

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

Vom Fachbereich Maschinenbau
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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

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Nomenclature

Some variables which are exclusively used locally are not included in this nomenclature. Units which arise from a local context are denoted by \mathcal{U} .

| Upper case latin letters | | Unit |
|--------------------------|--|-------------------------|
| A | General amplitude | \mathcal{U} |
| A_{fr} | Preexponential constant of the Arrhenius law | \mathcal{U} |
| C | General constant | — |
| C_e | Efficiency correction function | — |
| C_s | Smagorinsky coefficient | — |
| \mathcal{C} | Courant number | — |
| \mathcal{D} | Diffusion number | — |
| \mathcal{D}_k | Diffusion coefficient of the component k | m^2/s |
| E_a | Activation energy | J/mol |
| $E_{i,j}$ | Frequency spectrum | m^2/s |
| \mathcal{E} | Efficiency function | — |
| \mathcal{F} | Thickening factor | — |
| \mathcal{G} | Spatial filtering operator | $1/\text{m}^3$ |
| K | Flame stretch | $1/\text{s}$ |
| $L_{i,j}$ | Germano identity | 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 | kg/kmol |
| \mathcal{M}_k | Molar mass of the species k | 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 | \mathcal{U} |
| P_{TKE} | Production of the turbulent kinetic energy | m^2/s^3 |

| | | |
|-----------------|--|--------------------------------|
| \bar{P} | Modified pressure within the LES | Pa |
| Pr | Prandtl number | — |
| \dot{Q} | External source or sink of enthalpy | J/m ³ s |
| $R_{i,j}$ | Autocovariance | m ² /s ² |
| $R_{n,i,j}$ | Autocorrelation | m/s |
| \mathcal{R} | Perfect gas constant | J/kmol K |
| \mathcal{R} | General right hand side of an equation | \mathcal{U} |
| S | General surface | m ² |
| \mathcal{S} | Filtered rate of strain | 1/s |
| S_{ij} | Rate of strain | 1/s |
| S_g | Swirl number based on the geometry | — |
| S_m | Swirl number based on the momentum | — |
| T | Temperature | K |
| \mathcal{T} | Effective straining function | — |
| \mathcal{U} | Characteristic velocity | m/s |
| V | General volume | m ³ |
| V_F | Filtering volume | m ³ |
| $V_{k,i}$ | Diffusion velocity of the component k into direction i | m/s |
| \mathcal{X}_k | Symbol for species k | — |
| Y_k | Mass fraction of the species k | — |
| Y_{pv} | Reaction progress variable | — |
| $Y_{n,pv}$ | 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/s |
| c | Speed of sound | m/s |
| c_k | Molar concentration of the species k | mol/m ³ |
| c_p | Specific heat capacity of the mixture at constant pressure | J/kg K |
| c_{pk} | Specific heat capacity of the species k at constant pressure | J/kg K |
| f | Mixture fraction | — |
| $f_{k,i}$ | Volume force acting on the species k into direction i | m/s ² |
| \mathbf{f} | Is a function of | — |
| g_i | Acceleration of gravity into direction i | m/s ² |
| h | Specific enthalpy of the mixture | J/kg |
| h_k | Specific enthalpy of the species k | J/kg |
| k | Rate coefficient | \mathcal{U} |

| | | |
|--------------------|--|----------------------|
| 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 | kg/s ² m |
| q_i | Enthalpy flux into direction i | J/m ² s |
| r | General radius | m |
| r_{fr}, r_{br} | Reaction rate of the forward and backward reaction | mol/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 |
| $s_{l\Delta}$ | 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'_{Δ_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 |
| $\Delta h_{f,k}$ | 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 |
| $\Delta_{x,max}$ | Maximum grid size to capture the flame propagation | m |
| $\Delta_{x,min}$ | Minimum grid size for (spurious) flame stagnation | m |
| $\Delta_{R,H}$ | Reaction enthalpy | J/kg |
| Γ | General diffusion coefficient | \mathcal{U} |
| Φ | General scalar | \mathcal{U} |
| 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 |
| $\delta_{g(k)}^0$ | Flame thickness of the flamelet based on the gradient (of scalar k) | m |
| $\delta_{g(k)}^F$ | Flame thickness of the thickened flame based on the gradient (of species k) | m |
| δ_{ij} | Kronecker-symbol | — |
| $\delta_{\omega(k)}^0$ | FWHM thickness of the reaction zone from the flamelet (of scalar k) | m |
| $\delta_{\omega(k)}^F$ | FWHM thickness of the reaction zone from the thickened flame (of species k) | m |
| ϵ | General error | \mathcal{U} |
| $\epsilon_{\dot{m}}$ | Mass lack within the pressure correction scheme | kg/s |
| ϵ_{TKE} | Dissipation of the turbulent kinetic energy | m ² /s ³ |
| ϵ_{Δ} | Local error in the flame speed | m/s |
| $\epsilon_{g\Delta}$ | Global error in the flame speed | 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) | 1/m |
| λ | Thermal conductivity | W/m K |
| λ_E | Eigenvalue | \mathcal{U} |
| λ_T | Temperature conductivity | m ² /s |
| λ_w | Wavelength | m |
| μ | Dynamic viscosity | kg/s m |
| μ_t | Turbulent dynamic viscosity | kg/s m |
| ν | Kinematic viscosity | m ² /s |
| ν_t | Turbulent kinematic viscosity | 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 | kg/m ³ |
| ρ_s | Species (mass-) density | kg/m ³ |
| τ_{ij} | Components of the viscous stress tensor | kg/s ² m |
| φ | Arbitrary quantity | \mathcal{U} |
| ϕ | Equivalence ratio | — |
| $\dot{\omega}_k$ | Chemical source term of the component k | kg/m ³ s |

