edcSMOKE: A new combustion solver for stiff chemistry based on OpenFOAM®

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Symposium Multiscale-Multiphysics approaches for engineering applications
Contents

• Introduction
• EDC model and edcSMOKE
• Validation test cases
• Conclusions
• Prospects
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Combustion processes

• Laminar flame

• Turbulent flame

Most combustions in applications are turbulent combustions.

Source: www.guilford.eng.yale.edu

Source: crf.sandia.gov
Problems of combustion

• Pollution

Source: Everything You Need to Know about Nox, Charles Baukal et al., Tulsa, Okla

Source: combustion.mie.utoronto.ca/?page_id=402
Problems of combustion

• Dilemma

NO\textsubscript{x} formation trend with increased energy savings

Combustions modelling helps to find a solution to these issues with low cost.
Challenges of turbulent combustion modelling

**Multi-scale** (decades of scales) and **multi-physics** (fluid dynamics, chemical kinetics): detailed chemistry

**Prohibitive** number of tightly coupled equations for real fuels and systems ($5 + N_{sp}$) : high demand of computational resources

Adapted from R. Fox, Cambridge University Press (2002)
Turbulent combustion modelling approaches

Currently popular combustion models:

- Flamelet-like
  - SLFM, FPI/FGM
  - PDF presumed
- Eddy Dissipation Concept
  - Partially Stirred Reactor
- Transported PDF models
  - PDF computed

Accuracy, cost

Model selected: EDC

- Accuracy and cost are acceptable
- Detailed chemistry can be applied in EDC model
Turbulent combustion modelling approaches

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Eddy Dissipation Concept can be coupled to finite rate chemistry

- Mean reaction rate

\[
\bar{\omega}_k = - \frac{\bar{\rho} \gamma_\lambda^2}{\tau^* (1 - \gamma_\lambda^3)} (\bar{y}_k - y_k^*)
\]

\[
\bar{y}_k = \gamma_\lambda^3 y_k^* + \left(1 - \gamma_\lambda^3\right) y_k^0
\]

(Magnussen, 1996)

- Model parameters come from an energy cascade model

- Model constants

\[
C_\gamma = 2.1377 \quad C_\tau = 0.4083
\]

(Magnussen, 1996)
EDC model formulations

Different versions of EDC model are proposed by Magnussen et al.

\[ \bar{\omega}_k = -\frac{\bar{\rho} \gamma^3_\lambda}{\tau^* (1 - \gamma^3_\lambda)} (\tilde{y}_k - y_k^*) \]

\[ \tilde{y}_k = \gamma^3_\lambda y_k^* + (1 - \gamma^3_\lambda) y_k^0 \]  
('EDC1981')

\[ \bar{\omega}_k = -\frac{\bar{\rho} \gamma^2_\lambda}{\tau^* (1 - \gamma^3_\lambda)} (\tilde{y}_k - y_k^*) \]

\[ \tilde{y}_k = \gamma^3_\lambda y_k^* + (1 - \gamma^3_\lambda) y_k^0 \]  
('EDC1996')

\[ \bar{\omega}_k = -\frac{\bar{\rho} \gamma^2_\lambda}{\tau^* (1 - \gamma^2_\lambda)} (\tilde{y}_k - y_k^*) \]

\[ \tilde{y}_k = \gamma^2_\lambda y_k^* + (1 - \gamma^2_\lambda) y_k^0 \]  
('EDC2005')
Coupling of EDC model and OpenFOAM

**OpenFOAM® Framework**
- Complex 2D/3D geometries
  - structured and unstructured meshes
  - complex boundary conditions

**edcSMOKE**
- CFD code for turbulent reacting flows with detailed kinetic mechanisms – EDC model
  - edcSimpleSMOKE - steady
  - edcPimpleSMOKE - unsteady

**Numerical Libraries**
- Eigen
- RapidXML
- Boost C++
  - linear and nonlinear systems, ODE

**OpenSMOKE Library**
- Complex Gas-Phase Chemistry
  - homogeneous reactions
  - detailed transport properties
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Validation on flame combustion case:

