Abstract

HOFFIE, ANDREAS FRANK. Large Eddy Simulation of Spatially Developing Turbulent Reacting Shear Layers with the One-Dimensional Turbulence Model. (Under the direction of Dr. Tarek Echekki)

Large eddy simulation (LES) combined with the one-dimensional turbulence (ODT) model is used to simulate spatially developing turbulent reacting shear layers with high heat release and high Reynolds numbers. The LES-ODT results are compared to results from direct numerical simulations (DNS), for model development and validation purposes.

The LES-ODT approach is based on LES solutions for momentum and pressure on a coarse grid and solutions for momentum and reactive scalars on a fine, one-dimensional, but three-dimensionally coupled ODT subgrid, which is embedded into the LES computational domain. Although one-dimensional, all three velocity components are transported along the ODT domain. The low-dimensional spatial and temporal resolution of the subgrid scales describe a new modeling paradigm, referred to as autonomous microstructure evolution (AME) models, which resolve the multiscale nature of turbulence down to the Kolmogorov scales. While this new concept aims to mimic the turbulent cascade and to reduce the number of input parameters, AME enables also regime-independent combustion modeling, capable to simulate multiphysics problems simultaneously. The LES as well as the one-dimensional transport equations are solved using an incompressible, low Mach number approximation, however the effects of heat release are accounted for through variable density computed by the ideal gas equation of state, based on temperature variations. The computations are carried out on a three-dimensional structured mesh, which is stretched in the transverse direction. While the LES momentum equation is integrated with a third-order Runge-Kutta time-integration, the time integration at the ODT level is accomplished with an explicit Forward-Euler method. Spatial finite-difference schemes of third (LES) and first (ODT) order are utilized and a fully consistent fractional-step method at the LES level is used. Turbulence closure at the LES level is achieved by utilizing the Smagorinsky model. The chemical reaction is simulated with a global single-step, second-order equilibrium reaction with an Arrhenius reaction rate.

The two benchmark cases of constant density reacting and variable density non-reacting shear layers used to determine ODT parameters yield perfect agreement with
regards to first and second-order flow statistics as well as shear layer growth rate. The variable density non-reacting shear layer also serves as a testing case for the LES-ODT model to simulate passive scalar mixing. The variable density, reacting shear layer cases only agree reasonably well and indicate that more work is necessary to improve variable density coupling of ODT and LES. The disagreement is attributed to the fact that the ODT filtered density is kept constant across the Runge-Kutta steps. Furthermore, a more in-depth knowledge of large scale and subgrid turbulent kinetic energy (TKE) spectra at several downstream locations as well as TKE budgets need to be studied to obtain a better understanding about the model as well as about the flow under investigation. The local Reynolds number based on the one-percent thickness at the exit is \(\text{Re}_\delta \approx 5300\), for the constant density reacting and for the variable density non-reacting case. For the variable density reacting shear layer, the Reynolds number based on the 1% thickness is \(\text{Re}_\delta \approx 2370\). The variable density reacting shear layers show suppressed growth rates due to density variations caused by heat release. This has also been reported in literature. A Lewis number parameter study is performed to extract non-unity Lewis number effects. An increase in the Lewis number leads to a further suppression of the growth rate, however to an increase spread of second-order flow statistics.

Major focus and challenge of this work is to improve and advance the three-dimensional coupling of the one-dimensional ODT domains while keeping the solution correct. This entails major restructuring of the model. The turbulent reacting shear layer poses a physical challenge to the model because of its nature being a statistically stationary, non-decaying inhomogeneous and anisotropic turbulent flow. This challenge also requires additions to the eddy sampling procedure. Besides physical advancements, the LES-ODT code is also improved regarding its ability to use general cuboid geometries, an array structure that allows to apply boundary conditions based on ghost-cells and non-uniform structured meshes. The use of transverse grid-stretching requires the implementation of the ODT triplet map on a stretched grid. Further, advancing subroutine structure handling with global variables that enable serial code speed-up and parallelization with OpenMP are undertaken. Porting the code to a higher-level language, object oriented, finite-volume based CFD platform, like OpenFoam for example that allows more advanced array and parallelization features with graphics processing units (GPUs) as well as parallelization with the message passing interface (MPI) to simulate complex geometries is recommended for future work.
Large Eddy Simulation of Spatially Developing Turbulent Reacting Shear Layers with the One-Dimensional Turbulence Model

by

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A dissertation submitted to the Graduate Faculty of North Carolina State University in partial fulfillment of the requirements for the Degree of Doctor of Philosophy

Aerospace Engineering

Raleigh, North Carolina

2015

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Dedication

To my father

Hans Hoffie
(1946 - 2015)

for teaching me the importance of hard work, integrity and for encouraging me to think big. Forever remembered and treasured in our hearts.
Biography

Born in 1980 in Geislingen, Germany, the author grew up in Gussenstadt, located on the rural Swabian Alb in the southwest of Germany. From an early age, he helped his parents in the family guesthouse, restaurant and farm. Working the farm, he gained first hand experience with farming equipment and the skills to fix mechanical problems as they occurred.

His early interest in rocketry and his technical mind quickened by the idea of human space exploration, led to the decision to study Aerospace Engineering at the University of Stuttgart. After obtaining his Pre-Diploma (Bachelor equivalent) degree in 2005, Andreas decided to take part in an exchange program with Virginia Tech, culminating in a Master of Science degree in Mechanical Engineering, with a focus in fluid-dynamics and thermodynamics in 2006. With the completion of his Diploma-Engineer (Master equivalent) degree in Aerospace Engineering at the University of Stuttgart, with a focus in aero-thermodynamics and space systems in 2008, he gathered several years of experience in industry and research at Voith Heidenheim, Airbus Defense and Space Munich, the German Air Force in Erding and the German Aerospace Center (DLR) in Brunswick.

Because of his continued interest in propulsion and high speed aero-thermodynamics as well as the prospects of air-breathing rocket propulsion, the author realized that detailed and advanced turbulence models coupled with reacting flows are necessary in order to realize an optimum design. This fact led to the decision to study modeling and simulation of turbulent and reacting flows for his Doctoral research. While initially starting a Ph.D. program at the University of Buffalo in New York, he decided to transfer to North Carolina State University in August 2010 and is on course to complete his doctoral studies in Aerospace Engineering with a focus in turbulent reactive flow modeling and software development in December 2015.

In May 2015, Andreas married the young and beautiful Mary Brooke Cochrane, quite taken by her bi-lingual skills and interest in German culture. Besides family life, Andreas and Mary Brooke enjoy the outdoors, running, hiking, cycling and camping but also involvement in the local church community.
Acknowledgements

I want to express my gratitude to my advisor Dr. Tarek Echekki for giving me the opportunity to pursue Ph.D. research in the field of my interest, for guidance and advise over the years. I also want to thank my committee members, Dr. Hong Luo for his support, Dr. Jack Edwards for fruitful discussions and sharing technical insights, Dr. Frank Mueller for providing access to the ARC supercomputing platform.

I also want to thank my peers who contributed to the success of this work, Dr. Scott Mason (Lockheed Martin), for providing the original DNS code and for his availability to answer questions, Dr. Alan Kerstein, independent consultant and formerly at Sandia National Laboratories, for his availability for questions concerning ODT modeling, Dr. Dr. James Elliott (Sandia), for his advise from the computer science perspective, Dr. Lixiang Luo for helpful discussions about parallelization, Dr. David Fiala (Google), for his work as cluster administrator. I want to acknowledge the work of the secretaries Annie White, Eddie Nowell and Marilyn Cross, who help create a good work environment at the department.

Appreciation is also given to my friends, Dipl.-Ing. MSc. Max Rech, Dr. Marc Hoffmann, Dr. Maxwell Koobatian, Dr. Jesse Fulton and Dr. Alexander Franke, for their support and advise throughout my Ph.D. time. Also Bill Knouse, MS., Joseph Rajan, MS., Dr. Jan Büellesbach, Adam Brown, MS., Ricky Stevens, MA., Joseph Miller, DPT., Patrick Keene, MS., Dr. Christer Rajiv Akouala, soon to be Drs. Matthias Schmid, Edwin J. Walker Jr. and William Kish, Dr. Parth Shah, Dr. Shubham Sirivastava and Dr. Srinivasan Rasipuram.

I want to thank my family for their love and support over all these years, my mom and dad, Annemarie and Hans Hoffie, brothers Hans-Friedrich and Manfred Hoffie. Also my in-laws Carl and Brooke Ann Cochrane, Dr. Katharyn Cochrane, Loomis Cochrane and Abigail Cochrane.

The most sincere and heartfelt gratitude is given to my wife, Mary Brooke Hoffie for her never-ending love, patience and support, for being there for me when things were confusing, for her encouragement to push on and keep pursuing my dreams and for her great understanding that sometimes I had to choose Ph.D. research over her. This kind of selfless love is hard to find and that is why I married her.
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# List of Nomenclature

## Latin Letters

- $a$: Temperature Exponent
- $A$: Eddy size PDF coefficient
- $b$: Collision frequency
- $B_j$: Constant column matrix
- $c_i$: Kernel transformation amplitude, generic FD coefficient
- $c_p$: Specific heat at constant pressure
- $c_v$: Specific heat at constant volume
- $C$: Eddy rate parameter
- $C^D$: Divergence operator
- $C_\delta$: One-percent thickness growth rate
- $C^G$: Gradient operator
- $C_i$: Convection terms
- $C_i^m$: Generic finite-difference coefficient matrix
- $C_S$: Smagorinsky closure parameter
- $D$: Diffusivity
- $D_i$: Diffusive terms
- $E_i$: Energy column matrix
- $E$: Energy
- $E_a$: Activation energy
- $f$: Eddy size PDF
- $f_i$: External body force vector
- $F$: Fuel
- $g$: Eddy location PDF
- $G$: Filter function
- $h$: Enthalpy
- $h_0$: Standard enthalpy of formation
- $ied$: Ratio of LES to ODT resolution
- $i, j, k$: Index along $x, y, z$, dummy index
- $i1d, j1d, k1d$: 1D ODT index along $x, y, z$
- $in, jn, kn$: 1D ODT node index along $x, y, z$
\( J_{kj} \) Diffusive mass flux
\( k \) Turbulent kinetic energy
\( k_f, k_b \) Forward and backward reaction rate
\( K \) Kernel transformation function
\( l_e \) Eddy length
\( L \) Domain length
\( L_{x}, L_{y}, L_{z} \) Domain length along \( x, y, z \)
\( L_{j,k} \) Lagrangian multiplier
\( M \) Molecular mass
\( M \) Triplet map function
\( n \) Number of moles
\( N \) Total number of species (reactants, products)
\( N \) Resolution (number of grid points)
\( N_{\text{max}} \) Maximum number of eddy sampling trials
\( N_{\text{modes}} \) Total number of forcing modes
\( N_{r} \) Number of random phase changes per period
\( N_{x}, N_{y}, N_{z} \) Resolution along \( x, y, z \)
\( O \) Oxidizer
\( p \) Pressure
\( P \) Product
\( P_{e} \) Eddy acceptance probability
\( P_{\text{targ}} \) Eddy target probability
\( \dot{q}'' \) Surface heat flux
\( \dot{q}''' \) Volumetric heat source
\( Q_{j} \) Available kinetic eddy energy
\( r \) Velocity ratio
\( R \) Reactant, ratio of velocity ratios
\( \text{smin}, \text{smax} \) Minimum, maximum eddy index size
\( \dot{s} \) Source term (reaction rate)
\( \text{se} \) Index size of eddy
\( S_{ij} \) Strain rate tensor
\( t \) Time
\( T \) Temperature
\( T_{ij} \) Transfer matrix
\( U \) Velocity
\( U_1 \) Velocity of the high-speed stream
\( U_2 \) Velocity of the low-speed stream
\( U_m \) Mean velocity
\( u_i \) Velocity vector
\( u, v, w \) Streamwise, transverse, spanwise velocity component
\( x_i \) Coordinate vector
\( x, y, z \) Streamwise, transverse, spanwise coordinate
\( V \) Volume
\( X \) Mole fraction
\( Y \) Mass fraction
\( Z \) Viscous penalty parameter

**Greek Letters**

\( \alpha \) Non-dimensional temperature
\( \alpha_e \) Maximum allowable ODT energy for component redistribution
\( \beta \) Non-dim. activation energy (Schwab-Zeldovich number)
\( \beta_m \) Scaling parameter for eddy maturing condition
\( \gamma \) Adiabatic coefficient
\( \Gamma \) Magnitude of Oseen vortex
\( \alpha, \beta, \gamma \) Interpolation coefficients
\( \delta_{ij} \) Kronecker delta
\( \delta \) One-percent thickness
\( \delta_\omega \) Vorticity thickness
\( \Delta \) Filter width, difference, step size
\( \epsilon \) Power series coefficient
\( \epsilon \) Dissipation of turbulent kinetic energy
\( \epsilon_{SOR} \) Successive-over relaxation tolerance
\( \epsilon_p \) Relative magnitude of forcing perturbations
\( \zeta_k \) Runge-Kutta integration coefficient
\( \eta \) Kolmogorov length scale
\( \eta_i \)  
Spatial growth rate (imaginary)

\( \eta_r \)  
Stability wave number

\( \theta \)  
Momentum thickness

\( \Theta_r \)  
Randomly walked phase

\( \lambda \)  
Heat conductivity, wave length

\( \lambda_e \)  
Eddy rate distribution

\( \mu \)  
Dynamic viscosity

\( \nu \)  
Kinematic viscosity, stoichiometric coefficients

\( \nu_T \)  
Turbulent eddy viscosity

\( \xi_k \)  
Runge-Kutta integration coefficient

\( \xi \)  
Size of Oseen vortex

\( \rho \)  
Density

\( \sigma \)  
Hyperbolic tangent function shape parameter

\( \tau_{ij} \)  
Viscous shear stress tensor

\( \tau_e \)  
Eddy turn-over time

\( \tau_\nu \)  
Viscous time scale

\( \Phi \)  
Laplacian pressure, stability mode

\( \phi, \phi_i \)  
Scalar generic dependent variable, column matrix

\( \varphi, \varphi_i \)  
Generic dependent variable, vector

\( \xi \)  
Crank-Nicholson integration coefficient

\( \psi \)  
Crank-Nicholson integration coefficient

\( \omega \)  
Specific dissipation of turbulent kinetic energy

\( \omega_i \)  
Vorticity vector, temporal growth rate (imaginary)

\( \omega_r \)  
Oscillation frequency

\( \omega_{SOR} \)  
Relaxation parameter

\( \dot{\omega} \)  
Source term (net production rate)

\( \Omega \)  
Stochastic contribution due to stirring events
Subscripts

<table>
<thead>
<tr>
<th>Subscript</th>
<th>Description</th>
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<tbody>
<tr>
<td>( \varphi_0 )</td>
<td>Start location of eddy, inlet, fundamental mode</td>
</tr>
<tr>
<td>( \varphi_1 )</td>
<td>High-speed stream</td>
</tr>
<tr>
<td>( \varphi_2 )</td>
<td>Low-speed stream</td>
</tr>
<tr>
<td>( \varphi_a )</td>
<td>Advection</td>
</tr>
<tr>
<td>( \varphi_c )</td>
<td>Center</td>
</tr>
<tr>
<td>( \varphi_{ad} )</td>
<td>Adiabatic</td>
</tr>
<tr>
<td>( \varphi_d )</td>
<td>Dimensional quantity, diffusion</td>
</tr>
<tr>
<td>( \varphi_{DNS} )</td>
<td>DNS quantity</td>
</tr>
<tr>
<td>( \varphi_e )</td>
<td>Eddy</td>
</tr>
<tr>
<td>( \varphi_{elap} )</td>
<td>Elapsed</td>
</tr>
<tr>
<td>( \varphi_{ign} )</td>
<td>Ignition</td>
</tr>
<tr>
<td>( \varphi_{in} )</td>
<td>Inlet</td>
</tr>
<tr>
<td>( \varphi_f )</td>
<td>Flush</td>
</tr>
<tr>
<td>( \varphi_F )</td>
<td>Fuel</td>
</tr>
<tr>
<td>( \varphi_k )</td>
<td>Runge-Kutta sub-step, species index</td>
</tr>
<tr>
<td>( \varphi_{LES} )</td>
<td>LES quantity</td>
</tr>
<tr>
<td>( \varphi_m )</td>
<td>Mean quantity</td>
</tr>
<tr>
<td>( \varphi_{max} )</td>
<td>Maximum of quantity</td>
</tr>
<tr>
<td>( \varphi_{min} )</td>
<td>Minimum quantity</td>
</tr>
<tr>
<td>( \varphi_O )</td>
<td>Oxidizer</td>
</tr>
<tr>
<td>( \varphi_{ODT} )</td>
<td>ODT quantity</td>
</tr>
<tr>
<td>( \varphi_p )</td>
<td>Perturbation, parallel</td>
</tr>
<tr>
<td>( \varphi_{ref} )</td>
<td>Reference quantity</td>
</tr>
<tr>
<td>( \varphi_{RMS} )</td>
<td>Root-mean-squared (standard deviation)</td>
</tr>
<tr>
<td>( \varphi_s )</td>
<td>Stirring, serial</td>
</tr>
<tr>
<td>( \varphi_{samp} )</td>
<td>Sampling</td>
</tr>
<tr>
<td>( \varphi_{SOR} )</td>
<td>Successive over-relaxation</td>
</tr>
<tr>
<td>( \varphi_{targ} )</td>
<td>Target</td>
</tr>
<tr>
<td>( \varphi_T )</td>
<td>Turbulent/eddy quantity, Temperature</td>
</tr>
<tr>
<td>( \varphi_x )</td>
<td>Quantity along ( x )-direction</td>
</tr>
<tr>
<td>( \varphi_y )</td>
<td>Quantity along ( y )-direction</td>
</tr>
<tr>
<td>( \varphi_z )</td>
<td>Quantity along ( z )-direction</td>
</tr>
</tbody>
</table>
Superscripts