Indices

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

Chapter 1

Introduction

This work addresses the simulation of premixed combustion with regard to the application in stationary gas turbines and future aero engines. In the following the global background leading to the motivation of this work will be given. After that, the state of research in this area is briefly outlined followed by the concrete aims of this work. At the end of this chapter, the structure of this thesis is given.

1.1 Background

Within the combustion process chemically bound energy is transformed into heat. Herein the reaction takes place between the fuel and an oxidizer, often the oxygen contained in the air. Since its discovery many thousands of years ago, the thermal energy obtained from combustion was first exclusively used directly for example to heat or for food preparation. Mainly wood was used as fuel. Within the last centuries, machines have been designed to convert the heat into other forms of energy for the final usage, e.g. mechanical motion by the steam engine within the 18th century. Over the last 150 years major achievements have been obtained in the area of thermodynamics. The basic principles of the thermodynamic cycles which transform heat into mechanical energy developed in this time are still up to date. These can be found in coal power plants (Clausius-Rankine process¹) or stationary gas turbines (Joule process²) for electricity generation, in aero engines (open Joule process) to generate thrust or in internal combustion engines (Otto and Diesel process³). The fuels used are mostly coal, oil and gas.

Today combustion is the most important pillar to cover the energy demand of industrialized economies. Approximately 90 % of the primary energy consumption is obtained by combustion processes [21; 91; 243]. Due to the negative impact of the reaction products onto the local air composition [231] as well as onto the global climate [92; 232] these must be reduced. The plans to realize this are embedded in an area of tension between technological capabilities and economical and political interests. Furthermore, the efforts are counteracted by the increasing energy demand. This demand has doubled within the last 40 years [91] and will further increase according to all prognoses (e.g. [90]). The cause is the increasing industrialization of emerging and developing economies like India

¹Named after the physicists Rudolf Clausius (1822-1888) and William John Macquorn Rankine (1820-1872).

²Named after the physicist James Prescott Joule (1818-1889).

³Named after the inventor Nicolaus Otto (1832-1891) and the engineer Rudolf Diesel (1858-1913).

and China [233] whose today's per capita energy consumption is below the world average and significantly lower compared to fully developed economies [243]. Therefore, it is more realistic to water down further damage caused by the emissions than to actually reduce them in order to keep the climate change as little as possible [214].

Current measures are related to a better usage of the combustion as well as the utilization of other forms of energy. Regarding the optimization of combustion systems two steps are important.

The first step is the conversion of the chemically bound energy into heat. It is decisive for the composition and temperature of the burnt gases. One distinguishes between premixed and non-premixed combustion. Within non-premixed combustion, fuel and oxidizer are introduced separately into the combustor and react as soon as they approach each other, given the necessary activation energy is present. The essential advantage is the safety since no flammable mixture exists outside of the combustor. Within premixed combustion fuel and oxidizer are mixed before reaction occurs with the risk of flashback. Furthermore, this type of flame is prone to thermo-acoustic instabilities. Despite these difficulties, huge efforts are committed to optimize premixed combustion for its application since it enables to avoid high peak temperatures, mainly present at stoichiometric conditions which are always found in non-premixed flames. This is necessary to reduce the thermal formation of nitric oxides (NO and NO_2 , often summarized as NO_x) by the Zeldovich mechanism [258]. Since these constitute a major portion of the pollutants and contribute to acid rain, ozone formation and smog problems, strong regulations exist for all applications. Regarding these, the requirements for aero engines given by the *Committee on aviation environmental protection* (CAEP [89]) are hardly met by most of the devices which almost exclusively operate with non-premixed combustors. In view of future goals given by the *Advisory Council for Aeronautics Research in Europe* (ACARE [1; 2]) which include the reduction of NO_x emissions by 80 % (compared to CAEP 2) until 2020, the changeover to lean premixed combustors, as already used in stationary gas turbines [15], is planned [118]. Similar regulations exist for vehicles (e.g. European emission standards [53]).

