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Large Eddy Simulation of bluffbody stabilized flames using novel Flame Tracking method

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Outline

- Flame tracking-particle method
- Validation results
- First LES calculations
- Flame stabilization with flame holder
- 3D piloted premixed Bunsen burner
- Conclusions

Background

Frolov S.M., Ivanov V.S., Smetanyuk V.A., Basara B., Suffa M. Numerical simulation of propane - air turbulent flame acceleration in straight tubes of different length. **2009**

Frolov S.M., Ivanov V.S., Smetanyuk V.A., Basara B. Tracking of propagating turbulent flames and autoignition in enclosure. **2009**

Frolov S.M., Ivanov V.S. Combined Flame Tracking - Particle method for numerical simulation of deflagration-to-detonation transition. **2010**

Ivanov V. S., Frolov S. M. Numerical simulation of the operation process and thrust performance of an air-breathing pulse detonation engine in supersonic flight conditions. **2011**

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Objective:

develop a coupled Large Eddy Simulation – Flame Tracking method for premixed combustion

RANS vs. LES

RANS

$$\begin{aligned} \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{u}) &= 0, \\ \frac{\partial (\rho \vec{u})}{\partial t} + \nabla \cdot (\rho \vec{u} \vec{u}) &= -\nabla p + \nabla \cdot (\mathbf{\tau}_{\mathbf{m}} + \mathbf{\tau}_{\mathbf{t}}), \\ \frac{\partial (\rho E)}{\partial t} + \nabla \cdot (\rho \vec{u} H) &= \nabla \cdot \left[\vec{u} \cdot (\mathbf{\tau}_{\mathbf{m}} + \mathbf{\tau}_{\mathbf{t}}) + + (\vec{q}_{m} + \vec{q}_{t}) \right], \\ \rho &= pm/(RT) \end{aligned}$$

m – molecular t - turbulent

$$\boldsymbol{\tau}_t = 2\mu_t \left(\mathbf{S} - \frac{1}{3} \mathbf{I} \, \nabla \cdot \vec{u} \right) + \frac{2}{3} k \, \mathbf{I}, \quad \vec{q}_t = -\lambda_t \nabla T$$

LES

$$\begin{cases} \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{u}) = 0 \\ \frac{\partial (\rho \vec{u})}{\partial t} + \nabla \cdot (\rho \vec{u} \vec{u}) = -\nabla p + \nabla \cdot (\mathbf{\tau}_{\mathbf{m}} + \mathbf{\tau}_{SGS}) \\ \frac{\partial (\rho E)}{\partial t} + \nabla \cdot (\rho \vec{u} H) = \nabla \cdot \left[\vec{u} \cdot (\mathbf{\tau}_{\mathbf{m}} + \mathbf{\tau}_{SGS}) + (\vec{q}_{m} + \vec{q}_{SGS}) \right] \end{cases}$$

m – molecular sgs - subgrid

$$\mathbf{\tau}_{\text{SGS}} = 2\mu_{\text{SGS}} \left(\mathbf{S} - \frac{1}{3} \left(\nabla \cdot \vec{u} \right) \mathbf{I} \right) + \frac{2}{3} k_{\text{SGS}} \mathbf{I} , \ \vec{q}_{\text{SGS}} = -\lambda_{\text{SGS}} \nabla T$$

Smagorinsky model



RANS vs. LES

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m – molecular sgs - subgrid

$$\boldsymbol{\tau}_{\text{SGS}} = 2 \mu_{\text{SGS}} \left(\mathbf{S} - \frac{1}{3} \left(\nabla \cdot \vec{u} \right) \mathbf{I} \right) + \frac{2}{3} k_{\text{SGS}} \mathbf{I} \,, \; \vec{q}_{\text{SGS}} = -\lambda_{\text{SGS}} \nabla T$$

Smagorinsky model



Approach





- 1 cells with fresh mixture
- 2 nearest to flame cells with fresh mixture
- **3** mixed cells with flame front
- 4 nearest to flame cells with products

Flame Tracking method for RANS



Any combustion model:

Damkoeh Shelkin Zimont Gulder

Bradley Liu, Ziegler, Lenze Peters

Transition from RANS to LES

$$\frac{u_T}{u_n} = F(u', l, \delta, \dots)$$

Damkoehler
$$F = 1 + \frac{u'}{u_n}$$

Shelkin $F = \left(1 + \frac{{u'}^2}{u_n^2}\right)^{1/2}$
Zimont $F = 1 + 0.52 \left(\frac{u'}{u_n}\right)^{1/2} \left(\frac{u'l}{v}\right)^{1/4}$
Gulder $F = 1 + 0.62 \left(\frac{u'}{u_n}\right)^{1/2} \left(\frac{u_n l}{v}\right)^{1/4}$

Transition from RANS to LES

$$\frac{u_T}{u_n} = F(u', l, \delta, \dots)$$

 $F = \left(1 + \frac{u'^2}{u'^2}\right)^{1/2}$

Damkoehler $F = 1 \underbrace{\begin{pmatrix} u' \\ u \end{pmatrix}}_{u}$

Shelkin

Zimont
$$F = 1 + 0.52 \left(\frac{u'}{u_n} \right)^{1/2} \left(\frac{u'l}{v} \right)^{1/4}$$

Gulder $F = 1 + 0.62 \left(\frac{u'}{u}\right)^{1/2} \left(\frac{u_n l}{v}\right)^{1/4}$

- \rightarrow $u' \rightarrow u'_{sgs}$ $\mathbf{U}_{\mathrm{T}} \rightarrow \mathbf{U}_{\mathrm{TSGS}}$

Database: laminar flame

- Hydrogen
- Methane
- Propane
- n-Heptane
- n-Octane
- Decane
- Thetradecane
- **PRF95**
- Ethanol

Speed **Thickness** NO Soot CO $\mathbf{O2}$ Lewis number Viscosity

Pressure: 1-100 atm Temperature: 300-900 K All range of eq. ratios EGR: 0-60%

Advantages of the FTPM

Standard combustion model (CFM)



Flame tracking-particle method



Temperature



Validation: Combustion in enclosures (RANS)

Combustion in enclosures





Validation: Test calculations for LES combustion

Simple test case



Bell et al.





Different initial conditions



temperature





Flame stabilization with flame holder

Experiments





Stable flame



Screech mode

Buzz mode

G. Jourdain, L.-E. Eriksson

Experiments



Animation





Temperature snapshots



Profiles

instantaneous profiles of temperature

instantaneous profiles of velocity

averaged profiles of temperature



Flame blow-off

increase of stream velocity from 15 to 20 m/s



Flame blow-off

change equivalence ratio from 0.7 to 0.6



Bunzen burner

Experiments





Y.-C. Chen, N. Peters, G.A. Schneemann, N. Wruck, U. Renz, M. S. Mansour

Computation setup



Snapshots

temperature

velocity

turbulence





2	3	4	5	6	7	8	9	10



Results



Conclusions

- The algorithm of coupled Large Eddy Simulation Flame Tracking Method in 3D geometries has been developed and implemented into a CFD code.
- The method is (conditionally!) parameter free and very efficient in terms of CPU requirements.
- Results of calculations were **compared with experimental data**.
- The method can be readily applied to studies of **combustion phenomena in different applications.**

Advantages of the FTPM

Flame tracking-particle method



Standard combustion model (CFM) One kinetic mechanism for preflame postflame and flame reactions

Problem with calculation of the pollutants in the flame