$(\phi)'$ Reynolds fluctuation, reactant, first derivative, distinguished variable

$(\phi)''$ Favre fluctuation, second derivative, product

$(\phi)^*$ Interim quantity

$(\phi)^D$ Divergence

$(\phi)^G$ Gradient

$(\phi)^n$ $n$th time step

$(\phi)^{SGS}$ Sub-grid stress contribution

Operators

$(\overline{\phi})$ Reynolds-averaged quantity

$(\tilde{\phi})$ Favre-averaged quantity, filtering operation

$\langle \phi \rangle$ Spatially and temporally (RANS or FAVRE) averaged quantity

$\hat{(\phi)}$ Interpolation operation

$L(\phi)$ Laplacian operator

$\|\phi\|_2$ Euklidian $L_2$ norm

$\text{rad}(\phi)$ Radicant of a root

Dimensionless Numbers

CFL Courant Friedrichs Lewy Number

Da Damkohler number

Le Lewis number

Ma Mach Number

Pr Prandtl number

Re Reynolds number

Sc Schmidt number

Constants

$\pi$ Irrational circumferential number 3.142

$R_u$ Universal gas constant 8.314 J/(mol·K)
**Abbreviations**

<table>
<thead>
<tr>
<th>Abbreviation</th>
<th>Description</th>
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<tbody>
<tr>
<td>AME</td>
<td>Autonomous Microstructure Evolution Model</td>
</tr>
<tr>
<td>AMR</td>
<td>Adaptive Mesh Refinement</td>
</tr>
<tr>
<td>ANN</td>
<td>Artificial Neural Network</td>
</tr>
<tr>
<td>CMC</td>
<td>Conditional Moment Closure Model</td>
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<tr>
<td>CPU</td>
<td>Central Processing Unit</td>
</tr>
<tr>
<td>CFD</td>
<td>Computational Fluid Dynamics</td>
</tr>
<tr>
<td>DNS</td>
<td>Direct Numerical Simulation</td>
</tr>
<tr>
<td>DES</td>
<td>Detached Eddy Simulation</td>
</tr>
<tr>
<td>EDC</td>
<td>Eddy Dissipation Concept</td>
</tr>
<tr>
<td>EBU</td>
<td>Eddy Break-Up Model</td>
</tr>
<tr>
<td>FD</td>
<td>Finite-Difference</td>
</tr>
<tr>
<td>FDF</td>
<td>Filtered Density Function</td>
</tr>
<tr>
<td>FPDF</td>
<td>Filtered Probability Density Function</td>
</tr>
<tr>
<td>FPV</td>
<td>Filtered Progress Variable</td>
</tr>
<tr>
<td>GPU</td>
<td>Graphics Processing Unit</td>
</tr>
<tr>
<td>LES</td>
<td>Large Eddy Simulation</td>
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<tr>
<td>LEM</td>
<td>Linear Eddy Model</td>
</tr>
<tr>
<td>MPI</td>
<td>Message Passing Interface</td>
</tr>
<tr>
<td>ODT</td>
<td>One-Dimensional Turbulence Model</td>
</tr>
<tr>
<td>OpenMP</td>
<td>Open Source Multi-Processing</td>
</tr>
<tr>
<td>OpenFOAM</td>
<td>Open Source Field Operation And Manipulation Software</td>
</tr>
<tr>
<td>PCA</td>
<td>Principal Component Analysis</td>
</tr>
<tr>
<td>PDF</td>
<td>Probability Density Function</td>
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<tr>
<td>RANS</td>
<td>Reynolds-Averaged Navier-Stokes Simulations</td>
</tr>
<tr>
<td>SGS</td>
<td>Sub-Grid Stress</td>
</tr>
<tr>
<td>SGF</td>
<td>Sub-Grid Flux</td>
</tr>
<tr>
<td>TPF</td>
<td>Turbulent Premixed Flames</td>
</tr>
<tr>
<td>TNF</td>
<td>Turbulent Nonpremixed Flames</td>
</tr>
<tr>
<td>UFPV</td>
<td>Unsteady/Flamelet Progress Variable</td>
</tr>
<tr>
<td>U-RANS</td>
<td>Unsteady RANS</td>
</tr>
<tr>
<td>VLES</td>
<td>Very Large Eddy Simulation</td>
</tr>
</tbody>
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Chapter 1

Introduction

"When I meet God, I am going to ask Him two questions:
Why relativity? And why turbulence?
I really believe He will have an answer for the first."

Werner Heisenberg

The field of turbulent-reactive (turbulent and combustion) flows has undergone significant progress in the 1970s and 1980s due to the developments in computational fluid dynamics (CFD), but also due to the advancement of non-intrusive laser-based techniques. These advanced experimental measurements serve as standards for model validation purposes, and have been made publicly available by the "Turbulent Nonpremixed Flames" (TNF) and "Turbulent Premixed Flames" (TPF) workshops, starting in the 1990s.

This chapter serves as an introduction to the rather vast field of turbulence and combustion modeling. Three major approaches exist to simulate fluids - direct numerical simulation (DNS), large eddy simulation (LES) and Reynolds-averaged Navier-Stokes simulations (RANS) as well as combinations of these. While DNS does not require turbulence modeling, LES and RANS does. This chapter focuses on LES turbulence modeling only, while trying to give an overview of the many models used today with the focus on a paradigm shift introduced by the autonomous microstructure evolution (AME) models to which ODT belongs to.
After the introduction of aspects of turbulence modeling, the discussion shifts to explaining flow phenomena present in turbulent non-reacting and reacting shear layers. This discussion focuses on numerical as well as experimental findings. At the end of the chapter the objectives of this work are formulated and the chapter is then concluded by an outline of the discussions lying ahead.

### 1.1 Simulation of Turbulent and Reactive Flows

More recently, rapid progress has been achieved in modeling and simulation of turbulent-reactive flows. This is due to the availability of improved high-performance computing resources, which enabled the simulation of more realistic flows, with detailed description of turbulence and chemistry. On the other hand, the increasing demands of design margins of combustion technologies to become cleaner and more efficient is another driving factor for advancements in modeling and simulation. Such improved simulations will significantly reduce the overall turn-around times in the design process.

Turbulent combustion has long been identified as a continuum temporal and spatial multi-scale problem. Based on the spatially resolved turbulent scales of the flow, there are three simulation approaches: first, direct numerical simulation (DNS), which resolves all turbulent scales down to the Kolmogorov level; second, large eddy simulation (LES), which resolves large and models small turbulent structures; and third, Reynolds-averaged Navier-Stokes simulations (RANS), which models all turbulent scales and yields a temporally averaged solution. Formulating a model for the residual turbulent subgrid stresses (SGS) as they appear in the filtered (time or ensemble averaged) LES and RANS equations, is key challenge of all turbulence models and known as the ”Closure Problem”.

#### 1.1.1 Direct Numerical Simulation (DNS)

As DNS resolves all turbulent scales, it provides a complete and detailed information about the flow field and can thus be used as benchmark to validate LES and RANS turbulence models. For DNS simulations however, the number of required grid points scales exponentially with the Reynolds number based on the Kolmogorov length-scale, $\eta$ and time scale $\tau$ (the dissipation length scales). Such that for a cuboid domain of length...
1.1. Simulation of Turbulent and Reactive Flows

1. INTRODUCTION

L with homogeneous grid \((\Delta x = \Delta y = \Delta z)\) for example, the number of required grid points is given by

\[
N_{\text{DNS}}^3 = \left(\frac{L}{\eta}\right)^3 \left(\frac{T}{\tau}\right) \sim \Re_L^3.
\]

Therefore, due to computational limitations, Re number limitations for DNS exist. A higher resolution (grid points per volume) always goes along with a smaller time step to ensure numerical stability and to resolve all physical effects correctly in time. This is addressed by the CFL condition. DNS is also limited to simple geometries as it is based on finite-difference operators for structured grids.

1.1.2 Reynolds-Averaged Navier-Stokes Simulation (RANS)

The RANS governing equations are obtained by taking the time or ensemble average on the DNS governing equations, such that the solution of the governing equations corresponds to a statistically stationary flow. Due to averaging, all small scale information is lost and are represented by the Reynolds stress tensor in the governing equations, which introduces new unknowns into the system of equations. This term can only be represented by introducing new variables (model constants) and a formulation for a turbulence model. Famous turbulence models are the Spalart-Allmaras model, the mixing length model, \(k - \varepsilon\) or \(k - \omega\) models, for example. A timely resolved variant of RANS exists and is termed unsteady RANS or U-RANS [30, 111, 124].

1.1.3 Large-Eddy Simulation (LES)

Due to the limitations of DNS and RANS, a third approach has been developed by Smagorinsky [117], and later Deardorff [17], termed LES, which resolves large scales while small scales require modeling. Most LES turbulence models are derived from RANS models. The LES computational cost is comparable to that of RANS, but LES still has Reynolds number limitations. Over the past years, LES has gained more and more popularity due to increasing computational resources (Pope [103]) and has recently been applied to engineering flows, as presented in Sankaran, Menon et. al. [113], with application to gas-turbine combustor flows. An alternative to LES in order to save computational
resources, is V-LES (Very-Large Eddy Simulation), as presented in Magnato [66].

There are also Hybrid LES-RANS approaches (Fröhlich [22], Davidson [16]), such as detached-eddy simulation (DES), which uses RANS and LES in different regions, for example RANS for the near wall region and LES for regions which need to be timely resolved.

1.2 Turbulent Combustion Modeling for LES

Turbulent combustion modeling poses several challenges to the modeler, as combustion is a process with high heat release, which may involve a large number of species. Turbulent transport happens over a wide range of length and time scales, which many present models are not able to cover. In addition to that, turbulence-chemistry interactions are hard to describe physically. Turbulence increases the volumetric reaction rate and thus changes the flame structure. High heat release can lead to dissipation of turbulent kinetic energy due to increased viscosity or increase in baroclinic vorticity. These interactions are subject of current combustion modeling research.

As already mentioned above, filtering of the DNS governing equations results in LES subgrid-stress (SGS) and subgrid-flux (SGF) terms for velocities and scalars respectively, which need to be modeled with appropriate equations. Conventional turbulent subgrid closure models for large eddy simulation (LES) use adjustments of the model constants in their equations to simulate the desired regime. These include gradient diffusion approximations, such as the Smagorinsky model [117] and the dynamic model by Germano [24]. Gradient diffusion type models rely on deriving the closure information for unresolved physics using resolved scales. This method has severe limitations on turbulent mixing and combustion. One limitation is that non-unity Lewis number effects cannot be adequately modeled. In addition to that, counter-gradient diffusion effects have been observed in studies when high heat release is present, as done by Poinsot [102] and Veynante [122].

Modeling source terms for chemical reactions poses another major challenge in turbulent combustion modeling. These terms are generally non-linear and exist on very different time scales associated with different rates of complex reaction mechanisms, which can involve thousands of reactions and hundreds of species for practical fuels. Species source
terms also need close coupling to their diffusion terms, which heavily defines the flame structure, wrinkling and mixing. Large scale mixing increases the number of interfaces, which separate reactants and products or fuel and oxidizer in premixed and non-premixed cases respectively. Thus mixing affects scalar gradients which in turn influences rates of molecular transport and coupling with chemistry.

While large scale turbulence is coupled with small scale turbulence, reasonable assumptions can be made to attempt to partially decouple large and small turbulent scales. This is done by other conventional scale-separating models like the eddy-dissipation concept (EDC) or the eddy break-up (EBU) model, which are based on the comparison of rates of mixing versus rates of chemistry. More sophisticated approaches that have been developed are the flamelet model (Peters [93], Pitsch [99] and Ihme [38]). But also the conditional moment closure (CMC) model (Klimenko [54] and Bilger [7]) and the transported filtered density function (FDF) model (Pope [104]) or similar approaches with the presumed probability density function (PDF) models (Givi [27]).

Flamelet and CMC approaches represent reactive scalars through transport equations in phase space in terms of quantities that can be transported in physical space. A typical phase-space “coordinate” is the mixture fraction. The transport of a passive scalar, like the mixture fraction in physical space, reduces the number of scalar transport equations and eliminates source terms in the conservation equations. Such parametrization however, makes assumptions about the combustion mode and regime, which cannot be met uniformly in space and time.

Regime-independent turbulent combustion modeling however, allows to simulate configurations involving a combination of different regimes. For example extinction, reignition, soot formation, partial premixing, recirculation and multi-stage ignition, etc, while minimizing the required input parameters. Regime-independency is achieved with the temporally and spatially resolved low-dimensional representation of the relevant advection-diffusion-reaction coupling equations in physical space.

Two famous examples of regime-independent modeling is the linear eddy model (LEM) and the one-dimensional turbulence model (ODT). The LEM model has been initially developed by Kerstein [43] in 1988. Then later by McMurty, Menon and Kerstein [72]. The latest contributions are by Sannan, Weydahl and Kerstein [114]. The one-dimensional
turbulence model (ODT), has also been initially developed by Kerstein [49] in 1999 and later developed into ODTLES by McDermott [70] and by Gonzales-Juez, Schmidt and Kerstein [29] and others, but also by Cao and Echekki [13] into LES-ODT, which the work at hand is based on.

The family of models of this new paradigm is summarized under the term "autonomous microstructure evolution" (AME) [51]. The defining feature of the AME paradigm in the context of flow simulation is that a representation of small scale processes is adopted (locality principle) that yield through process evolution collective behaviors that correspond to continuum flow. The AME paradigm accommodates processes rather than particles as its primitive elements. In the formulation explained here (ODT), the primitive elements are associated with vortical motion ("a process"), rather than vortices per se. The key attributes of the primitive elements introduced here is that their process is implemented on a one-dimensional spatial domain.

In summary, the approaches of LES simulation of turbulent reactive flows may be classified under the following three categories: (1) moment closure methods such as the ones based on the flamelet approach and the conditional moment closure (CMC) approach, and (2) filtered mass-density function (FDF) methods as well as probability density (PDF) methods and assumed PDF methods, and last but not least (3) one-dimensional stochastic (or AME) approaches, such as LEM and ODT. A brief, more detailed review about the flamelet, CMC and AME models is given below.

1.2.1 Flamelet Model

The underlying assumption for flamelet modeling is that chemical time scales are short enough so that reactions occur in a thin layer around stoichiometric mixture, where the layer is on a scale that is smaller than the small scales of turbulence (Peters [93]). Following this idea, a small instantaneous flame element embedded in a turbulent flow has the same attributes as a small laminar flame - a so-called flamelet. The flamelet model takes into account finite-rate chemistry. There are essentially two strategies of flamelet modeling depending on the independent parameter variable used to tabulate values in a library. The first strategy is to use the scalar dissipation rate, the second is to use the reaction progress variable.
1.2. Turbulent Combustion Modeling for LES

Using the scalar dissipation rate as the underlying parameter, there are steady state (Kempf [42], Raman and Pitsch [105]) and transient flamelet models for non-equilibrium finite rate chemistry in a Lagrangian (Pitsch and Steiner [101]) and Eulerian (Pitsch [98]) formulation. The unsteady flamelet equations are solved to provide the filtered scalar quantities using a presumed filtered probability density function (presumed FPDF) of the mixture fraction. The downside of using the scalar dissipation rate as parameter is that it has to be properly determined. Also, the flamelet model cannot predict extinction and re-ignition, as solutions are not unique to for one scalar dissipation rate value.

Due to these weaknesses, Pierce and Moin [96] suggested a second flamelet approach, which is based on the progress variable, the flamelet/progress variable (FPV) model. The transport equations are for the filtered progress variable and the filtered chemical source term is closed with the flamelet library and the presumed joined FPDF of mixture fraction and progress variable. As validation cases have shown (Pierce and Moin [96]), the progress variable approach is able to capture the unsteady, filtered flame dynamics as observed in the experiments. According to Ihme [38], the steady-state assumption at low scalar dissipation rate, especially during re-ignition is inaccurate. Therefore, an extension to an unsteady flamelet library formulation has been proposed by Pitsch and Ihme [100] and Ihme and See [39], termed as the unsteady flamelet/progress variable (UFPV) model. However, providing the correct joint filtered probability density function (FPDF) of the mixture fraction and the progress variable remains still a challenge. Following these modeling approaches and the attempt to predict more complex combustion phenomena, requires in turn more closure models, additional variables, and potentially increases the uncertainty about model accuracy.