Sandia flame D
Sandia flame D: experimental and numerical set-up

Flame details

Fuel: CH₄/Air (25%, 75% mass)

Pilot: mixture of C₂H₂/H₂/air/CO₂/N₂

Reynolds number: 22,400

Geometry

Fuel nozzle diameter: 7.2 mm

Coflow diameter: 18.2 mm

Computational details

Domain: 2D axisymmetric (150 x 650 mm)

Computational grid: ~4600 cells

Solver: steady edcSimpleSMOKE

Turbulent model: RANS k-epsilon

Kinetic schemes

GRI3.0: 53 species, 325 reactions

PolimiC1C3HTNOX: 114 species, 2,105 reactions

Source: Robert Barlow and Jonathan Frank, Sandia Laboratories
Sandia flame D: modelling results of mean temperature profiles

![Graphs showing temperature profiles at different x/d values.](image_url)
Validation on flame combustion case:

DLR flame A
DLR flame A: experimental and numerical set-up

Flame details
Fuel: CH$_4$/Air/N$_2$ (22.1%, 33.2%, 44.7% volume)

Co-flow: air and 0.8% mole fraction H$_2$O

Reynolds number: 15,200

Geometry
Fuel nozzle diameter: 8.0 mm
Coflow diameter: 140 mm

Computational details
Domain: 2D axisymmetric (190 x 1000 mm)

Computational grid: ~3500 cells
Solver: steady edcSimpleSMOKE
Turbulent model: RANS k-epsilon

Kinetic schemes
GRI3.0: 53 species, 325 reactions

Source: www.sandia.gov/TNF/DataArch/DLRflames.html
DLR flame A: modelling results of mean CO$_2$ mass fraction profiles
Validation on flameless (MILD) combustion case:

Adelaide Jet in Hot Co-flow (JHC) burner
MILD (flameless) combustion

The Moderate or Intense Low oxygen Dilution (MILD) combustion:

• Preheated oxidizer stream
• Distributed reaction zone
• No visible flame

Advantages:

• High efficiency
• Low NOx and CO emissions
Adelaide Jet in Hot Co-flow (JHC) burner
JHC burner: experimental and numerical set-up

**Flame details**
- **Fuel**: CH\textsubscript{4}/H\textsubscript{2} (50%, 50% volume)
- **Co-flow**: mixture of CH\textsubscript{4}/H\textsubscript{2} /air/CO\textsubscript{2}/H\textsubscript{2}O/CO/N\textsubscript{2}/O\textsubscript{2}
- **Co-flow Temperature**: 1300 K
- **Reynolds number**: 10,000

**Geometry**
- **Fuel nozzle diameter**: 4.25 mm
- **Coflow diameter**: 82.0 mm

**Computational details**
- **Domain**: 2D axisymmetric (254 x 1000 mm)
- **Computational grid**: ~30,000 cells
- **Solver**: unsteady edcPimpleSMOKE
- **Turbulent model**: RANS k-epsilon
- **Kinetic schemes (Nox free)**
  - **KEE**: 17 species, 58 reactions
  - **GRI3.0**: 36 species, 219 reactions
  - **SAN_DIEGO**: 50 species, 247 reactions
Modelling results: Comparison of mean Temperature profiles from different EDC model formulations

K-epsilon model constant $C_{1\epsilon} = 1.60$. 
Modelling results: Comparison of mean Temperature profiles from different detailed chemistry mechanisms

Axial 30 mm

Axial 60 mm

Axial 120 mm

Centerline
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Conclusions

• Satisfactory prediction results can be obtained with the edcSMOKE solvers;

• Both the steady and unsteady solvers give relative good results in prediction;

• The EDC combustion model can be adopted in flame and flameless combustion;

• Large mechanisms can be used in combination with this solver.
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Prospects

• Chemistry reduction method is supposed to be implemented to save the computational time;

• Using Large Eddy Simulation to solve part of the turbulence;

• Compare the EDC model with Partially Stirred Reactor (PaSR) combustion model.
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Thank you

Questions?

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