Large Eddy Simulation of Premixed Combustion Using Artificial Flame Thickening Coupled with Tabulated Chemistry

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vorgelegt von

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Erklärung

Hiermit erkläre ich, dass ich die vorliegende Arbeit, abgesehen von den in ihr ausdrücklich genannten Hilfen, selbständig verfasst habe.

Datum, Unterschrift

Preface

This thesis originated from my work as a doctoral candidate at the Institute for Energy and Power Plant Technology at the University of Technology in Darmstadt. Therefore, at first, I would like to cordially thank the head of the institute Prof. Dr. Johannes Janicka for this opportunity as well as for his confidence placed in me for the autonomous conduction of this work.

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Darmstadt, January 2012 Guido Künne

Contents

Nomenclature

Some variables which are exclusively used locally are not included in this nomenclature. Units which arise from a local context are denoted by $\mho$.

Upper case latin letters		**Unit**
A	General amplitude	$\mho$
A_{fr}	Preexponential constant of the Arrhenius law	$\mho$
C	General constant	–
C_{e}	Efficiency correction function	–
C_{s}	Smagorinsky coefficient	–
$\mathcal{C}$	Courant number	–
$\mathcal{D}$	Diffusion number	–
$\mathscr{D}_k$	Diffusion coefficient of the component k	$\mathrm{m^2/s}$
E_{a}	Activation energy	$\mathrm{J/mol}$
$E_{i,j}$	Frequency spectrum	$\mathrm{m^2/s}$
$\mathscr{E}$	Efficiency function	–
$\mathscr{F}$	Thickening factor	–
$\mathcal{G}$	Spatial filtering operator	$\mathrm{1/m^3}$
K	Flame stretch	$\mathrm{1/s}$
$L_{i,j}$	Germano identity	$\mathrm{m^2/s^2}$
Le_k	Lewis number of the species k	–
$\mathcal{L}$	Characteristic length scale	m
$\mathcal{M}$	Molar mass of the mixture	$\mathrm{kg/kmol}$
$\mathcal{M}_k$	Molar mass of the species k	$\mathrm{kg/kmol}$
N_{cv}	Number of control volumes	–
N_{r}	Number of reactions	–
N_{s}	Number of species	–
$\mathcal{O}$	In the order of	–
P	Probability	$\mho$
P_{TKE}	Production of the turbulent kinetic energy	$\mathrm{m^2/s^3}$

$\overline{P}$	Modified pressure within the LES	Pa
Pr	Prandtl number	–
$\dot{Q}$	External source or sink of enthalpy	$^{\mathrm{J}}/_{\mathrm{m^3\,s}}$
$R_{i,j}$	Autocovariance	$^{\mathrm{m^2}}/_{\mathrm{s^2}}$
$R_{\mathrm{n},i,j}$	Autocorrelation	$^{\mathrm{m}}/_{\mathrm{s}}$
$\mathcal{R}$	Perfect gas constant	$^{\mathrm{J}}/_{\mathrm{kmol\,K}}$
$\mathscr{R}$	General right hand side of an equation	$\mho$
S	General surface	m^2
$\mathcal{S}$	Filtered rate of strain	$^{1}/_{\mathrm{s}}$
S_{ij}	Rate of strain	$^{1}/_{\mathrm{s}}$
S_{g}	Swirl number based on the geometry	–
S_{m}	Swirl number based on the momentum	–
T	Temperature	K
$\mathscr{T}$	Effective straining function	–
$\mathcal{U}$	Characteristic velocity	$^{\mathrm{m}}/_{\mathrm{s}}$
V	General volume	m^3
V_{F}	Filtering volume	m^3
$V_{k,i}$	Diffusion velocity of the component k into direction i	$^{\mathrm{m}}/_{\mathrm{s}}$
$\mathcal{X}_k$	Symbol for species k	–
Y_k	Mass fraction of the species k	–
Y_{pv}	Reaction progress variable	–
$Y_{\mathrm{n,pv}}$	Normalized reaction progress variable	–
Z_k	Element mass fraction of the element k	–
$\mathcal{Z}$	Stability function of the time integration scheme	–