1.2.2 Conditional Moment Closure (CMC)

The conditional moment closure (CMC) model has been independently developed by Klimenko [54] and Bilger [7] for RANS. This approach solves exact transport equations for mixture fraction conditioned means of reactive scalars. Kim and Pitsch [53] applied the model to LES simulations, Navarro-Martinez [87] applied the LES-CMC approach to non-premixed, piloted, turbulent jet diffusion flames, which shows better predictions than the RANS-CMC approach [108].
One of the disadvantages of the model is that it only provides an approximate closure for chemical source terms because the mean chemical source terms are dependent on the conditional mean values (Chen [15]). Moreover, predicting extinction and re-ignition and determining scalar dissipation rate still pose challenges, as the CMC equations share many similarities with the transient flamelet (UFPV) model. Refinements of these models require adding additional transport equations as for the case of the flamelet model. Additional transport equations require additional closure models and add complexity, more parameters, but also computational cost.

1.2.3 Transported Filtered Density Function Approach (FDF)

The transported filtered density function approach has originally been introduced by Pope [104] in 1990. The model has proven its capability so simulate local extinction and re-ignition (Chen [15]). The transport equation is based on one-point one-time information, such that multi-point information, like molecular mixing needs to be modeled, which can be a restriction as discussed in Pitsch [99]. The joint scalar FDF transport equation is represented by a system of notional particles and cannot be solved by the finite volume or finite difference method. The accuracy of the model scales with the square root of the number of notional particles and thus the computational cost becomes significant for LES-FDF simulations. Muradoglu [86] suggested a hybrid scheme, where the energy equation is solved using the transport equation but the chemical source term is obtained through the joint PDF. Zhang and Haworth [127] used FDF with unsteady RANS. In contrast to flamelet and CMC, the FDF approach does not make assumptions about the combustion mode, thus the only challenge in FDF modeling remains with mixing models and computational cost.

1.2.4 Autonomous Microstructure Evolution (AME) Models

As mentioned above, novel regime-independent multiphysics models (or AME models) can overcome assumptions over the combustion regime. Regime-independency for turbulent flows describes the ability to simulate simultaneously different flow regimes in combustion like extinction and re-ignition, multiple phases (soot formation), partial premixing,
recirculation and multi-stage ignition, etc. This is accomplished with low-dimensional spatial and temporal resolution of the subgrid scales on an actual subgrid, meaning by enabling microstructures to evolve autonomously on the physical subgrid. In the case of LEM and ODT, the subgrid is one-dimensional. This helps to keep the simulation affordable. Resolving the LES subgrid scales on a mesh, allows to couple advection, diffusion and reaction processes directly and deterministically from the inertial subrange down to the Kolmogorov limit. This aligns well with the LES strategy, which resolves scales far enough below the flow-dependent energy-containing scales so that the unresolved motions are within the inertial subrange.

The main role of unresolved motion is presumed to be cascading the mesh-resolved kinetic energy to smaller, unresolved scales. The dissipation is incorporated using eddy viscosity. Information of the flow between the resolved and unresolved scales is exchanged by down-scaling (for example interpolation) or up-scaling (for example filtering) of the flow quantities from the LES grid to the subgrid and vice versa. Combining the three-dimensional LES solution with the one-dimensional solution also allows to resolve three-dimensional effects and simulate boundary conditions more accurately.

For practical three-dimensional simulations, one-dimensional ODT line segments are associated with each control volume of an LES element in all three orthogonal directions. This procedure is denoted as ODTLES formulation (Gonzales-Juez, Schmidt and Kerstein [29]) or LES-ODT formulation, (Cao & Echekki [13]), which are the two predominant strategies to couple LES and ODT.

1.2.4.1 Linear Eddy Model (LEM)

The linear eddy model (LEM), originally developed and proposed by Kerstein [43] in 1988, addresses the challenge to simulate turbulent mixing and combustion at all turbulent length and time scales. As mentioned above, this is accomplished by spatially and temporally resolving subgrid turbulent advection, diffusion and reaction on a one-dimensional domain in physical space. The advantage over other models is that the two primary mechanisms that govern the scalar mixing process, turbulent eddy turn-over events and molecular diffusion as well as reaction, are treated distinctively. Diffusion-reaction equations are integrated in time on a one-dimensional domain. The advection
process is simulated stochastically by eddy turn-over events, which is realized by means of a mathematical triplet-map, which simulates the strain and the rotational folding effects of vortical motion, [43].

The model has been applied to shear layers and to axi-symmetric flow by Kerstein (see [44], [45]). It also has been used to study microstructure of diffusive scalar mixing fields, jet diffusion flames, finite-rate chemistry (extinction and re-ignition) and multi-stream mixing, see Kerstein [46], [47], [48]. McMurtry [72] predicted the decay of a scalar in homogeneous turbulence using LEM for wide ranges of Reynolds and Schmidt numbers. Goldin and Menon [28] used LEM for steady-state turbulent combustion.

While the cases cited above were stand-alone LEM cases only, McMurtry et al. [74] applied LEM as LES subgrid closure to a hydrogen-air flame for the first time. Menon et al. [75] then further explored LEM-LES for premixed and non-premixed combustion flows and used a ”splicing method” to transport the scalar subgrid information across cell boundaries. In a further advancement, Zimberg et al. [128] investigated mixing, multiphase flows (soot) and radiation effects within the LEM-LES context; and Sone [118] simulated fuel-air mixing in an internal combustion engine within the LEM-LES context. The latest contributions to LEM have been made by Sannan [114], for unsteady flows with improved three-dimensional performance.

However, size, frequency and distribution of the eddies have to be known a-priori. A predefined energy spectrum is used to do that by choosing parameters that govern the random event sequence. Also, LEM has been designed to be a mixing model and the velocity information is not present at the small turbulent scales.

### 1.2.4.2 One-Dimensional Turbulence Model (ODT)

In order to overcome the limitations to know turbulence properties a-priori, in 1999 Kerstein [49] developed a new model, called one-dimensional turbulence (ODT) Model. ODT limits the input parameters and also has detailed velocity information available at the smallest turbulent scales. Therefore, ODT is a method to simulate the dynamic fluctuations of turbulent motion along a notional, one-dimensional line of sight of an actually three-dimensional flow (Schmidt [115]). In other words, while LEM is a mixing model, ODT is a turbulence model, which solves for velocities at the subgrid scale. The
1.3. Non-Reacting and Reacting Shear Layers

The present study applies the LES-ODT context to reacting and non-reacting shear layers. Shear layers are important phenomena in nature as well as in engineering. This chapter gives a detailed problem description and shall serve as a brief review of the work done on shear layers experimentally and numerically. A more general overview of reacting and non-reacting shear layers is also given in Dimotakis [19] and Ho & Huerre [34] respectively.

1.3.1 Problem Description

Figure 1.1 depicts a possible experimental shear layer setup. Two parallel streams of fluid at different velocities $U_1$ and $U_2$, where $U_1 > U_2$ are initially separated by a plate, but...
then are allowed to interact at the end of the plate.

Mason [69] discusses the Kelvin-Helmoltz roll-up of a shear layer. Linear stability theory predicts that for a range of Reynolds numbers, the shear layer becomes unstable. In nature, the differently developed boundary layers on either side of the plate provide enough disturbances to trigger the primary instability, the so-called Kelvin-Helmholtz instability. These instabilities form one-dimensional waves and eventually two-dimensional "rollers", so-called vortices with vorticity components in the transverse \((y)\) direction. The disturbance-interactions from the two streams lead to combination of vortices from each stream and in turn, to their amplification in the downstream direction, which leads to formation of larger and larger vortices. This process entrains fluid from the other stream, which causes the growth (spread) of the shear layer along the streamwise \((x)\) direction. In literature, this phenomenon is also known as Kelvin-Helnholtz roll-up.

In the transition phase, vortices with vorticity components in the streamwise direction begin to emerge, which are called "rib" vortices. At high enough Reynolds numbers, the interaction of spanwise and streamwise vortices produce three-dimensional structures that lead to mixing enhancement. When the shear layer is dominated by large-scale structures, it is considered to be fully turbulent.

The shear layer can be characterized by several parameters, such as the shearing inten-
1.3. Non-Reacting and Reacting Shear Layers

1.3.1 Introduction

If \( r = U_2/U_1 \), if \( U_1 > U_2 \), the mean (time-averaged) thickness \( \delta \), quantified by 1% profile thickness, the vorticity thickness \( \delta_\omega \) and the momentum thickness \( \theta \). Common definitions of the Reynolds number are for example \( \text{Re}_x = \Delta U x/\nu \), \( \text{Re}_\delta = \Delta U \delta/\nu \), \( \text{Re}_\theta = \Delta U \Theta/\nu \), with \( \Delta U = U_1 - U_2 \) and \( \nu \) the kinematic viscosity. The shear layer is fully turbulent for \( \text{Re}_x > 10^6 \), where the flow shows self-similar behavior and the main thickness is linearly within the downstream distance.

In the reacting case, the free-streams contain fuel and oxidizer respectively, which chemically react when mixed with each other. When the reaction rates are fast compared to flow rates, the reaction occurs in a thin flame sheet wrinkled and stretched by the large scale velocities. When the reaction rates are small compared to the flow rates, the reaction zone becomes thicker. The Damköhler number compares chemical time scale to flow (or mixing) time scale.

Shear layers with significant heat release, usually involving hydrocarbon fuels, will significantly alter its structure, as the fluid mechanics are coupled with chemistry through density variations. Mason [69] gives also an overview on experimental as well as numerical findings on non-reacting and reacting shear layers.

1.3.2 Non-Reacting Shear Layers

1.3.2.1 Experimental Work

Brown and Roshko [8] in 1974 already, studied the planar, turbulent shear layer between gases with different densities by means of a spark shadowgraph. Their observations have shown that the turbulent region is dominated by large scale structures (\( \text{Re}_x \approx 10^6 \)). The conclusion was that these structures were responsible for turbulent mixing and shear layer growth. In parallel to these studies, Winant and Browand [125] were also looking at the vortex pairing effect in a water tunnel experiment, at moderate Reynolds numbers (\( \text{Re}_\theta \approx 500 \)). From their observations, vortex pairing was described as originating from flow instabilities.

The discovery of dominant large scale structures in shear layers led to a paradigm shift about how researchers thought about turbulence. Consequently, Oster and Wygnanski [88] looked at the effects of two-dimensional forcing of two air streams at Reynolds
numbers of $\text{Re}_\theta \approx 10^4$. At low forcing amplitudes, the initial growth rate was greater than for the unforced case, as excitation promotes vortex pairing. With increasing amplitudes, vortex pairing after initial growth was suppressed, due to resonance. The observations have also shown that pairing resumes after the resonance region, however with loss of self-similar behavior of the layer. The studies have also shown that varying the frequency has similar effects on the initial growth rate, which suggested that vortex pairing is related to the subharmonics of the initial instability frequency.

Ho and Huang [33] studied the effects of subharmonics on vortex pairing in a water tunnel. The findings showed that the presence of subharmonics is a necessity for pairing and controlling of the growth of the layer. Small forcing near the subharmonics of the most unstable frequency resulted in localized pairing. When forced at the first subharmonic, vortices paired at a fixed location, and when forced at the second subharmonic vortices paired at a fixed location and the resulting vortex pairs at another fixed location. Forcing near the most unstable mode, prevents growth because of resonance. One further important outcome was that linear inviscid stability theory is able to predict most of the phenomena observed in forced shear layers.

Bernal [6] presents an investigation into small-scale, three-dimensional shear layer structures, which increase mixing but do not break down large-scale structures. The small three-dimensional structures form at transition as a result of earlier instabilities and have streamwise vorticity components (rib vortices). These observations were confirmed by Jimenez [40], Lasheras, Cho and Maxworthy [61], Lasheras and Choi [60].

At a later time, Huang and Ho [37], Tung and Kleis [121], found that the wavelength of the secondary instability is approximately two-thirds of the wavelength of the fundamental mode of spanwise instability. Pierrehumbert and Widnall [97] confirm the value of two-thirds in their theoretical work.

1.3.2.2 Numerical Simulations

The first numerical studies of forced shear layers have been performed by Patanik et al. [92] in 1976, by Knight [55] in 1979 and by Riley and Metcalfe [107] in 1980. Riley and Metcalfe showed with their three-dimensional DNS simulations that forcing near the most unstable mode reduces shear layer growth, therefore suggesting that out-of-phase
subharmonic perturbations were required to enhance vortex pairing.

Looking at incompressible, spatially developing forced shear layers at low Reynolds numbers, Lowery and Reynolds [65] found good agreement of growth rates compared to experiments (Oster and Wygnanski [88]). Another important finding was that the shear layer entrained more fluid from the high-speed side and thus moved toward the low-speed side. This asymmetry has also been confirmed by experiments of Dimotakis [18]. Ghoniem and Ng [25] did similar studies by using vortex element methods.

Lowery and Reynolds emphasis that forcing resembles the randomness of a natural shear layer, leading to non-linear growth rates. The forcing was implemented by perturbing the inflow with random noise, which was intended to emulate the small-scale structures in which case the spanwise vortices developed naturally, with a spacing consistent with the wavelength of the most unstable mode. This study has proven that inlet-forcing in numerical simulations leads to increased production and pairing of vortices.

Sandham and Reynols [112] confirmed the finding that by forcing the fundamental and subharmonic modes with random phases leads to natural shear layer behavior with asymmetric entrainment.

Moser and Rogers [82] examined the temporally developing shear layer, however a lack of both, large-scale pairing and streamwise rib vortices was found. The importance of rib vortices in temporally evolving shear layers has been studied in Moser and Rogers [81], Knio and Ghoniem [57], but also by Buell [9], Buell and Mansour [11] and Knio and Ghoniem [56].

1.3.3 Reacting Shear Layers

1.3.3.1 Experimental Work

The majority of experiments concerning the reacting shear layer have been performed by Mungal and co-workers at California Institute of Technology. For a hydrogen $H_2$ and fluorine $F_2$ reaction, and at low heat release. Mungal and Dimotakis [83] found that as for the non-reacting case, mixing and entrainment were dominated by large-scale structures, which are hot regions, separated by entrainment tongues of cooler fluid. The asymmetric behavior was also found by flipping fuel and oxidizer side, which led to two different mean
temperature profiles, as the flow would bend toward the low speed side.

Mungal, Hermanson and Dimotakis [85] have shown that over an increasing range of Reynolds numbers from $Re_\delta \approx 4 \cdot 10^4$ to $2 \cdot 10^5$, the maximum mean temperature decreased, yielding to not self-similar temperature profiles.

In the presence of heat release, a thinning of the shear layer was observed by Hermanson, Mungal and Dimotakis [31]. This was surprising, but the increase in heat volumetric expansion, led to a decrease of fluid entrainment. Wallace [123] argued that reduced entrainment is due to the production of baroclinic torque.

In later studies, Mungal and Frieler [84] looked at the influence of the Damköhler number (Da) on the formation of reaction products. For larger than one but decreasing Da numbers ($10 > Da > 1$), the maximum mean temperature and production-rates of products decreased. At $Da \approx 1$, chemistry was described as slow and for $Da \geq 10$, the flow was chemically "frozen", meaning reaction time was much larger than the mixing time.

1.3.3.2 Numerical Simulations

McMurtry et al. [73] was one of the first to study the incompressible turbulent-reacting shear layer at low Reynolds numbers and with simple, single-step reaction. They were able to confirm the experimental observation (Wallace [123] and Hermanson et al. [31]) that heat release decreases product formation, entrainment and layer thickness.

Metcalfe et al. [76] found that the decrease in shear layer growth was due to both, thermal expansion during the laminar mixing period and the production of baroclinic torque. Also, increase in temperature, meaning decrease in density, lowered the production rate of turbulent kinetic energy.

Ghoniem, Knio and Krishnan [26] studied Damköhler number effects of a planar jet at high Reynolds numbers. Increasing the Da number led to a thinning of the reaction zone. Three-dimensional DNS simulations of reacting shear layers have been undertaken by Knio and Ghoniem [58], as well as Park, Metcalfe and Hussain [91], who found that rib vortices can lead to noticeable reaction enhancement.

Mechanisms of volumetric heat expansion and baroclinic torques that cause reduction in shear layer growth for the reacting case were studied by Higuera and Moser [32] for the
temporal and by Soteriou and Ghoniem [119] for the spatial shear layer. Chen, Riley and McMurtry [14] have looked into effects of heat release in the context of Reynolds-stress transport, scalar transport and $k - \epsilon$ modeling, like Mason and Rutland have done in [68].

1.4 Objective

The intent of this work is to advance the current LES-ODT formulation, as introduced by Cao and Echekki [13], by applying it to more general and practical flows as they occur in science and engineering. As an example flow, the spatially developing turbulent reactive shear layer is chosen, such that a model extension from decaying (highly unsteady) homogeneous isotropic turbulent reacting flows to statistically stationary, non-decaying inhomogeneous anisotropic turbulent reacting flows has been found necessary and is presented in the following. This includes a more advanced and precise three-dimensional coupling of the one-dimensional subgrid of the ODT domains and additions to the eddy sampling procedure. The model is then validated against DNS results with regards to growth rate and first and second order flow statistics. Another advancement was to enable the variable density formulation, by computing the density on the ODT subgrid and passing it back to LES through filtering.