The second step consists of the conversion of the heat into mechanical energy by the thermodynamic cycle. The most environment-friendly method is the combustion of gaseous fuels in combined cycle power plants. By using a high temperature level Joule process followed up by a Clausius-Rankine process of lower temperature, an overall efficiency above 60 % can be obtained [239]. Currently, this technology is somewhat limited by the availability of natural gas since the known resources, even though considerable in amount, are quite concentrated to only a few countries led by the Russian Federation, Iran and Katar [235]. Therefore coal power plants are often employed by countries like Germany or China which have a vast amount of own coal resources. However, these have a lower efficiency (approximately 47 %) and emit significantly more carbon dioxide attributed to the fuel.

On the side of renewable energies, hydro power, geothermal energy, ocean energy, wind

energy, solar energy and biomass are found. Their contribution to the production of energy will significantly increase in the future [237] whereby the distribution among each other is open due to the partially young technology [221]. Herein hydro power is limited by geodesic conditions. Currently wind- and solar energy exhibit high rates of growth. Both technologies are promising, but have a low energy density when compared to conventional power plants which limits their applicability in densely populated regions like Europe. Furthermore, the energy production depends on the weather. Therefore, the ability to store and transport energy is decisive for their implementation. To store the energy, thermal (e.g. steam accumulator), mechanical (e.g. pump storage), electrical (e.g. capacitors) and chemical storages (e.g. batteries) are used [236]. Regarding the latter one, the synthetic production of fuels (hydrogen or methane) is also under development which can then be used for combustion in combined cycle power plants [238]. In the area of biomass, the systematic planting of biofuel-plants for combustion is applied besides the usage of bio-waste. At this, the consumption of carbon dioxide during the growth shall establish a neutral balance. During the last years this technology also exhibits high rates of growth but competes with food regarding the acreage.

Hence, regarding the overall energy situation the following can be summarized. Due to the increasing energy demand which is currently covered by renewable energies by only a small fraction with limited rates of growth, also in the future the majority of energy will be obtained by conventional combustion processes, mostly in gas- and coal power plants and internal combustion engines⁴. Thereby, the fraction of renewable energies will significantly increase at which combustion acts either supporting e.g. to ensure the base load, complementary e.g. by biofuels, or even technology-completing via synthetic fuels. Within all of these, premixed combustion plays a decisive role.

1.2 Motivation of this work

The simulation of physical processes becomes increasingly important within research and development. The demand basically arises for two reasons. First, expensive experiments (e.g. crash experiments) should at least be reduced or even completely replaced by simulations. Furthermore, the simulation reveals more information, e.g. the load and deformation of individual components instead of the macroscopic recording by high speed cameras. These information in turn can be used for a better understanding of the process and thus for its optimization. These demands are faced by the current capabilities of the simulation. While several processes like elastic deformations can already be computed very accurately, numerous examples exist whose simulation is desirable but the results need to be taken with a pinch of salt which limits its application. One of these applications is the simulation of flows generally referred to as computational fluid dynamics (CFD). Already the occurrence of turbulent structures can often only be approximated. The complexity gets further increased by mixing processes e.g. between fuel and oxidizer as well as their chemical reaction such that the simulation is no longer able to correctly

⁴The role of nuclear energy is uncertain, since, especially after the recent incidents in Fukushima, it is a difficult political / emotional discussion.

describe the situation. The causes for the deficiency are the incomplete theoretical description of the process as well as the available computing capacities. The latter one is currently much more restrictive since the understanding of the physical mechanism and its mathematical description are generally very good. The demand for computing capacities arises from the necessity to resolve the relevant phenomena. Herein, the length scales involved vary by several orders of magnitude ranging from the reaction kinetics up to the combustor geometry. Therefore, the simulation cannot capture the overall process. Hence, the current improvements of the simulation result from the increasing computing capacities as well as from the development of methods to simplify the problem without too restricting assumptions. The latter one is subject of this work.