Lower case latin letters		**Unit**
a	Strain rate (counter flow configuration)	$^{1}/_{\mathrm{s}}$
c	Speed of sound	$^{\mathrm{m}}/_{\mathrm{s}}$
c_k	Molar concentration of the species k	$^{\mathrm{mol}}/_{\mathrm{m^3}}$
c_{p}	Specific heat capacity of the mixture at constant pressure	$^{\mathrm{J}}/_{\mathrm{kg\,K}}$
$c_{\mathrm{p}k}$	Specific heat capacity of the species k at constant pressure	$^{\mathrm{J}}/_{\mathrm{kg\,K}}$
f	Mixture fraction	–
$f_{k,i}$	Volume force acting on the species k into direction i	$^{\mathrm{m}}/_{\mathrm{s^2}}$
$\mathfrak{f}$	Is a function of	–
g_i	Acceleration of gravity into direction i	$^{\mathrm{m}}/_{\mathrm{s^2}}$
h	Specific enthalpy of the mixture	$^{\mathrm{J}}/_{\mathrm{kg}}$
h_k	Specific enthalpy of the species k	$^{\mathrm{J}}/_{\mathrm{kg}}$
k	Rate coefficient	$\mho$

l	General length	m
l_{I}	Integral length scale	m
l_{m}	Mixing length (Prandtl's mixing-length hypothesis)	m
m_k	Mass of the species k	kg
p	Pressure	$\mathrm{kg}/\mathrm{s^2 m}$
q_i	Enthalpy flux into direction i	$\mathrm{J}/\mathrm{m^2 s}$
r	General radius	m
$r_{\mathrm{fr}}, r_{\mathrm{br}}$	Reaction rate of the forward and backward reaction	$\mathrm{mol}/\mathrm{m^3 s}$
s	Coordinate in the flame reference frame	m
s_{a}	Absolute flame speed	m/s
s_{l}	Laminar flame speed	m/s
$s_{\mathrm{l}\Delta}$	Numerically computed laminar flame speed obtained on a certain grid size	m/s
s_{T}	Turbulent flame speed	m/s
t	Time	s
t_{I}	Integral time scale	s
u_i	Velocity (into direction i)	m/s
$u'_{\Delta_{\mathrm{e}}}$	Velocity fluctuation on the test filter Δ_{e}	m/s
v'	Characteristic vortex velocity	m/s
x_{F}	Flame position	m
x_i or x, y, z	Cartesian coordinate	m

Upper case greek letters — Unit

Δ_{e}	Test filter size for the ATF model	m
$\Delta h_{\mathrm{f},k}$	Enthalpy of formation of the species k	J/kg
Δ_{t}	Time step size	s
Δ_{T}	General time interval	s
Δ_{x}	Grid size (also Δ_{y} or Δ_{z} if direction is relevant)	m
$\Delta_{\mathrm{x,max}}$	Maximum grid size to capture the flame propagation	m
$\Delta_{\mathrm{x,min}}$	Minimum grid size for (spurious) flame stagnation	m
$\Delta_{\mathrm{R,H}}$	Reaction enthalpy	J/kg
Γ	General diffusion coefficient	℧
Φ	General scalar	℧
Ξ	Flame wrinkling factor	–
Ω	Flame sensor	–

Lower case greek letters — Unit

α	Alignment angle between scalar layers in a stratified flame	Radian
γ	Isentropic exponent	–

δ	General flame thickness	m
δ^{T}	Thickness of the turbulent flame brush	m
$\delta^{0}_{\mathrm{g}(k)}$	Flame thickness of the flamelet based on the gradient (of scalar k)	m
$\delta^{\mathrm{F}}_{\mathrm{g}(k)}$	Flame thickness of the thickened flame based on the gradient (of species k)	m
δ_{ij}	Kronecker-symbol	–
$\delta^{0}_{\omega(k)}$	FWHM thickness of the reaction zone from the flamelet (of scalar k)	m
$\delta^{\mathrm{F}}_{\omega(k)}$	FWHM thickness of the reaction zone from the thickened flame (of species k)	m
ϵ	General error	℧
$\epsilon_{\dot{m}}$	Mass lack within the pressure correction scheme	$\mathrm{kg/s}$
ϵ_{TKE}	Dissipation of the turbulent kinetic energy	$\mathrm{m^2/s^3}$
ϵ_{Δ}	Local error in the flame speed	$\mathrm{m/s}$
$\epsilon_{\mathrm{g}\Delta}$	Global error in the flame speed	$\mathrm{m/s}$
ζ	Stretched coordinate in the context of the ATF model	m
η_{K}	Kolmogorov length scale	m
θ	Rotation angle of the movable block	Radian
κ	Wave number (in the energy spectrum)	$\mathrm{1/m}$
λ	Thermal conductivity	$\mathrm{W/m\,K}$
λ_{E}	Eigenvalue	℧
λ_{T}	Temperature conductivity	$\mathrm{m^2/s}$
λ_{w}	Wavelength	m
μ	Dynamic viscosity	$\mathrm{kg/s\,m}$
μ_{t}	Turbulent dynamic viscosity	$\mathrm{kg/s\,m}$
ν	Kinematic viscosity	$\mathrm{m^2/s}$
ν_{t}	Turbulent kinematic viscosity	$\mathrm{m^2/s}$
ν'_k	Stoichiometric coefficient of species k on the reactant side	–
ν''_k	Stoichiometric coefficient of species k on the product side	–
ξ_i	Local, cell oriented logical coordinate	–
π	Circular constant (number pi)	–
ρ	(Mass-) density of the mixture	$\mathrm{kg/m^3}$
ρ_{s}	Species (mass-) density	$\mathrm{kg/m^3}$
τ_{ij}	Components of the viscous stress tensor	$\mathrm{kg/s^2\,m}$
φ	Arbitrary quantity	℧
ϕ	Equivalence ratio	–
$\dot{\omega}_k$	Chemical source term of the component k	$\mathrm{kg/m^3\,s}$