Two benchmark cases are identified to isolate variable density and chemistry effects. The first is a constant density reacting case and the second is a variable density non-reacting case. These are chosen to determine ODT simulation parameters. The model with the newly found parameters is then applied to a fully reacting shear layer with variable density. A non-unity Lewis number parameter study is conducted showing influence on growth rate and flow statistics. The second benchmark case of variable density non-reacting shear layer is a demonstration of passive scalar mixing.

Besides physical model advancements, the LES-ODT code capabilities are also advanced by implementing a new data format that allows three-dimensional array elements to be addressed in conventional orthogonal index notation, while at the same time saving memory. This is because the ODT resolution is only comparable to the DNS resolution in one specific spatial direction but not at any given point in space. Reducing the resolution
means saving computational cost. Statistical contributions of the ODT model account for information loss due to reduced resolution. This new data format also allows to generalize domain geometries from cubes to arbitrary cuboid geometries. In addition to that, grid stretching capabilities based on generic finite difference operators and definition of boundary conditions based on ghost points have also been implemented.

Transition to a massively parallel formulation with the aid of the message passage interface (MPI) and graphics processing units (GPUs) is recommended for the future. During that transition, the code should be ported to a modern high-level language, object-oriented CFD platform like OpenFoam, which uses a finite volume formulation that enables to simulate flows in more complex geometries.

1.5 Outline

In order to achieve the objectives outlined above, first, physical modeling aspects are discussed and the strategy to combine LES and ODT is presented in great detail in Chapter 2. This includes LES and ODT governing equations and details of the ODT model with advective, diffusive and turbulence transport, as well as reaction closure terms. The chapter concludes with a set of non-dimensionalized governing equations and scaling numbers, which are the working equations for the present study.

Chapter 3 discusses the numerical solution to the LES and ODT governing equations, coupling of the two solution procedures, implementation of the data format and grid stretching. Then, the geometrical problem set-up, initial and boundary conditions are addressed in Chapter 4, with a detailed discussion on parameter choices and a discussion on the parallel scalability of the code.

Chapter 5 presents the results for the non-reacting shear layer as well as different reacting shear layer cases, including a non-unity Lewis number parameter study. All of the findings are summarized in Chapter 6, alongside with recommendations for future work. A detailed illustration on the fractional step method to solve the DNS governing equations is given in Appendix A.
Chapter 2

Physical Modeling

The novel formulation of LES-ODT is based on the coupling of the LES governing equations for mass, momentum and pressure only with the corresponding one-dimensional deterministic-stochastic ODT governing equations, which resolve momentum and reactive scalars at the subgrid level. Key of this formulation is to address important couplings between turbulent transport and the molecular reaction and diffusion processes at the LES subgrid scales.

Different variants of the LES-ODT method have been studied. Balasubramanian, Sedhai and Echekki implemented a formulation, which advects the ODT domains on the flame brush in a Lagrangian fashion ([3], [116]). In the Cao and Echekki formulation [13], which is used as a starting point for the work at hand, the ODT domains are fixed in space. This conforms to an Eulerian description of the flow field. Further discussions of the model are given in Cao [12] as well as in Echekki and Mastorakos [20].

The present form of the Eulerian LES-ODT model does not use ODT information for LES momentum closure, however a well-established closure model, the Smagorinsky model is used. Using ODT information for LES closure terms will involve additional modeling elements to establish consistency and is recommended for future work.

In the following sections, the LES governing equations are presented, then coupling between LES and ODT is discussed with regards to spatial, temporal, corrective and variable density coupling. Then the ODT governing equations are presented and a presentation and summary of the non-dimensional working equations conclude this chapter.
2.1 LES-ODT Modeling Strategy

The ODT formulation simulates the time evolution of velocities and scalars along a one-dimensional domain. This domain represents a notional line of sight through turbulent flow, as illustrated in Figure 2.1. In Cartesian coordinates and in the Eulerian context, such a one-dimensional domain can be thought to be aligned with the \((x_1)\)-coordinate for example. Along this line, the turbulent signal \((\varphi(x_1))\) can be decomposed into a mean or filtered part \((\bar{\varphi})\) and into a fluctuating part \((\varphi'')\).

![Figure 2.1: Interpretation of ODT as a notional line of sight, [71].](image)

Contribution along this line can be spatially and temporally resolved, whereas contributions from the second \((x_2)\) and third \((x_3)\) orthogonal directions need to be modeled. The same principle applies for notional lines parallel to the other two coordinate directions. The following sections discuss the modeling efforts needed to overcome the difficulties associated with capturing three-dimensional effects with one-dimensional domains.

Figure 2.2 shows the embedded ODT domains as a three-dimensional lattice in the LES computational domain, illustrated here with one LES cell. The ODT domains are aligned with the LES cell edges. An ODT node is defined as the intersection point of three orthogonal ODT domains. In the present work the ODT grid is aligned in such a way that the ODT node coincides with the LES node. The ODT grid points between the
ODT nodes are called intra-nodes.

It is important to see that at the ODT node, all three orthogonal directions are resolved, such that no modeling is necessary. This is different for the intra-nodes. Only the direction under consideration is resolved where unresolved contribution need to be modeled.

![Three-dimensional alignment of LES cell and ODT domains](image)

**Figure 2.2: Three-dimensional alignment of LES cell and ODT domains**

The ODT domain alignment with the LES cell as illustrated in Figure 2.2 shows a special case. In general, ODT domains do not need to be aligned with the cell edges and ODT nodes do not have to coincide with LES nodes. However, flexible ODT domain alignment needs to be re-implemented in the updated ODT formulation and thus is deferred to future work.

The ODT concept of the work at hand contains three key features to simulate turbulent reactive transport on the subgrid: (1) a representation of the advection process, (2) a representation of the molecular diffusion and reaction process and (3) a representation of one-dimensional turbulent stirring event with a stochastic process involving instantaneous mappings, emulating an eddy turn-over event. These processes and events are explained thoroughly in Section 2.3: "ODT Governing Equations", a presentation of the LES governing equations follows next.
2.2 LES Governing Equations

In LES-ODT, the LES governing equations cover only the large scale motion using mass and momentum conservation as well as pressure transport. By performing a density-averaged (Favre-averaged) filtering operation on the Navier-Stokes equations the filtered LES governing equations are obtained. As a starting point, the DNS governing equations as presented in Mason are chosen [69]. The LES governing equations are then obtained as:

**LES Continuity**

\[
\frac{\partial \bar{\rho}}{\partial t} + \frac{\partial \bar{\rho} \bar{u}_i}{\partial x_i} = 0
\]  

(2.1)

**LES Momentum**

\[
\frac{\partial (\bar{\rho} \bar{u}_i)}{\partial t} = -\frac{\partial (\bar{\rho} \bar{u}_i \bar{u}_j)}{\partial x_j} - \frac{\partial \bar{p}}{\partial x_i} + \bar{\rho} \bar{f}_i + \frac{\partial \bar{\tau}_{ij}^{SGS}}{\partial x_j},
\]  

(2.2)

which, when assuming incompressibility and negligible external forces (gravity, etc.) reduces to

\[
\bar{\rho} \frac{\partial \bar{u}_i}{\partial t} = \left[ -\bar{\rho} \bar{u}_j \frac{\partial \bar{u}_i}{\partial x_j} - \bar{\rho} \frac{\partial \bar{\tau}_{ij}}{\partial x_j} \right] + \left\{ \frac{\partial \bar{\tau}_{ij}^{SGS}}{\partial x_j} \right\}.
\]  

(2.3)

This equation has been decomposed into a resolved part (terms inside brackets ‘[ ]’), and an unresolved part (terms inside braces ‘{ }’), which is expressed in terms of a subgrid scale stress tensor \( \bar{\tau}_{ij}^{SGS} \), given as

\[
\bar{\tau}_{ij}^{SGS} = \bar{\rho}(\bar{u}_i \bar{u}_j - \bar{u}_i \bar{u}_j).
\]  

(2.4)

The viscous stress tensor \( \bar{\tau}_{ij} \) is expressed in terms of the dynamic viscosity \( \mu \) and the strain rate tensor, \( S_{ij} \)

\[
\bar{\tau}_{ij} = 2\mu S_{ij},
\]  

(2.5)

where

\[
S_{ij} = \frac{1}{2} \left( \frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i} \right) - \frac{2}{3} \delta_{ij} \frac{\partial \bar{u}_k}{\partial x_k}.
\]  

(2.6)
2.2. LES Governing Equations

The symbol “-” corresponds to spatial filtering by a function $G$ with a characteristic filter size $\Delta$, such that a generic filtered quantity $\bar{\varphi}$, defined at a spacial position, $x$, and time, $t$ is expressed as

$$\bar{\varphi}(x,t) = \int_{\Delta} \varphi(x',t) \cdot G(x - x', \Delta) dx'.$$  \hfill (2.7)

The Symbol “∼” corresponds to Favre filtering

$$\tilde{\varphi}(x,t) = \frac{\rho \varphi}{\bar{\rho}}.$$ \hfill (2.8)

The flow quantity $\varphi$ may then be expressed as a sum of a filtered, or LES resolved component and a residual component, representing the turbulent fluctuations, as introduced in Figure 2.1

$$\varphi = \tilde{\varphi} + \varphi''.$$ \hfill (2.9)

The filtered density is computed by spatially filtering the ODT density, which is evaluated on the subgrid based on the ideal gas equation of state. The equation of state in its original form is given in Eq. (2.27) and in its non-dimensionalized form in Eq. (2.115). The fluid is driven by pressure variations that are computed with the poisson equation for pressure, which is derived by combining the continuity equation and the momentum equations. The poisson equation for pressure is derived in the next chapter and given in Eq. (3.13), following the Fractional-Step Method and the numerical Runge-Kutta time integration scheme.

The subgrid stresses $\tau_{ij}^{SGS}$ given in Eq. (2.4) are the closure terms and need to be modeled using an LES turbulence model. The most common model used is the Smagorinsky model, which defines

$$\tau_{ij}^{SGS} = 2\bar{\rho} \nu_T S_{ij},$$ \hfill (2.10)

with the turbulent kinematic viscosity $\nu_T$ given as

$$\nu_T = (C_S \Delta)^2 \left(2\overline{S_{ij}S_{ij}}\right)^{1/2},$$ \hfill (2.11)

with $C_S$ being the Smagorinsky constant, which depends on the filter type, numerical method and flow conditions. For homogeneous isotropic turbulence, the most commonly
used value of $C_S$ is 0.2. $\Delta$ represents the filter width, which for LES simulations is equivalent to the grid spacing $\Delta = (\Delta x, \Delta y, \Delta z)$. The definition of the viscous subgrid stress as given in Eq. (2.10), is analogous to the definition of the viscous stress tensor, given in Eq. (2.5), where the turbulent dynamic viscosity ($\mu_T$) has been replaced with the turbulent kinematic viscosity ($\nu_T = \mu_T/\rho$). The definition for the strain-rate tensor is given in Eq. (2.6).

2.2.1 Non-Dimensionalization

In order to make the governing equations independent of the problem size, the governing equations are usually non-dimensionalized. In this work, the following relations are used

\[
\begin{align*}
x_i &= \frac{(x_i)_d}{L_{\text{ref}}} & u_i &= \frac{(u_i)_d}{U_{\text{ref}}} & \rho &= \frac{\rho_d}{\rho_{\text{ref}}} & T &= \frac{T_d - T_{\text{ref}}}{T_{\text{ad}} - T_{\text{ref}}} \\
t &= \frac{t_d U_{\text{ref}}}{L_{\text{ref}}} & p &= \frac{p_d}{\rho_{\text{ref}} \cdot R_u/M \cdot T_{\text{ref}}} & \end{align*}
\]

where subscripts $d$ and 'ref' denote dimensioned quantity and reference quantity, respectively. The choice to scale pressure thermodynamically as opposed to hydrodynamically is important for the low Mach number approximation. Pressure is expressed in terms of the universal gas constant $R_u$ and the molecular mass $M$. Other symbols are analogous to generally accepted conventions. The non-dimensionalized governing equations then become

LES Continuity

\[
\frac{\partial \tilde{\rho}}{\partial t} + \frac{\partial \tilde{\rho} \tilde{u}_i}{\partial x_i} = 0 \tag{2.13}
\]

LES Momentum

\[
\frac{\partial \tilde{u}_i}{\partial t} = -\tilde{u}_j \frac{\partial \tilde{u}_i}{\partial x_j} - \frac{1}{\gamma M_a^2 \rho} \frac{\partial \tilde{p}}{\partial \tilde{x}_i} + \frac{1}{\rho \text{Re}} \left[ \frac{\partial^2 \tilde{u}_i}{\partial \tilde{x}_j^2} + \frac{1}{3} \frac{\partial}{\partial \tilde{x}_i} \left( \frac{\partial \tilde{u}_j}{\partial \tilde{x}_j} \right) \right] + \frac{\partial}{\partial \tilde{x}_j} \left( \tilde{u}_i \tilde{u}_j - \tilde{u}_i \tilde{u}_j \right) \tag{2.14}
\]

with the traditional scaling factors
Mach number
\[ \text{Ma} = \frac{U_{\text{ref}}}{\sqrt{\gamma \cdot R_u / M \cdot T_{\text{ref}}}}; \quad \gamma = \frac{c_p}{c_v} \]  
(2.15)

and Reynolds number
\[ \text{Re} = \frac{\rho_{\text{ref}} L_{\text{ref}} U_{\text{ref}}}{\mu}. \]  
(2.16)

\( \gamma \) is the adiabatic coefficient and \( c_p \) and \( c_v \) are the specific heats under constant pressure and volume, respectively.

### 2.2.2 Low Mach Number Approximation

In order to avoid the restrictions on the numerical integration time step due to high frequency acoustic waves, it is common to do a low Mach number approximation. This supports density changes due to heat release, but suppresses acoustic waves. As a result, the density is only a function of temperature. According to Rutland [110], the approximate equations are derived by expanding the dependent variable in a power series in terms of the parameter \( \epsilon = \gamma \text{Ma}^2 \ll 1 \) for an arbitrary flow quantity \( \varphi \)

\[ \varphi = 1 + \epsilon \varphi + \epsilon^2 \varphi^2 + \ldots . \]  
(2.17)

Substituting this into the governing equations and collecting zeroth-order results, the continuity equation remains unchanged from the original form. The zeroth order momentum equation reduces to

\[ \nabla p^{(0)} = 0, \]  
(2.18)

which is quite different from its original form and states that the zeroth order pressure is spatially constant. The assumption that the zeroth order pressure is constant in time as well replaces the pressure in the equation of state with an arbitrary constant such that

\[ p^0 = \text{const.} = p_0. \]  
(2.19)

The equation of state is evaluated at the ODT subgrid level. It is given in its original form in Eq. (2.27) and in its non-dimensionalized form in Eq. (2.115).

The momentum equation is identical to its original form, except that the pressure is
first-order whereas density and velocity are zeroth order, such that the final form of the momentum equation becomes (while neglecting the superscripts)

\[
\frac{\partial \tilde{u}_i}{\partial t} = -\tilde{u}_j \frac{\partial \tilde{u}_i}{\partial x_j} - \frac{1}{\bar{\rho}} \frac{\partial \bar{p}}{\partial x_i} + \frac{1}{\rho \text{Re}} \left[ \frac{\partial^2 \tilde{u}_i}{\partial x_j^2} + \frac{1}{3} \frac{\partial}{\partial x_i} \left( \frac{\partial \bar{u}_j}{\partial x_j} \right) \right] + \frac{\partial}{\partial x_j} (\bar{u}_i \tilde{u}_j - \bar{u}_i \bar{u}_j). \tag{2.20}
\]

## 2.3 ODT Governing Equations

The ODT governing equations are evaluated in space and advanced in time on each individual ODT node as well as on each individual intra-node on the one-dimensional ODT domains in a Cartesian (orthogonal) coordinate system. The three-dimensionally intersecting one-dimensional domains without the LES cell are illustrated in Figure 2.3.

![ODT Domain Diagram](image-url)

Figure 2.3: Three-dimensional intersection of ODT domains.

The temporal and spatial resolutions are implemented to resolve the subgrid scale physics and therefore the associated resolution requirements are similar to those needed for direct numerical simulation. While the LES solution for velocity is evaluated numerically on a coarse grid, it is possible to interpolate it onto a finer ODT grid, while maintaining reasonable separation between LES-resolved and LES-unresolved (i.e. ODT) scales.