1.3 State of research

Due to the above mentioned complexity, a wide range of applications and developments of combustion simulations exists. Herein, besides statistically stationary premixed and non-premixed flames, globally transient processes like ignition and extinction, flashback and thermo-acoustic instabilities belong to the **phenomena** considered. At this, the **configurations** used vary significantly. Starting from one- and two-dimensional domains of small extent, also full scale gas turbine combustors or internal combustion engines including complex inlet and outlet ducts have been simulated. Accordingly, various **numerical methods** exist for the three simulation approaches given by the time-averaged description (RANS), the large eddy simulation (LES) and the direct numerical simulation (DNS). Herein, structured one- or multi-block meshes with cubic or curved cells, or unstructured meshes are employed for the spatial discretization depending on the complexity. Fixed as well as moving meshes to follow for example the piston movement are used. Also adaptive schemes exist to refine the mesh according to local criteria.

Amongst these topics a mutually exclusive interaction exists. In this respect the consideration of detailed chemical processes is not possible in the simulation of real combustors due to the large range of different length scales and vice versa [168]. Often times this is also not necessary. Currently, detailed chemistry DNS are conducted in small scale cubic domains as well as LES of realistic complex geometries where these details are not captured. Both approaches are incomplete and profit from the knowledge gained mutually. Within this exchange, ignition sequences [256], flame-vortex interactions [177] or stratification processes [72; 135; 136] are often investigated separately to obtain information about the underlying physics and to derive models for the simulation techniques with a lower resolution. In these detailed studies, the increasing computing capacities already allow the simultaneous simulation of numerous phenomena as recently done by Yoo et al. [257] who studied the stabilization mechanism of a turbulent ethylene flame by means of DNS with reduced chemistry. But, for these simulations the most powerful high performance computers are employed yielding immense costs [31].

Regarding the simulation of realistic geometries, LES has established as an appropriate technique in the research community. It allows the simulation of complex devices and—contrary to the RANS technique which is currently the industrial standard due to the

low computing costs— converges towards the DNS solution with increasing resolution. By resolving only the large scale structures LES enables the simulation of turbulent flows within affordable computational costs. Especially simulations of combustion processes profit from the explicit computation of the fluctuations which determine the transient field of scalar quantities (e.g. [20; 96; 113]). Despite the fact that already several simulations of real combustors have been carried out [68], a huge research demand exists to improve the modeled part that accounts for the unresolved turbulent structures and chemical processes. Regarding the subgrid turbulence, besides the general questions regarding the LES [180], additional issues arise for combustion simulations related to the fluctuation of scalar quantities [240]. But, the essential modeling demand is associated with the treatment of the chemical reaction since even the largest length scales of the chemistry are generally smaller than the grid size. Hence, the treatment of detailed chemistry is impossible and the combustion model aims at reproducing the most important properties of the reaction on the LES mesh. For premixed combustion this is the propagation speed of the flame and its wrinkling. Various approaches, often adopted from RANS models (see [51; 174]), exist but many of them are unable to predict the laminar flame speed, a vital property with the increasing resolution available. Currently often used and capable of that are the artificially thickened flame model (ATF) [38] and the G-equation [172] or flame surface density (FSD) [80] approach. The ideas behind them are fundamentally different. Within ATF, the length scales of the flame are artificially increased until they can be resolved on the LES mesh and the correct flame speed can be computed, generally with strongly reduced chemical mechanisms. Within the G-equation and FSD approach, the flame is treated like a kinematic surface which propagates with a prescribed velocity. Hence, not the chemistry itself but rather its implication is modeled. Both approaches are established with continuous improvements of details. Their predicting capabilities assessed using generic burners where detailed experimental data exists, are generally satisfying. At this, the ATF model is more universal since it contains no restricting assumptions regarding a certain flame structure. The kinematic approach on the other hand assumes a premixed flame propagation but has a lower amount of unresolved wrinkling for this flame mode.

Besides the prediction of statistically stationary flames, LES is currently also used for the investigation of important intrinsically transient processes. One of these are thermo-acoustic phenomena in which the heat release induced by combustion interacts with the pressure field of the flow. Under certain conditions depending on the combustor geometry an unstable amplification can occur which causes severe problems in the development of premixed combustors with low pollutant emissions [87]. Therefore, this thermo-acoustic instability is currently addressed by several research groups. Again, in a supplementary process, theoretical considerations [149] as well as LES of generic flames [61] and complete combustors [217] are conducted. Again, the chemistry is often treated by ATF or the G-equation. Besides the thermo-acoustic phenomena, ignition/flame propagation, blowoff or flashback are transient processes currently addressed by LES. For example Boileau et al. [16] simulated the ignition sequence of a whole annular combustor. Regarding flashback, by explicitly computing three-dimensional turbulent structures, the LES offers the ability to gain a better understanding of the physical processes as a complementary tool to