Indices

$\cdot'$	Temporal fluctuation
$\cdot_0$	Characteristics of large scale structures
$\cdot_\mathrm{b}$	State in the burnt gas
$\cdot_\mathrm{br}$	Backward reaction
$\cdot_\mathrm{D}$	One node towards the downwind direction
$\cdot_\mathrm{eq}$	Equilibrium (conditions)
$\cdot_\mathrm{F}$	Fuel
$\cdot_\mathrm{fr}$	Forward reaction
$\cdot_\mathrm{l}$	Lean flammability limit
$\cdot_\mathrm{max}$	Maximum
$\cdot_\mathrm{min}$	Minimum
$\cdot_\mathrm{N,E,S,W,T,B}$	One node towards the north, east, south, west, top, bottom direction
$\cdot_\mathrm{n,e,s,w,t,b}$	North, east, south, west, top, bottom face of a control volume
$\cdot_\mathrm{O}$	Oxidizer
$\cdot_\mathrm{pv}$	Progress variable
$\cdot_\mathrm{proj}$	Into projection direction
$\cdot_\mathrm{r}$	Rich flammability limit
$\cdot_\mathrm{ref}$	Reference conditions ($T = 298.15\,\mathrm{K}$, $p = 101\,325\,\mathrm{Pa}$)
$\cdot_\mathrm{rms}$	Temporal standard deviation (root mean square)
$\cdot_\mathrm{sgs}$	Subgrid-scale
$\cdot_\mathrm{ss}$	Substep
$\cdot_\mathrm{st}$	Stoichiometric conditions
$\cdot_\mathrm{tp}$	Turning point value
$\cdot_\mathrm{u}$	State in the unburnt gas
$\cdot_\mathrm{U}$ / $\cdot_\mathrm{UU}$	One node / two nodes towards the upwind direction

Operators

$\langle\cdot\rangle$	Temporal average
$\bar{\cdot}$	Spatial (LES) filter
$\tilde{\cdot}$	Density weighted spatial filter
$\hat{\cdot}$	Test filter (Germano)

Dimensionless numbers

Da	Damköhler number
Fo	Fourier number
Gr	Grashof number

Ka	Karlovitz number
Le	Lewis number
Ma	Mach number
Pr	Prandtl number
Ra	Rayleigh number
Re	Reynolds number
Re_t	Turbulent Reynolds number
Re_Δ	Subgrid turbulent Reynolds number (Charlette et al.)
Sc	Schmidt number
Sc_k	Schmidt number of the species k
Sc_t	Turbulent Schmidt number

Abbreviations

ATF	Artificially thickened flame
CDS	Central difference scheme
CFD	Computational fluid fynamics
CPU	Central processing unit
DNS	Direct numerical simulation
DZ	Diffusion zone
FGM	Flamelet generated manifolds
FWHM	Full width at half maximum
LES	Large eddy simulation
OZ	Oxidation zone
PDF	Probability density function
PIV	Particle image velocimetry
PLIF	Planar laser-induced fluorescence
RANS	Reynolds averaged Navier Stokes
RK	Runge-Kutta
RZ	Reaction zone
TKE	Turbulent kinetic energy
TVD	Total variation diminishing
URANS	Unsteady Reynolds averaged Navier Stokes