The component of the unresolved turbulent scales \( \varphi'' \) (see Eq.(2.9), and Fig. 2.1) is
represented by a stochastic process, which is referred to as "stirring events" in this work. Stirring events emulate the eddy turnover process in ODT. This is symbolized by $\Omega$ in the ODT governing equations. Therefore, ODT governing equations feature both, deterministic convective and diffusive-reactive and stochastic contributions. Recalling that at the ODT node, all directions are fully resolved, as discussed in Section 2.1, one can consequently write for ODT conservation equations governing the nodes

Node Momentum

$$\frac{\partial u_i}{\partial t} = \left[ -\bar{u}_j \frac{\partial u_i}{\partial x_j} + \frac{1}{\rho} \frac{\partial \tau_{ij}}{\partial x_j} + \Omega_{uj} \right], \quad (2.21)$$

Node Energy

$$\frac{\partial T}{\partial t} = \left[ -\bar{u}_j \frac{\partial T}{\partial x_j} + \frac{1}{\rho c_p} \left( \frac{\partial q''_j}{\partial x_j} - \sum_{k=1}^{N} h_k \bar{\omega}_k + q''' \right) + \Omega_{T} \right], \quad (2.22)$$

Node Species

$$\frac{\partial Y_k}{\partial t} = \left[ -\bar{u}_j \frac{\partial Y_k}{\partial x_j} + \frac{1}{\rho} \frac{\partial J_{k,j}}{\partial x_j} + \frac{\bar{\omega}_k}{\rho} + \Omega_{Y_k} \right]. \quad (2.23)$$

The solution at the nodes have a true 3D content, which is reflected in the formulation of the node governing equations. The intra-nodes are governed by one-dimensional equations which are written in such a way that the resolved coordinate component is along the ODT domain under consideration and the unresolved contributions are from the second and third orthogonal component, which need to be modeled. Therefore, cyclic permutations of the indices keep the equations valid. From the perspective of the ($x_1$)-direction, the normalized, one-dimensional ODT governing equations then become
2.3. ODT Governing Equations

2. PHYSICAL MODELING

1D Momentum

\[
\frac{\partial u_i}{\partial t} = \left[ -\bar{u}_1 \frac{\partial u_i}{\partial x_1} + \frac{1}{\rho} \frac{\partial \tau_{i1}}{\partial x_1} + \Omega_{ui} \right]_{\text{resolved}} + \left\{ -\left( \bar{u}_2 \frac{\partial u_i}{\partial x_2} + \bar{u}_3 \frac{\partial u_i}{\partial x_3} \right) + \frac{1}{\rho} \left( \frac{\partial \tau_{i2}}{\partial x_2} + \frac{\partial \tau_{i3}}{\partial x_3} \right) \right\}_{\text{modeled}}, \tag{2.24}
\]

1D Energy

\[
\frac{\partial T}{\partial t} = \left[ -\bar{u}_1 \frac{\partial T}{\partial x_1} + \frac{1}{\rho c_p} \left( \frac{\partial \dot{q}''_1}{\partial x_1} - \sum_{k=1}^{N} h_k \dot{\omega}_k + \dot{\dot{q}}'''' \right) \right]_{\text{resolved}} + \left\{ -\left( \bar{u}_2 \frac{\partial T}{\partial x_2} + \bar{u}_3 \frac{\partial T}{\partial x_3} \right) + \frac{1}{\rho c_p} \left( \frac{\partial \dot{q}''_2}{\partial x_2} + \frac{\partial \dot{q}''_3}{\partial x_3} \right) \right\}_{\text{modeled}}, \tag{2.25}
\]

1D Species

\[
\frac{\partial Y_k}{\partial t} = \left[ -\bar{u}_1 \frac{\partial Y_k}{\partial x_1} + \frac{1}{\rho} \frac{\partial J_{k1}}{\partial x_1} + \dot{\omega}_k + \Omega_{Yk} \right]_{\text{resolved}} + \left\{ -\left( \bar{u}_2 \frac{\partial Y_k}{\partial x_2} + \bar{u}_3 \frac{\partial Y_k}{\partial x_3} \right) + \frac{1}{\rho} \left( \frac{\partial J_{k2}}{\partial x_2} + \frac{\partial J_{k3}}{\partial x_3} \right) \right\}_{\text{modeled}}. \tag{2.26}
\]

As already indicated, terms inside the brackets ‘[]’ are resolved contributions and terms inside the braces ‘{ }’ are contributions that require modeling. In the above equations, \( \bar{u}_j \) is the large-scale advective velocity from LES. \( T \) is the temperature, \( Y_k, h_k, \dot{\omega}_k \) and \( J_{kj} \) are the \( k \)th species mass fraction (of \( N \) total species), total enthalpy, production rate and diffusive flux in the \( j \)th direction; \( \dot{q}'' \) is the heat flux and \( \dot{q}'''' \) the volumetric heat addition (e.g. radiation). The density is evaluated with the ideal gas equation, which closes the system of equations

\[
p = \rho R_u T \sum_k \frac{Y_k}{M_k}, \tag{2.27}
\]
where $R_u$ is the universal gas constant and $M_k$ the molecular mass.

The ODT governing equations are solved by decomposing the physical contributions for advection, diffusion-reaction and stirring into separate "events" of which each progresses at its own time step. Mathematically, this can be done by splitting the operators for each contribution and the final solution is obtained by superposition of the individual solutions. In the following subsections, each physical contribution is discussed individually in greater detail.

### 2.3.1 Advective Transport

The advective transport as formulated in the ODT governing equations for the nodes Eqs. (2.21) - (2.23) as well as for the intra-nodes, Eqs. (2.24) - (2.26) is based on deterministic advancement of the flow quantities on the subgrid. As the splitting of the governing equations into a nodal update and into an intra-node update already indicates, the present ODT formulation represents the advective contributions by a two-step process, consisting of node-advection and one-dimensional advection.

During the advection event, the nodes are updated first and the intra-nodes are updated second, while the unresolved contributions of the intra-nodes are based on linear interpolation of the fully resolved three-dimensional nodal information. This interdependency is indicated in Figure 2.3. The ODT nodes are depicted as a larger point in grey and the intra nodes are depicted as smaller points in black. The ODT domains are illustrated as lines and the arrows along these lines indicate the possible advection directions along such one-dimensional domains and illustrate how three-dimensional advection is possible at each node. The ODT subgrid extends throughout the computational domain in a likewise manner, meaning each node supports a three-dimensional intersection of one-dimensional domains.

The advection process itself uses the large-scale convective velocity $\tilde{u}_j$ interpolated from the LES grid to the ODT subgrid. The advection process is therefore referred to as "mean" or "filtered" advection. The decomposed form of the advection event for the node update can then be written as
2.3. ODT Governing Equations

Node Momentum Advection
\[
\frac{\partial u_i}{\partial t} = \left[ -\tilde{u}_j \frac{\partial u_i}{\partial x_j} \right]_{\text{resolved}},
\]  
(2.28)

Node Energy Advection
\[
\frac{\partial T}{\partial t} = \left[ -\tilde{u}_j \frac{\partial T}{\partial x_j} \right]_{\text{resolved}},
\]  
(2.29)

Node Species Advection
\[
\frac{\partial Y_k}{\partial t} = \left[ -\tilde{u}_j \frac{\partial Y_k}{\partial x_j} \right]_{\text{resolved}}.
\]  
(2.30)

And from the \((x_1)\)-perspective, the one-dimensional advection for the intra-node update can then be written as consisting of resolved and modeled contributions

1D Momentum Advection
\[
\frac{\partial u_i}{\partial t} = \left[ -u_1 \frac{\partial u_i}{\partial x_1} \right]_{\text{resolved}} + \left\{ -\tilde{u}_2 \frac{\partial u_i}{\partial x_2} - \tilde{u}_3 \frac{\partial u_i}{\partial x_3} \right\},
\]  
(2.31)

1D Energy Advection
\[
\frac{\partial T}{\partial t} = \left[ -u_1 \frac{\partial T}{\partial x_1} \right]_{\text{resolved}} + \left\{ -\tilde{u}_2 \frac{\partial T}{\partial x_2} - \tilde{u}_3 \frac{\partial T}{\partial x_3} \right\},
\]  
(2.32)

1D Species Advection
\[
\frac{\partial Y_k}{\partial t} = \left[ -u_1 \frac{\partial Y_k}{\partial x_1} \right]_{\text{resolved}} + \left\{ -\tilde{u}_2 \frac{\partial Y_k}{\partial x_2} - \tilde{u}_3 \frac{\partial Y_k}{\partial x_3} \right\}.
\]  
(2.33)

Again, for the second and third orthogonal directions \((x_2,x_3)\), the transport equations look analogously, except that the indices need to be rotated cyclically. The ‘\(\tilde{\text{ }}\)’-symbol
indicates an interpolation operation of unresolved contributions from the complementary orthogonal directions onto the ODT domain under consideration. This interpolation operation is based on nodal values, which contain appropriately resolved flow information, as discussed above (see Fig. 2.3). The numerical implementation aspects as well as numerical solution of the advection step is discussed in Chapter 3.

### 2.3.2 Diffusion-Reaction Transport

Like the advective transport, the diffusion-reaction step in ODT is based on deterministic advancement of the subgrid solution. Analogous to the discussions above, the diffusion contributions can be written as a decomposed form of the ODT governing equations and then further decomposed into a node and an intra-node update. The diffusive-reactive advancement contains source terms for chemical reaction (the reaction rate term) and for radiation (volumetric heat addition term). For the node update the gradients are fully resolved in all three dimensions.

**Node Momentum Diffusion**

$$\frac{\partial u_i}{\partial t} = \left[ \frac{1}{\rho} \frac{\partial \tau_{ij}}{\partial x_j} \right]_{\text{resolved}}, \quad (2.34)$$

**Node Energy Diffusion**

$$\frac{\partial T}{\partial t} = \left[ \frac{1}{\rho c_p} \left( \frac{\partial q''_{ij}}{\partial x_j} - \sum_{k=1}^{N} h_k \dot{\omega}_k + q''' \right) \right]_{\text{resolved}}, \quad (2.35)$$

**Node Species Diffusion**

$$\frac{\partial Y_k}{\partial t} = \left[ \frac{1}{\rho} \left( \frac{\partial J_{k,j}}{\partial x_j} + \dot{\omega}_k \right) \right]_{\text{resolved}}. \quad (2.36)$$

And for the one-dimensional diffusion the intra-node update needs to be split into a resolved and an unresolved (modeled) part.
1D Momentum Diffusion

\[
\frac{\partial u_i}{\partial t} = \left[ \frac{1}{\rho} \frac{\partial \tau_{i1}}{\partial x_1} \right]_{\text{resolved}} + \left\{ \frac{1}{\rho} \left( \frac{\partial \tau_{i2}}{\partial x_2} + \frac{\partial \tau_{i3}}{\partial x_3} \right) \right\}_{\text{modeled}},
\]  

(2.37)

1D Energy Diffusion

\[
\frac{\partial T}{\partial t} = \left[ \frac{1}{\rho c_p} \left( \frac{\partial q_{i1}'''}{\partial x_1} - \sum_{k=1}^{N} h_k \omega_k + \dot{q}_{i1}''' \right) \right]_{\text{resolved}} + \left\{ \frac{1}{\rho c_p} \left( \frac{\partial q_{i2}'''}{\partial x_2} + \frac{\partial \dot{q}_{i3}'''}{\partial x_3} \right) \right\}_{\text{modeled}},
\]  

(2.38)

1D Species Diffusion

\[
\frac{\partial Y_k}{\partial t} = \left[ \frac{1}{\rho} \left( \frac{\partial J_{k,1}}{\partial x_1} + \dot{\omega}_k \right) \right]_{\text{resolved}} + \left\{ \frac{1}{\rho} \left( \frac{\partial J_{k,2}}{\partial x_2} + \frac{\partial \dot{J}_{k,3}}{\partial x_3} \right) \right\}_{\text{modeled}}.
\]  

(2.39)

As for the advection step, the time advancement in the diffusion update for the second and third orthogonal directions \((x_2,x_3)\) looks analogously, except that the indices need to be rotated cyclically. The ‘\(\hat{}\)’-symbol indicates an interpolation operation of unresolved contributions from the complementary orthogonal directions onto the ODT domain under consideration. This interpolation operation is based on nodal values, which contain appropriately resolved flow information, as discussed above. The numerical implementation aspects as well as numerical solution of the diffusion step is discussed in Chapter 3.

In the following discussion, the diffusion-reaction equations are further broken down into their elements by replacing analytical expressions for the momentum-, heat flux- and species-diffusion, as well as reaction-rate and volumetric heat addition (radiation). For that reason, momentum, energy and species equation are considered separately.
2.3.1 ODT Governing Equations

2.3.2.1. Momentum Diffusion

Considering the ODT diffusion contribution for node and intra-nodes given in Eqs. (2.34, 2.37) and substituting the expression for the viscous shear stress tensor by combining Eq. (2.5) and Eq. (2.6)

\[ \tau_{ij} = \mu \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) - \frac{2}{3} \mu \left( \delta_{ij} \frac{\partial u_k}{\partial x_k} \right) \]

one obtains after a few steps of simplification the

Node Momentum Diffusion

\[ \frac{\partial u_i}{\partial t} = \left[ \nu \left( \frac{\partial^2 u_i}{\partial x_j^2} + \frac{1}{3} \frac{\partial}{\partial x_i} \left( \frac{\partial u_j}{\partial x_j} \right) \right) \right] \]

(2.40)

1D Momentum Diffusion

\[ \frac{\partial u_i}{\partial t} = \left[ \nu \left( \frac{\partial^2 u_i}{\partial x_1^2} + \frac{1}{3} \frac{\partial}{\partial x_i} \left( \frac{\partial u_1}{\partial x_1} \right) \right) \right] + \left\{ \nu \left( \chi \right) \right\} \]

(2.41)

with

\[ \chi = \frac{1}{3} \frac{\partial}{\partial x_i} \left( \frac{\partial u_1}{\partial x_1} \right) \]

(2.42)

Applying the non-dimensionalization relations Eq. (2.12), to the node and intra-node momentum diffusion, one can rewrite the

Node Momentum Diffusion

\[ \frac{\partial u_i}{\partial t} = \left[ \frac{1}{\rho \text{Re}} \left( \frac{\partial^2 u_i}{\partial x_j^2} + \frac{1}{3} \frac{\partial}{\partial x_i} \left( \frac{\partial u_j}{\partial x_j} \right) \right) \right] \]

(2.43)
2.3. ODT Governing Equations

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1D Momentum Diffusion

\[
\frac{\partial u_i}{\partial t} = \left[ \frac{1}{\mu \text{Re}} \left( \frac{\partial^2 u_i}{\partial x_1^2} + \frac{1}{3} \frac{\partial}{\partial x_1} \left( \frac{\partial u_1}{\partial x_1} \right) \right) \right] \text{resolved} + \left\{ \frac{1}{\mu \text{Re}} \phi \right\} \text{modeled}. \tag{2.44}
\]

2.3.2.2 Energy Diffusion and Reaction Source Terms

Considering the ODT temperature diffusion contribution for node and intra-nodes given in Eqs. (2.35, 2.38), substituting the expression for heat flux, as described by Fourier’s law of heat conduction

\[
\dot{q}_j'' = -\lambda \frac{\partial T}{\partial x_j}, \tag{2.45}
\]

(\(\lambda\) being the heat conductivity) and neglecting radiation (volumetric heat source)

\[
\dot{q}''' = 0, \tag{2.46}
\]

one obtains

Node Energy Diffusion

\[
\frac{\partial T}{\partial t} = \left[ \frac{1}{\rho c_p} \left( \frac{\partial^2 T}{\partial x_j^2} - \sum_{k=1}^{N} h_k \dot{\omega}_k \right) \right] \text{resolved}, \tag{2.47}
\]

1D Energy Diffusion

\[
\frac{\partial T}{\partial t} = \left[ \frac{1}{\rho c_p} \left( \frac{\partial^2 T}{\partial x_1^2} - \sum_{k=1}^{N} h_k \dot{\omega}_k \right) \right] \text{resolved} + \left\{ \frac{1}{\rho c_p} \left( \frac{\partial^2 T}{\partial x_2^2} + \frac{\partial^2 T}{\partial x_3^2} \right) \right\} \text{modeled}. \tag{2.48}
\]

In the following, the formulation for the heat release term due to reaction (or reactive source term) (\(\sum h_k \dot{\omega}_k\)) is considered more closely. Any arbitrary set of chemical reactions can be represented by

\[
\sum_{k=1}^{N} \nu_{k,i}^\prime R_k = \sum_{k=1}^{N} \nu_{k,i}'' P_k, \tag{2.49}
\]
where $\nu'$ and $\nu''$ are the stoichiometric coefficients for reactants and products of species $k$ of the $i$th reaction. $N$ is the total number of species, and in the following $M$ represents the total number of reactions.

As products are being formed (or "produced") from chemically interacting reactants, one can define a forward reaction rate for products (production rate), expressed as a concentration of species of product $[P_k]$ and reactant $[R_k]$

$$\frac{d[P_k]}{dt} = k_{f,i} \prod_{k=1}^{N} [R_k]^{\nu'_{k,i}},$$

(2.50)

analogously one can define a backward reaction rate for reactants (depletion rate)

$$\frac{d[R_k]}{dt} = k_{b,i} \prod_{k=1}^{N} [P_k]^{\nu''_{k,i}},$$

(2.51)

where $k_f$ and $k_b$ are forward and backward reaction rate constants, defined as

$$k_i = b_i T^{a_i} \cdot \exp\left[\frac{-E_{a,i}}{R_a T}\right],$$

(2.52)

with $b_i$ the collision frequency, $a_i$ the temperature exponent and $E_{a,i}$ the activation energy. These variables are reaction specific, and the relation is commonly known as Arrhenius law, or law of mass action.

