar Preheated ~ 673K Equivalence Ratio ~ 0.43-0.5 Turbulence Grid is included



Mesh ~ 7M cells ~ 0.1mm in shear layers

Flame Lengths



RANS overestimates the flame length (independent of chemistry scheme) due to the EDC underestimating the volume fraction

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CO



Clearly dependent on the chemistry scheme.

Since CO oxidation is a much slower process, it will also be influenced by turbulent diffusion.



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EDC Volume Fraction Change



The EDC correctly predicts increase of volume fraction when scales are resolved but is limited to 0.75 of the cell size.



Major and Minor Species Profiles



Log-scale used on CH3, CH2O, CO, OH to emphasize distribution and interaction with resolved turbulent eddies. CO, as expected, interacts the most with turbulence. Restricted © Siemens AG 20XX

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Finite-Rate Effects near Lean Blow-Out Conditions



Equivalence Ratio Change indicates increase of flame-length but is under-predicted due to neglect of heat losses.

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Volume Fraction in Scale-Resolved Simulations



Is clearly a problem since the constant is based on a full cascade happening in each cell \rightarrow over-estimates the volume fraction

The partial cascade can be estimated by equating the resolved dissipation (filter-size) to the fine-structure dissipation (Fureby, 2012).

This introduces the filter-size into the expression and removes the constant volume fraction assumption

If the mesh is resolved beneath the fine-structure scale, Kolmogorov quantities start to determine reactor residence time and a quasi-laminar reaction rate is calculated similar to DNS.

Length Scale degenerates to Kolmogorov size

Reaction rate degenerates to laminar rate

$$\gamma^* = \min\left(\sqrt{\frac{\Delta\epsilon}{6} \left(\frac{3}{2k}\right)^{1.5}}, 1\right)$$

$$\widetilde{\dot{\omega_i}} = \min\left(\frac{\rho\xi^2}{\left(1-\xi^3\right)\tau^*}\left(Y_i^* - Y_i^0\right); \dot{\omega_i}^*\right)$$

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Modified Volume Fraction in DES



The volume fraction is now calculated and does not need to be 'clipped' as in the original version of the EDC

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Modified Volume Fraction in DES



Fine structure length scales reflect partial cascade but when normalized by Kolmogorov scales, the modification mainly affects the smaller scales.

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Summary

- 1. Scale resolution is of more value than chemistry resolution.
- 2. The EDC hypothesis in a partially resolved eddy-cascade simulation (L/DES) is not right since the original proposition by Magnussen (1989) was developed for RANS.
- 3. For the EDC to work with partial cascades (flamelet regime or low turbulence), the reaction rate should allow a volume fraction of 1.

Questions?



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