Consequently, one can define a net production rate for each species $k$

$$\dot{\omega}_k = \sum_{i=1}^{M} (\nu''_{k,i} - \nu'_{k,i}) \left( k_{f,i} \prod_{k=1}^{N} [R_k]^{\nu'_{k,i}} - k_{b,i} \prod_{k=1}^{N} [P_k]^{\nu''_{k,i}} \right).$$

(2.53)

In the following, the backward reaction is neglected. The species concentration can be expressed as

$$[R_k] = \frac{n_k}{V} = \frac{X_k p}{R_u T},$$

(2.54)

In this equation, $X_i$ is the mole fraction for species $k$ and $p$ is the total pressure of the mixture. Oftentimes it is more convenient to have the production rate (or net production
rate) in units of \([\text{kg}/(\text{m}^3\text{s})]\) and not in \([\text{mol}/(\text{cm}^3\text{s})]\). This can be achieved by simply multiplying the expression for the reaction rate by the molecular mass \(M_k\) of species \(k\). Additionally, recalling the equation of state for a mixture as already formulated in Eq. (2.27)

\[ p = \rho R_u T \sum_{k=1}^{N} \frac{Y_k}{M_k} \]

and the identity

\[ X_k = \frac{Y_k/M_k}{\sum_{k=1}^{N} Y_k/M_k}, \quad (2.55) \]

one can write the net production rate in terms of mass fractions \(Y_k\)

\[ \dot{\omega}_k = M_k \sum_{i=1}^{M} (\nu_{k,i}'' - \nu_{k,i}') \left\{ k_f,i \prod_{k=1}^{N} \left( \frac{\rho Y_k}{M_k} \right) \nu_{k,i}' \right\}. \quad (2.56) \]

The chemistry considered in this work is further greatly simplified. The entire reaction system is assumed as a single-step reaction of fuel (F) and oxidizer (O) and can thus be represented by one reaction equation \((M = 1)\). Also the molar stoichiometric oxidizer-to-fuel ratio is unity and the reaction results in a single product (P). Therefore the general reaction system equation (Eq. (2.49)) becomes

\[ F + O \rightarrow P, \quad (2.57) \]

where

\[ \nu_F' = 1 \quad \nu_O' = 1 \quad \nu_P' = 0 \]
\[ \nu_F'' = 0 \quad \nu_O'' = 0 \quad \nu_P'' = 1. \quad (2.58) \]

One further assumptions are that all of the participating species have the same molecular mass \(M_F = M_O = M_P = M\) and that the temperature exponent \(a\) is zero, such that Eq. (2.56) returns for the production rate

\[ \dot{\omega} = \rho^2 Y_F Y_O \frac{b}{M} \cdot \exp \left( \frac{-E_a}{R_u T} \right) \quad (2.59) \]

and

\[ \dot{\omega}_F = -\dot{\omega} \quad \dot{\omega}_O = -\dot{\omega} \quad \dot{\omega}_P = \dot{\omega}. \quad (2.60) \]
With this information one can quantify the heat release term due to reaction in Eqs. (2.35) and (2.38), where \( h_k \) is really the standard enthalpy of formation \( \Delta h_{f,k}^0 \) for species \( k \), such that

\[
- \sum_{k=1}^{N} h_k \dot{\omega}_k = - \sum_{k=1}^{N} \dot{\omega}_k \Delta h_{f,k}^0 = \dot{\omega} \left( \Delta h_{f,F}^0 + \Delta h_{f,O}^0 - \Delta h_{f,P}^0 \right) \tag{2.61}
\]

and with

\[
\Delta h_{f,F}^0 + \Delta h_{f,O}^0 - \Delta h_{f,P}^0 = c_p \left( T_{ad} - T_{ref} \right) \tag{2.62}
\]

the final expression for the heat release due to reaction becomes

\[
- \sum_{k=1}^{N} h_k \dot{\omega}_k = \dot{\omega} c_p \left( T_{ad} - T_{ref} \right). \tag{2.63}
\]

\( T_{ad} \) is the adiabatic flame temperature and \( T_{ref} \) is the reference temperature.

Using the non-dimensionalization relations again, as given in Eqs. (2.12), one can write the non-dimensional diffusion-reaction contributions in ODT for

**Node Energy Diffusion**

\[
\frac{\partial T}{\partial t} = \left[ \frac{1}{\rho \text{RePr}} \frac{\partial^2 T}{\partial x_j^2} + \dot{s} \right] \tag{2.64}
\]

**1D Energy Diffusion**

\[
\frac{\partial T}{\partial t} = \left[ \frac{1}{\rho \text{RePr}} \frac{\partial^2 T}{\partial x_j^2} + \dot{s} \right] + \left\{ \frac{1}{\rho \text{RePr}} \left( \frac{\partial^2 T}{\partial x_2^2} + \frac{\partial^2 T}{\partial x_3^2} \right) \right\} \tag{2.65}
\]

and the production rate was rewritten in form of a reaction rate by

\[
\dot{s} = \frac{\dot{\omega}}{\rho} = D \rho Y_F Y_O \cdot \exp \left( \frac{-\beta (1 - T)}{1 - \alpha (1 - T)} \right). \tag{2.66}
\]
2.3. ODT Governing Equations

The following traditional non-dimensional scaling factors are used for

Prandtl number

$$ Pr = \frac{c_p \mu}{\lambda}, \quad (2.67) $$

non-dimensional temperature

$$ \alpha = \frac{T_{ad} - T_{ref}}{T_{ad}}, \quad (2.68) $$

non-dimensional activation energy (Schwab-Zeldovich Number)

$$ \beta = \frac{E_a \alpha}{R_u T_{ad}}, \quad (2.69) $$

and the Damköhler number, defined as

$$ Da = \frac{L_{ref}/U_{ref}}{\left[ \frac{b}{M \rho_{ref}} \cdot \exp \left( -\frac{\beta}{\alpha} \right) \right]^{-1}}. \quad (2.70) $$

In the special case of homogeneous isotropic turbulence, the ODT temperature diffusion contributions for the nodes and the intra-nodes can be written as

Node and 1D Temperature Diffusion

$$ \frac{\partial T}{\partial t} = \left[ \frac{3}{\rho \text{RePr} \frac{\partial^2 T}{\partial x_1^2}} + \hat{s} \right]_{\text{resolved}}. \quad (2.71) $$

As in homogeneous isotropic turbulence the gradients in each directions are identical, multiplying the current value by a factor of 3 is deemed to be a viable approximation. The equation above is written from the $x_1$ perspective. The expression for the complementary orthogonal second and third directions are analogous. From the numerical perspective however, one needs to pay attention that the node value is only updated only once.
2.3. ODT Governing Equations

2.3.2.3 Species Diffusion and Species Source Terms

Considering the ODT species diffusion contribution for node and intra-nodes given in Eqs. (2.36, 2.39) and substituting the expression for species diffusive flux for species \(k\), as described by Fick’s law

\[
J_{k,j} = \rho D_k \frac{\partial Y_k}{\partial x_j}
\]  

(2.72)

one can write for

**Node Species Diffusion**

\[
\frac{\partial Y_k}{\partial t} = \left[ D \frac{\partial^2 Y_k}{\partial x_j^2} + \dot{\omega}_k \right]_{\text{resolved}},
\]  

(2.73)

**1D Species Diffusion**

\[
\frac{\partial Y_k}{\partial t} = \left[ D \frac{\partial^2 Y_k}{\partial x_1^2} + \dot{\omega}_k \right] + \left\{ D \left( \frac{\partial^2 Y_k}{\partial x_2^2} + \frac{\partial^2 Y_k}{\partial x_3^2} \right) \right\}_{\text{modeled}},
\]  

(2.74)

where a constant diffusion constant (diffusivity) \(D_k = D\) has been assumed. By using the non-dimensionalization expressions in Eq. (2.12), the above species diffusion equations for nodes and one-dimensional domains can be written in non-dimensional form for

**Node Species Diffusion**

\[
\frac{\partial Y_k}{\partial t} = \left[ \frac{1}{\rho \text{RePrLe}} \frac{\partial^2 Y_k}{\partial x_j^2} - \dot{s} \right]_{\text{resolved}},
\]  

(2.75)

**1D Species Diffusion**

\[
\frac{\partial Y_k}{\partial t} = \left[ \frac{1}{\rho \text{RePrLe}} \frac{\partial^2 Y_k}{\partial x_1^2} - \dot{s} \right] + \left\{ \frac{1}{\rho \text{RePrLe}} \left( \frac{\partial^2 Y_k}{\partial x_2^2} + \frac{\partial^2 Y_k}{\partial x_3^2} \right) \right\}_{\text{modeled}}.
\]  

(2.76)

The reaction rate (source terms) for fuel and oxidizer are identical \((\dot{s}_F = \dot{s}_O = \dot{s})\), as
defined by Eq. (2.60) and with $\dot{s} = \hat{\omega}/\rho$. The Lewis number Le as another traditional non-dimensional scaling number has been introduced above, which is defined as

$$Le = \frac{\lambda}{\rho_{\text{ref}} c_p D}$$

and relates thermal diffusivity to mass diffusivity.

Equivalent to the temperature diffusion, in the special case of homogeneous isotropic turbulence, the ODT species diffusion contributions for the nodes and the intra-nodes can be written as

Node and 1D Species Diffusion

$$\frac{\partial Y_k}{\partial t} = \left[ \frac{3}{\rho \text{Re} \text{Pr} Le} \frac{\partial^2 Y_k}{\partial x_1^2} - \dot{s} \right]_{\text{resolved}}.$$  \hspace{1cm} (2.78)

In homogeneous isotropic turbulence the gradients in each directions are equivalent, therefore multiplying the gradient of each resolved quantity by a factor of 3 is deemed to be a viable approximation. In essence, this means that no terms for the diffusion contribution need to be modeled. This simplification is not valid for advective transport however. In advection, quantities depend on a directional transport, whereas in diffusion directionality is not present, as long as the flow considered is homogeneous and isotropic. The equation above is written from the $x_1$ perspective. The expression for the complementary orthogonal second and third directions ($x_1$ and $x_2$) are analogous.

### 2.3.3 Turbulent Transport

The stochastic stirring events, which model the turbulent motions are symbolized as $\Omega$ in the ODT governing equations for the nodes (Eqs. (2.21)-(2.23)) and for the intra-nodes (Eqs. (2.24)-(2.26)). For velocities $\Omega_u$, represents the turbulent contributions, and for temperature and species mass fractions $\Omega_T$ and $\Omega_{Y_k}$ are representatives respectively. The mathematical expression for the temporal advancement of the stirring event in the governing equations is recalled here in a decomposed form as
2.3. ODT Governing Equations

Node and 1D Momentum Stirring

\[ \frac{\partial u_i}{\partial t} = \Omega u_i \]  

(2.79)

Node and 1D Energy Stirring

\[ \frac{\partial T}{\partial t} = \Omega_T \]  

(2.80)

Node and 1D Species Stirring

\[ \frac{\partial Y_k}{\partial t} = \Omega Y_k. \]  

(2.81)

The time advancement of generating turbulent eddy turnover motions consists in fact of seven consecutive steps, however. These are:

1. **Eddy Size Selection,** \( l_e \)
   
   This procedure is elaborated in greater detail in Section 2.3.3.1: ”Eddy Sampling”. \( l_e \) denotes the physical eddy length.

2. **Eddy Location Selection,** \( x_{j,0} \),
   
   which is also addressed in Section 2.3.3.1. \( x_{j,0} \) is the physical coordinate of the start location of the eddy. Index ”j” is the index indicating the three coordinate directions \( x_1, x_2 \) and \( x_3 \).

3. **Eddy Rate Distribution Function Evaluation,** \( \lambda_e(l_e, x_{j,0}, \tau_e) \),
   
   discussed in Section 2.3.3.2. The eddy rate is a function of eddy size \( (l_e) \), eddy location \( (x_{j,0}) \) and characteristic eddy turn-over time \( (\tau_e) \), which in turn is dependent on the flow field velocities and therefore on the flow time scale \( (t) \).

4. **Eddy Acceptance Probability Evaluation,** \( P_e(f, g, \lambda_e, dt_s) \),
   
   discussed in Section 2.3.3.3. The acceptance probability depends on the presumed probability density functions (PDF’s) for eddy size \( (f = f(l_e)) \) and eddy location \( (g = g(x_{j,0})) \); the eddy rate distribution function \( (\lambda_e) \) and the stirring time step \( dt_s \).

5. **Eddy Rejection Tests**
   
   Sampled eddies are rejected, if they are smaller or larger than the allowed, predefined size; if their location does not meet the boundary conditions; if they do not
6. **Triplet Map Execution**

If the eddy is accepted, the triplet map is executed and the pressure scrambling model is applied (see Section 2.3.3.2).

7. **Stirring Time Step Adjustment**

The stirring time step \( dt_s \) is adjusted if the eddy acceptance probability \( P_e \) is far from the desired target probability \( P_{\text{targ}} \), but is being kept within predefined bounds of \( dt_{s,\text{min}} \) and \( dt_{s,\text{max}} \), as discussed in Section 2.3.3.4.

### 2.3.3.1 Eddy Sampling

In order to be able to evaluate an eddy acceptance probability \( P_e \) (see Sec 2.3.3.3), presumed probability density functions (PDF’s) \( f(l_e) \) and \( g(x_{j,0}) \) for physical eddy size \( l_e \) and location \( x_{j,0} \) are necessary. They are not unique and can assume any shape.

According to Kerstein [49] and Echekki [21], a reasonable shape of the eddy size distribution is

\[
f(l_e) = \frac{A}{l_e^2}. \tag{2.82}
\]

\( A \) is a constant that can be determined by the PDF definition

\[
\int_{l_{e,\text{min}}}^{l_{e,\text{max}}} f(l_e) dl_e = 1, \tag{2.83}
\]

and substituting Eq. (2.82) into Eq. (2.83) to

\[
A = \frac{l_{e,\text{min}} \cdot l_{e,\text{max}}}{l_{e,\text{max}} - l_{e,\text{min}}}, \tag{2.84}
\]

with \( l_{e,\text{min}} \) the smallest eddy and \( l_{e,\text{max}} \) the largest eddy.

The presumed eddy location PDF is uniform over each ODT domain of length \( L \) and given as

\[
g(x_{j,0}) = \frac{1}{L}. \tag{2.85}
\]
2.3. ODT Governing Equations

2.3.3.2 Eddy Rate Distribution Function

In order to be able to understand the expression for the eddy rate distribution function \( \lambda_e \), as given in Eq. (2.104), one needs to understand the physical contributions of each of its dependencies first. For that reason, a discussion about how turbulent motion is modeled within the ODT context follows next.

Turbulent Motion in ODT

Turbulent motion is emulated through discrete but stochastic eddy turnovers, termed "eddy events" or "stirring events". Each eddy event consists of two mathematical operations. One is a triplet map representing the fluid displacements associated with a notional turbulent eddy. The other is a modification of the velocity profiles in order to implement pressure-induced energy redistribution among velocity components and net kinetic-energy gain or loss due to equal-and-opposite changes of the gravitational potential energy. This process is also known as "return to isotropy principle" or "pressure-scrambling model". These operations are represented symbolically by the following mapping expressions and are termed "kernel transformation", for velocities \( u_i \) and scalars \( \phi_i \)

\[
\begin{align*}
    u_i(x_j) & \rightarrow u_i [M(x_j)] + c_i K(x_j), \\
    \phi_i(x_j) & \rightarrow \phi_i [M(x_j)],
\end{align*}
\]

(2.86a)

(2.86b)

According to this prescription, fluid at location \( M(x_j) \) is moved to location \( x_j \) by the mapping operation, thus defining the map in terms of its inverse \( M(x_j) \). This mapping is applied to all fluid properties. The additive term \( c_i K(x_j) \) affects only the velocity components, where \( c_i \) is the amplitude and \( K(x_j) \) is the kernel transformation function. It implements the kinetic-energy exchanges, addressed by the pressure-scrambling model.

Triplet Map

The triplet map is one member of a class of mapping procedures that obey conservation laws. For an eddy of physical size \( l_e \) in the range of \([x_{j,0}, x_{j,0} + l_e]\) the triplet map is defined in Kerstein [51]. Omitting the "\( j \)" index symbolizing the three cartesian coordinate directions, and letting \( l_e = l \) for simplicity, one can write
2.3. ODT Governing Equations

\[ M(x) = x_0 + \begin{cases} 
3(x - x_0) & \text{if } x_0 \leq x \leq x_0 + 1/3l \\
2l - 3(x - x_0) & \text{if } x_0 + 1/3l \leq x \leq x_0 + 2/3l \\
3(x - x_0) - 2l & \text{if } x_0 + 2/3l \leq x \leq x_0 + l \\
(x - x_0) & \text{otherwise} 
\end{cases} \]  \quad (2.87)

The mapping procedure can be divided into three steps: (1) compression, (2) copy and (3) inversion. The compression step shrinks property profiles within an interval \([x_0, x_0 + l]\) to a third of their original extent, and then fills the interval with three compressed copies of the profiles. The middle copy is inverted, or reversed, which maintains the continuity of mapped properties and introduces the rotational folding effect of turbulent eddy motion, as given in Figure 2.4. Property fields outside the size-l interval are unaffected.

![Figure 2.4: Triplet map procedure from McDermott, [71].](image)

The present form of the LES-ODT formulation uses a discrete numerical implementation of the triplet map, given by McDermott [71]

\[ M(i) = i_0 + \begin{cases} 
3(i - i_0) & \text{if } i_0 \leq i \leq i_0 + 1/3se \\
2l - 3(i - i_0) & \text{if } i_0 + 1/3se \leq i \leq i_0 + 2/3se \\
3(i - i_0) - 2se & \text{if } i_0 + 2/3se \leq i \leq i_0 + se \\
(i - i_0) & \text{otherwise} 
\end{cases} \]  \quad (2.88)

where 'se' is the interval size (or interval length) of an eddy with start location \(i_0\) and
end location \( i_0 + se \), spawning the interval \([i_0, i_0 + se]\). The physical length of the eddy can be recovered with \( l_e = se \cdot \Delta x_{j,ODT} \).

Due to the nature of the mapping procedure, the number of discrete intervals (\( 'se' \)) should be a multiple of 3. Since however a triplet map with an eddy size of 3 discrete intervals does not change the property profile, the minimum eddy size is 6 discrete ODT intervals (\( \Delta x_{j,ODT} \)). Figure 2.5 illustrates the discrete triplet map. In this figure, the dashed line is the original profile and the dotted line is the post-map profile.

![Figure 2.5: Discrete triplet map, McDermott [71].](image)

**Pressure-Scrambling Model**

Previous studies have shown that the triplet map can alter the potential energy (Wunsch and Kerstein [126]). In order to enforce energy conservation, a kernel transformation function \( K \) has been added to the mapping operation (Eq. (2.86a)), which is defined as

\[
K(x_j) = x_j - M(x_j),
\]

i.e. its value is equal to the distance that the local fluid element is displaced. It is nonzero only within the eddy interval, and it integrates to zero so that the process does not change the total \( (x_3\text{-integrated}) \) momentum of individual velocity components. It provides a
2.3. ODT Governing Equations

mechanism for kinetic energy redistribution among velocity components, enabling the model to simulate the tendency of turbulent eddies to drive the flow towards isotropy, constrained by the requirement of total (kinetic plus potential) energy conservation during the eddy event (which is non-dissipative). At the same time this process emulates pressure-velocity interactions, which are pressure-induced kinetic energy redistributions among velocity components.

To quantify these features of eddy energetics, and thereby specify the coefficients \( c_i \) in Eq. (2.86a), it is helpful to consider the kinetic energy for one velocity component of an individual eddy (again omitting the "j" index and letting \( l_e = l \) for simplicity)

\[
E_i = \frac{1}{2} \rho \int u_i^2(x) dx. \tag{2.90}
\]

Due to triplet mapping and kernel transformation, the change in kinetic energy is

\[
\Delta E_i = \frac{1}{2} \rho \int_{x_0}^{x_0+l} \left[ (u_i(M(x)) + c_i K(x))^2 - u_i^2(x) \right] dx
\]

\[
= \rho c_i l^2 u_{i,K} + \frac{2}{27} \rho c_i^3 l^3, \tag{2.91}
\]

where the energy conservation of triplet maps

\[
\int_{x_0}^{x_0+l} \left[ (u_i(M(x))^2 - u_i^2(x) \right] dx = 0 \tag{2.92}
\]

and the definition for \( u_{i,K} \)

\[
u_i, K = \frac{1}{l^2} \int_{x_0}^{x_0+l} u_i(M(x)) K(x) dx \tag{2.93}
\]

has been used. Now Eq. (2.91) can be solved for \( c_i \), returning

\[
c_i = \frac{27}{4l} \left( -u_{i,K} \pm \sqrt{u_{i,K}^2 + \frac{8}{27} \frac{\Delta E_i}{\rho l}} \right). \tag{2.94}
\]

A more explicit form of \( \Delta E_i \) is necessary in order to implement it numerically. Following
the ”return-to-isotropy principle”, Kerstein [52] postulated

\[ \Delta E_i = \alpha_e \sum T_{ij} Q_j, \]  

(2.95)

with \( Q_j \) the available kinetic energy, \( \alpha_e \) a free parameter and transfer matrix \( T_{ij} \)

\[ T := \frac{1}{2} \begin{pmatrix} -2 & 1 & 1 \\ 1 & -2 & 1 \\ 1 & 1 & -2 \end{pmatrix}. \]  

(2.96)

The parameter \( \alpha_e \) defines the maximum of allowable energy that can be exchanged between velocity components. If \( \alpha_e = 0 \), there is no energy exchange and if \( \alpha_e = 2/3 \), there is equi-partition in the pressure scrambling model.

\( \Delta E_i \) and \( Q_j \) needs to be found first. The maximum energy that can be removed from a velocity component can be obtained by maximizing \( -\Delta E_i \) with respect to \( c_i \) in Eq. (2.91). \( Q_j \) is then set equal to that value

\[ Q_j = \frac{27}{8 \rho l u_{i,K}^2}, \]  

(2.97)

which when substituting into Eq. (2.91) and then into Eq. (2.95), gives the result for the kernel amplitudes ([52], [12])

\[ c_i = \frac{27}{4l} \left[ -u_{i,K} + \text{sgn}(u_{i,K}) \sqrt{u_{i,K}^2 + \alpha_e \sum_j T_{ij} u_{j,K}^2} \right]. \]  

(2.98)

**Rate Distribution Function**

Key to the overall performance of the model is the procedure for determining the sequence of eddy events during the simulated flow realization. The eddy event frequencies should occur with frequencies comparable to the turbulent eddy turnover time \( \tau_e \). The expected number of eddies occurring during a stirring time step interval \( dt_s \), whose parameter values are within \( dx_j \) of \( x_{j,0} \) and within \( dl_e \) of \( l_e \), is defined by the eddy rate distribution,
2.3. ODT Governing Equations

(Kerstein et al. [52])

\[ \lambda_e(x_{j,0}, l_e, \tau_e) = \frac{\text{events}}{\text{location} \times \text{size} \times \text{time}} = \frac{C}{l_e^2 \tau_e(x_{j,0}, l_e, t)}, \tag{2.99} \]

where \( C \) scales the eddy event rate. In particular, this parameter scales the speed of the kinetic energy cascade down to viscosity. For high \( C \), the cascade is fast, for low \( C \) the cascade is slow. To estimate the eddy time scale \( \tau_e \), Kerstein et al. [52], looked at the turbulent kinetic energy, associated with each mapping interval and by applying dimensional analysis they obtain (omitting "\( j \)", letting \( l_e = l, \tau_e = \tau \))

\[ \frac{\rho l^2}{\tau^2} \sim \sum_j B_j Q_j, \tag{2.100} \]

with \( B_j \) arbitrary constants and \( Q_j \) the available kinetic energy of component \( j \), along an ODT domain, as given in Eq. (2.97). Combining Eq. (2.100) with Eqs. (2.95)-(2.97), one obtains

\[ \left( \frac{l}{\tau} \right)^2 \sim u_{i,K}^2 + \alpha_e \sum_j T_{ij} u_{j,K}^2. \tag{2.101} \]

This corresponds to the available kinetic energy of the velocity component \( u_i \), with the first term representing the added energy and the second term the redistributed energy.

Another effect that influences the eddy time scale is viscous damping. If the eddy time scale is much larger than the viscous time scale, the eddy event should be prohibited. A viscous penalty constant \( Z \) is introduced and added to the right hand side [52]

\[ \left( \frac{l}{\tau} \right)^2 \sim u_{i,K}^2 + \alpha_e \sum_j T_{ij} u_{j,K}^2 - Z \frac{\nu^2}{l^2}. \tag{2.102} \]

The viscous time scale is given as

\[ \tau_\nu \sim \frac{l^2}{\nu}. \tag{2.103} \]

Combining Eqs. (2.103), with the definition (2.99) one obtains an expression for the eddy
rate distribution function as

\[
\lambda_e(l_e, x_{j,0}, \tau_e) = \frac{C \nu}{l_e^4} \left( \frac{u_{i,K} l_e}{\nu} \right)^2 + \alpha_e \sum_j T_{i,j} \left( \frac{u_{j,K} l_e}{\nu} \right)^2 - Z.
\]  

(2.104)

If the discriminant under the root is negative, the sampled eddy will be rejected. The role of \( Z \) is to impose a threshold eddy Reynolds number that must be exceeded to allow eddy occurrence. In near-wall flow, the transition from the viscous layer to the buffer layer is sensitive to this threshold and hence to \( Z \). For \( Z > 0 \), eddies are suppressed entirely when local values of the eddy Reynolds number are sufficiently small. For \( Z = 0 \), the argument of the square root is a scaled form of the net available energy. Thus, for given \( x_{j,0} \) and \( l_e \), with \( Z = 0 \) is simply the dimensionally consistent relation between the net available energy and the length and time scales of eddy motion, where the associated time scale is the inverse of the (approximately normalized) eddy rate, \( \lambda_e \). Thus, Eq. (2.99) may be viewed as a representation of a mixing-length phenomenology within the ODT framework. This phenomenology is the basis of many turbulence modeling approaches. In particular, it is central to LES closures based on eddy viscosity, hence the analogy between conventional LES and the LES-ODT methodology.

### 2.3.3.3 Eddy Acceptance Probability

The explicit reconstruction of the eddy rate distribution \( \lambda_e \) in Eq. (2.104) as the flow evolves is numerically too costly. Therefore, the rejection method, as described by Ross [109] and by L’Ecuyer [63] and employed by Kerstein [49] and Echekki [21] is used in the present formulation. This method involves eddy sampling based on an arbitrary sampling distribution (a random number) that is designed to over-sample all eddies. True rates are computed only for sampled eddies and are used to determine the eddy acceptance probability. The acceptance probability as defined in Echekki [21] is given as

\[
P_e = \frac{\lambda_e(l_e, x_{j,0}, \tau_e) dt_s}{f(l_e) g(x_{j,0})},
\]

(2.105)
with $dt_s$ the stirring time step between eddy events and the presumed probability density functions (PDF’s) $f(l_e)$ and $g(x_{j,0})$ for eddy size $l_e$ and start location $x_{j,0}$, as given in Section 2.3.3.1. The eddy rejection procedure as used in the formulation at hand is discussed in greater detail in the following section.

### 2.3.3.4 Eddy Sampling and Rejection Test Procedure Summary

As introduced above, the eddy rate is computed based on accepted eddies only. This section summarizes equations and findings from within the turbulent transport section regarding sampling and rejection of eddies.

The eddies are selected based on their size ($l_e$) and start location ($x_{j,0}$), according to the size and location probability distributions $f(l_e)$ and $g(x_{j,0})$, as given in Eqs. (2.82) and (2.85). The condition is that the eddy size ($l_e$) needs to be within predefined eddy sizes ($l_{e,\text{min}}$ and $l_{e,\text{max}}$) and meet the boundary conditions.

In order to compute the acceptance probability $P_e$ (Eq. (2.105)), one needs to compute the eddy rate distribution $\lambda_e$ (Eq. (2.104)) first. However, the immediate step is to compute the radicand of the eddy rate distribution function

$$\text{rad}(\lambda_e) = \left( \frac{u_{i,K}l_e}{\nu} \right)^2 + \alpha_e \sum_j T_{i,j} \left( \frac{u_{j,K}l_e}{\nu} \right)^2 - Z. \quad (2.106)$$

The eddy is rejected, if

$${\text{TEST 1:}} \quad \text{rad}(\lambda_e) < 0. \quad (2.107)$$

In order to increase the chance of accepted eddies, but also to save simulation time, an "intensified sampling" cycle has been introduced, such that the procedure tries at least a defined amount of times before before skipping the stirring event and only sampling at the next time interval $[t_{ODT} + dt_s]$ again.

Next, the acceptance probability is computed

$$P_e = \frac{\lambda_e dt_s}{f \cdot g} \quad (2.108)$$
and the eddy is rejected, if $P_a$ is smaller than a random number ($\text{rand()}$) in the interval $[0; 1]$

\[
\text{TEST 2: } P_e < \text{rand()} .
\]  

(2.109)

Third, the elapsed physical time is computed

\[
t_{\text{elap}} = \frac{x_{i,0}}{U_m}, \quad \text{where} \quad U_m = \frac{1}{2} (u_{i,\text{max}} + u_{i,\text{min}})
\]  

(2.110)

and compared to the eddy turn-over time

\[
\tau_e = \frac{C}{l_e^2 \lambda_e} .
\]  

(2.111)

The eddy is rejected if the eddy is immature

\[
\text{TEST 3: } t_{\text{elap}} < \beta_m \tau_e ,
\]  

(2.112)

where $\beta_m$ is a free parameter in the range $[0, 1]$. This test corresponds to an ”eddy maturing condition” and avoids large eddies at the inlet and enables the turbulence to build up downstream, as described in Echekki [21].

If the eddy passes all tests, the constants (amplitudes) for the kernel transformation $c_i$ Eq. (2.94) are being computed, the triplet map Eq. (2.87) is executed and the kernel transformation completed.

The stirring advancement accounts for adjusting the time step $dt_s$ based on the sampled data and the target probability, $P_{\text{targ}}$ and the current maximum probability, which is the acceptance probability $P_e$.

\[
dt_s^{\text{new}} = dt_s^{\text{old}} \frac{P_{\text{targ}}}{P_e},
\]  

(2.113)

with the condition that $dt_s^{\text{new}}$ lies within the boundaries of $dt_{s,\text{min}}$ and $dt_{s,\text{max}}$. This condition is revisited after a defined number of iterations. Further details about the numerical implementation of turbulent transport in the present formulation of ODT is discussed in Section 3.
2.3.4 Equation of State

The equation of state closes the system of ODT governing equations. For convenience the relation from Eq. (2.27) shall be recalled here

\[ p = \rho R_u T \sum_{k=1}^{N} \frac{Y_k}{M_k}, \]

which under the assumptions discussed in Section 2.3.2.2: \( \sum_k Y_k = 1, M_k = M, N = 3 \), will simplify to

\[ p = \rho \frac{R_u T}{M}. \tag{2.114} \]

With the non-dimensionalization relations given in Eq. (2.12), the equation of state becomes

\[ p_0 = \rho \left( 1 + T \left( \frac{\alpha}{1 - \alpha} \right) \right). \tag{2.115} \]

2.4 Summary of Non-Dimensional Working Equations

A non-dimensional set of LES-ODT governing equations which are used in this work, can be summarized and assembled following the discussion of this chapter.

2.4.1 LES Governing Equations

LES Continuity

\[ \frac{\partial \tilde{\rho}}{\partial t} + \frac{\partial \tilde{\rho} \tilde{u}_i}{\partial x_i} = 0 \tag{2.116} \]

LES Momentum

\[ \frac{\partial \tilde{u}_i}{\partial t} = -\tilde{u}_j \frac{\partial \tilde{u}_i}{\partial x_j} - \frac{1}{\tilde{\rho}} \frac{\partial \tilde{\rho}}{\partial x_i} + \frac{1}{\rho \text{Re}} \left[ \frac{\partial^2 \tilde{u}_i}{\partial x_j^2} + \frac{1}{3} \frac{\partial}{\partial x_i} \left( \frac{\partial \tilde{u}_j}{\partial x_j} \right) \right] + \frac{\partial}{\partial x_j} (\tilde{u}_i \tilde{u}_j - \tilde{u}_i \tilde{u}_j) \tag{2.117} \]
2.4.2 ODT Governing Equations

2.4.2.1 ODT Node Governing Equations

Node Momentum
\[
\frac{\partial u_i}{\partial t} = \left[ -\tilde{u}_j \frac{\partial u_i}{\partial x_j} + \frac{1}{\rho \text{Re}} \left( \frac{\partial^2 u_i}{\partial x_j^2} + \frac{1}{3} \frac{\partial}{\partial x_i} \left( \frac{\partial u_j}{\partial x_j} \right) \right) + \Omega_{u_i} \right]
\] (2.118)

Node Energy
\[
\frac{\partial T}{\partial t} = \left[ -\tilde{u}_j \frac{\partial T}{\partial x_j} + \frac{1}{\rho \text{RePr} \frac{\partial^2 T}{\partial x_j^2}} + \dot{s} + \Omega_T \right]
\] (2.119)

Node Species
\[
\frac{\partial Y_k}{\partial t} = \left[ -\tilde{u}_j \frac{\partial Y_k}{\partial x_j} + \frac{1}{\rho \text{RePrLe} \frac{\partial^2 Y_k}{\partial x_j^2}} - \dot{s} + \Omega_{Y_k} \right]
\] (2.120)

2.4.2.2 ODT 1D Governing Equations

\[
\frac{\partial u_i}{\partial t} = \left[ -\tilde{u}_1 \frac{\partial u_i}{\partial x_1} + \frac{1}{\rho \text{Re}} \left( \frac{\partial^2 u_i}{\partial x_1^2} + \frac{1}{3} \frac{\partial}{\partial x_1} \left( \frac{\partial u_1}{\partial x_1} \right) \right) + \Omega_{u_i} \right]
\] + \left\{ -\tilde{u}_2 \frac{\partial u_i}{\partial x_2} - \tilde{u}_3 \frac{\partial u_i}{\partial x_3} + \frac{1}{\rho \text{Re}} \left( \chi \right) \right\}
\] (2.121)

\[
\frac{\partial T}{\partial t} = \left[ -\tilde{u}_1 \frac{\partial T}{\partial x_1} + \frac{1}{\rho \text{RePr} \frac{\partial^2 T}{\partial x_1^2}} + \dot{s} + \Omega_T \right]
\] + \left\{ -\tilde{u}_2 \frac{\partial T}{\partial x_2} - \tilde{u}_3 \frac{\partial T}{\partial x_3} + \frac{1}{\rho \text{RePr}} \left( \frac{\partial^2 T}{\partial x_2^2} + \frac{\partial^2 T}{\partial x_3^2} \right) \right\}
\] (2.122)

\[
\frac{\partial Y_k}{\partial t} = \left[ -\tilde{u}_1 \frac{\partial Y_k}{\partial x_1} + \frac{1}{\rho \text{RePrLe} \frac{\partial^2 Y_k}{\partial x_1^2}} - \dot{s} + \Omega_{Y_k} \right]
\] + \left\{ -\tilde{u}_2 \frac{\partial Y_k}{\partial x_2} - \tilde{u}_3 \frac{\partial Y_k}{\partial x_3} + \frac{1}{\rho \text{RePrLe}} \left( \frac{\partial^2 Y_k}{\partial x_2^2} + \frac{\partial^2 Y_k}{\partial x_3^2} \right) \right\}
\] (2.123)
2.4. Summary of Non-Dimensional Working Equations

Modeled (Unresolved) Momentum Diffusion Contributions

\[ \chi = \frac{1}{3} \frac{\partial}{\partial x_i} \left( \frac{\partial u_1}{\partial x_1} \right) \bigg|_{i \neq 1} + \left( \frac{\partial^2 u_i}{\partial x_i^2} + \frac{1}{3} \frac{\partial}{\partial x_i} \left( \frac{\partial u_2}{\partial x_2} \right) \right) + \left( \frac{\partial^2 u_i}{\partial x_3^2} + \frac{1}{3} \frac{\partial}{\partial x_i} \left( \frac{\partial u_3}{\partial x_3} \right) \right) \]

Reaction Rate

\[ \dot{s} = D_a \rho Y_F Y_O \cdot \exp \left( -\frac{\beta(1 - T)}{1 - \alpha(1 - T)} \right) \]

Equation of State

\[ p_0 = \rho \left( 1 + T \left( \frac{\alpha}{1 - \alpha} \right) \right) \]

2.4.2.3 Non-Dimensional Scaling Factors

Mach number

\[ Ma = \frac{U_{ref}}{\sqrt{\gamma \cdot \frac{R_u}{M} \cdot T_{ref}}} \]

Reynolds number

\[ Re = \frac{\rho_{ref} L_{ref} U_{ref}}{\mu} \]

Prandtl number

\[ Pr = \frac{c_p \mu}{\lambda} \]

Lewis number

\[ Le = \frac{\lambda}{\rho_{ref} c_p D} \]

Non-Dimensional Temperature

\[ \alpha = \frac{T_{ad} - T_{ref}}{T_{ad}} \]

Non-Dimensional Activation Energy (Schwab-Zeldovich number)

\[ \beta = \frac{E_a \alpha}{R_u T_{ad}} \]

Damköhler number

\[ Da = \frac{L_{ref} / U_{ref}}{\left[ \frac{b}{M \rho_{ref} \cdot \exp (-\beta / \alpha)} \right]^{-1}} \]

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Chapter 3

Numerical Solution

The first version of the Eulerian LES-ODT code was originally developed by Cao & Echekki [12], proposing a first approach to three-dimensional ODT subgrid coupling and containing all the necessary ingredients of the LES-ODT concept. This code was derived from a DNS code developed by Mason [69], who adopted the code from Al-Shaalan [1].

During the course of this work, several limitations of the model as well as code layout have been identified. This includes the three-dimensional coupling of ODT domains at the subgrid level, variable density coupling, grid stretching, boundary conditions, the ability to use other geometries than a cube, array structures, code performance and speed-up.

The challenge of coupling one-dimensional ODT domains in a three-dimensional fashion has been discussed thoroughly in Chapter 2. The following sections give an overview and discussion about the numerical solution procedure used to solve the LES governing as well as the ODT governing equations. LES-ODT coupling is addressed in greater detail also, with the addition of numerical aspects. The chapter concludes with spatial discretization aspects, grid stretching and how the triplet map has been implemented on stretched grids. A special emphasis is also given to the implementation the eddy sampling procedure.

The DNS governing equations are presented in Chapter 5, Section 5.1. While the solution procedure of the momentum equation, is analogous to the LES governing equations, a solution procedure overview to the scalar equations is given in Appendix A.
3.1 LES Governing Equations

Mason [69] presents a modified fractional-step (time-splitting) method of Peyret and Taylor [94] to solve DNS governing equations. This method can also be applied to solve LES governing equations. It decomposes convection and diffusion terms of the momentum equation, Eq. (2.2). In discrete form ($\partial \to \delta$, $d \to \Delta$), the momentum equation becomes

$$\frac{\delta \tilde{u}_i}{\delta t} = -\frac{1}{\rho} \frac{\delta p}{\delta x_i} - C_i + D_i,$$

(3.1)

with the convection terms $C_i$

$$C_i = \tilde{u}_j \frac{\delta \tilde{u}_i}{\delta x_j} - \frac{\delta}{\delta x_j}(\tilde{u}_i\tilde{u}_j - \tilde{u}_i\tilde{u}_j).$$

(3.2)

According to Mason [69], it is necessary to insure conservation of momentum and kinetic energy in discretized form. This can be accomplished by using the identity

$$\tilde{u}_j \frac{\delta \tilde{u}_i}{\delta u_j} = \frac{1}{2} \frac{\delta \tilde{u}_j}{\delta x_i} - \tilde{u}_j \left( \frac{\delta \tilde{u}_j}{\delta x_i} - \frac{\delta \tilde{u}_i}{\delta x_j} \right),$$

(3.3)

as suggested by Mansour, Ferziger and Reynolds [67], such that the convective terms become with the convection terms $C_i$

$$C_i = -\frac{1}{2} \frac{\delta \tilde{u}_j}{\delta x_i} - \tilde{u}_j \left( \frac{\delta \tilde{u}_j}{\delta x_i} + \frac{\delta \tilde{u}_i}{\delta x_j} \right) - \frac{\delta}{\delta x_j}(\tilde{u}_i\tilde{u}_j - \tilde{u}_i\tilde{u}_j).$$

(3.4)

The diffusion terms $D_i$ can be written as

$$D_i = \frac{1}{\rho \text{Re}} \left[ \frac{\delta^2 \tilde{u}_i}{\delta x_i^2} + \frac{\delta}{3} \frac{\delta}{\delta x_i} \left( \frac{\delta \tilde{u}_j}{\delta x_j} \right) \right].$$

(3.5)

The fractional step method can be divided into four major steps. First, the convective and diffusive terms are integrated in time by utilizing a Runge-Kutta time stepping method yielding predicted (interim) velocities ($\tilde{u}_j^*$). Second, under the restriction that the interim velocity field satisfies continuity for each Runge-Kutta step, a Poisson equation for pressure is solved. Third, the pressure gradient is used to correct the predicted velocity.
And finally fourth, the continuity equation is monitored at each Runge-Kutta time step additionally to insure solution convergence. This sequence is illustrated and summarized in Fig. 3.1. The figure serves as an outlook on the discussion to follow as the fully discretized forms of the governing equations are solved, as presented in the next sections. These steps can then be divided into predictor, pressure solution, corrector step and continuity check steps.

![Fractional step method to solve the LES momentum equation.](image)

**Figure 3.1:** Fractional step method to solve the LES momentum equation.

### 3.1.1 Predictor Step

The convection and diffusion terms are integrated in time using an explicit third-order Runge-Kutta scheme, as proposed by Le and Moin [62], where each time step is divided into three substeps, or stages \( k \), with \( k = 1, 2, 3 \), such that the predicted interim velocities
are given by
\[ \bar{u}_i^* = \bar{u}_i^{(k-1)} + \Delta t \left[ -\xi_k \left( -C_{i-1}^k + D_{i-1}^k \right) - \zeta_k \left( -C_{i-2}^k + D_{i-2}^k \right) \right], \quad (3.6) \]

with \( \Delta t \) the global time step and integration coefficients \( \xi_k \) and \( \zeta_k \) given by
\[
\begin{align*}
\xi_1 &= 8/15 & \xi_2 &= 5/12 & \xi_3 &= 3/4 \\
\zeta_1 &= 0 & \zeta_2 &= -17/60 & \zeta_3 &= -5/12
\end{align*}
\]

where
\[ \sum_{k=1}^{3} (\xi_k + \zeta_k) = 1. \quad (3.8) \]

For each Runge-Kutta step \( k \) the time step \( dt_k \) is given as
\[ \Delta t_k = (\xi_k + \zeta_k) \Delta t \quad (3.9) \]

such that
\[ \Delta t_1 = \frac{8}{15} \Delta t \quad \Delta t_2 = \frac{5}{12} \Delta t \quad \Delta t_3 = \frac{1}{3} \Delta t. \quad (3.10) \]

The scheme is considered self-starting at \( k = 1 \), as the values \( C_i^{-1} \) and \( D_i^{-1} \) are not needed because \( \zeta_1 = 0 \).

### 3.1.2 Pressure Solution

The discrete continuity equation for each sub-step is given by
\[ \frac{\delta \rho^k}{\delta t} + \frac{\delta (\bar{\rho}^k \bar{u}_i^k)}{\delta x_i} = 0. \quad (3.11) \]

When combined with the velocity evolution due to the pressure gradient, from Eq. (3.1), while omitting convective and diffusive terms at this point, one obtains
\[ \frac{\bar{u}_i^k - \bar{u}_i^*}{\Delta t_k} = -\frac{1}{\bar{\rho}^k} \frac{\delta \rho^k}{\delta x_i}. \quad (3.12) \]
Solving for \( \tilde{u}_i^k \) and substituting into Eq. (3.12), one gets a poisson equation for pressure that implicitly satisfies continuity at each Runge-Kutta sub step, based on the predicted velocities \( \tilde{u}_i^* \)

\[
\frac{\delta^2 p^k}{\delta x_i^2} = \frac{1}{\Delta t_k} \left[ \frac{\delta \rho^k}{\delta t} + \frac{\delta \left( \rho^k \tilde{u}_i^* \right)}{\delta x_i} \right].
\]  

(3.13)

The time evolution of the density is obtained by employing a simple first order, backward-difference approximation at each Runge-Kutta substep, given as

\[
\begin{align*}
\frac{\delta \rho^1}{\delta t} &= \frac{\rho^1 - \rho^0}{\Delta t_1} \\
\frac{\delta \rho^2}{\delta t} &= \frac{\rho^2 - \rho^0}{\Delta t_1 + \Delta t_2} \\
\frac{\delta \rho^3}{\delta t} &= \frac{\rho^3 - \rho^0}{\Delta t}.
\end{align*}
\]  

(3.14a)

(3.14b)

(3.14c)

At \( k = 0 \), and with \( n \) being the current time iteration, the global time is \( t = n \Delta t \) and at \( k = 3 \), the global time is \( t = (n + 1) \Delta t \).

In order to solve the Poisson equation for pressure, a Gauss-Seidel iteration scheme with successive over-relaxation (SOR) is employed. In a three-dimensional grid, the scheme is given as

\[
p_{ijk}^{n+1} = (1 - \omega_{\text{SOR}})p_{ijk}^n + \omega_{\text{SOR}} \left( \frac{R_{ijk}^n - \Phi_{ijk}^n}{L_{xijk} + L_{yijk} + L_{zijk}} \right),
\]  

(3.15)

for iteration level \( n \), with relaxation parameter \( \omega_{\text{SOR}} \) and Laplacian operators \( L \), given as

\[
L(p) = \frac{\delta}{\delta x_i} \left( \frac{\delta p}{\delta x_i} \right) = (C_j^D C_j^G) p,
\]  

(3.16)

with \( C_j^D \) and \( C_j^G \) the divergence and gradient operators in the \( j \)th direction. \( R_{ijk}^n \) is the right-hand side of Eq. (3.13) and \( \Phi_{ijk}^n \) is given as

\[
\Phi_{ijk}^n = L(p)|_{ijk} - (L_{xijk} + L_{yijk} + L_{zijk}) p_{ijk}^n.
\]  

(3.17)
Convergence is achieved, when

\[ \| p^{n+1} - p^n \|_2 \leq \varepsilon_{\text{SOR}}, \]  

(3.18)

where \( \varepsilon_{\text{SOR}} \) is some prescribed tolerance, given in Chapter 4. A value of 1.1 for the successive over-relaxation parameter \( \omega_{\text{SOR}} \) is usually used.

### 3.1.3 Corrector Step, Continuity Check

The final velocity field is obtained by updating the predicted velocities \( \tilde{u}_i^* \) with the pressure gradient

\[ \tilde{u}_i^k = \tilde{u}_i^* - \frac{\Delta t_k \delta p^k}{\bar{\rho} \delta x_i}. \]  

(3.19)

This is done using a first order backward Euler approximation. The restriction that the new velocity field satisfies the continuity equation as given in Eq. (3.11) must be met. This closes the Runge-Kutta Loop, as displayed in Fig. 3.1. The Runge-Kutta loop is executed \( k \) times, meaning three-times for the utilized three-stage Runge-Kutta. After the Runge-Kutta advancement is complete, the time step is completed and the solution is advanced to the next time level.

### 3.1.4 Closing Remarks

Discrete derivative operators do not possess the same mathematical properties as continuous ones. This is known as the ”issue of operator consistency”. These differences show most predominantly in the Laplacian operator in the poisson equation (Eq. (3.15)). A solution is considered to be ”consistent” if the numerical operators on both sides of the equation are the same.

In addition to that, since the governing equations are solved in non-conservative form, the divergence operator (convective terms) must be the same for all governing equations, for the numerical integration scheme to be ”fully consistent”. The diffusion terms remain unaffected. If just the Laplacian operator is consistent, the formulation is considered to be ”quasi-consistent”. Mason [69], discusses the issue of operator consistency in greater detail with regards to solving the poisson equation for pressure.
3.2 LES-ODT Coupling

Section 3.3 discusses the time integration of the ODT governing equations for the nodes as given in Eqs. (2.118)-(2.120), and for the intra-nodes as given in Eqs.(2.121)-(2.123). However, before looking at the solution of the single ODT events, which are advection, diffusion-reaction and stirring in greater detail, an overview is given first on how the ODT solution procedure is coupled in space and time with the LES solution and among itself.

The ODT solver is called from within the LES time loop, as illustrated in Figure 3.2.

![Figure 3.2: LES-ODT time advancement.](image)

The LES-ODT solution procedure is somewhat more complicated however. It includes
initialization of the LES and the ODT field, solving the LES governing equations, correction of the ODT velocity field by LES, advancing the ODT solution in advection, diffusion-reaction, stirring and passing the ODT density back to the LES solution, in the case of variable density flow. These couplings are of spatial and temporal nature and explained next in further detail.

3.2.1 Spatial Coupling

As discussed in Section 2.1 and shown in Figures 2.1 and 2.2, the one-dimensional ODT domains are embedded into the LES domain and are aligned with the LES grid in a defined fashion. The coupling of ODT domains is done three-dimensionally at an ODT node.

3.2.2 Temporal Coupling

The ODT sub-steps, advection, diffusion-reaction and stirring, are advanced physically "in parallel". Numerically, these processes are executed in series, each with their own time step for advection \( \Delta t_a \), diffusion-reaction \( \Delta t_d \) and stirring \( \Delta t_s \), but in alternating order. This is illustrated in Figure 3.3.

The ODT time step is equal to the LES time step \( \Delta t_{ODT} = \Delta t_{LES} \), but is shifted by \( \Delta t_{LES}/2 \). This is done because a synchronization step is necessary between LES and ODT. The large scale velocities of LES and ODT are synchronized at the end of each LES time step (beginning of each ODT time step). And for the case of a variable density flow, the filtered ODT density is passed back to LES. This is illustrated in Fig. 3.4, with arrows between the LES and ODT time levels, labeled with \( \tilde{u}_{i,LES} \) and \( \tilde{\rho}_{ODT} \). In Figures 3.3 and 3.4 \( \Delta t_{ODT} \) has been replaced with \( \Delta t_{LES} \), because they are equal and for ease of understanding of the illustration. This principle has already been discussed in Cao [13], but is mentioned here again for completeness.

As the ODT time step falls in the middle of the LES interval, assuming that ODT properties (density, etc.) are constant over one LES interval, is a valid, but it may be a crude approximation. This simplifies the solution procedure greatly for variable density flow (Sec. 3.2.4).
Synchronizing the ODT large scale velocity with the LES velocity is termed "correction coupling". This describes a "downscaling process", moving information from large scales to smaller scales. This process is explained in Section 3.2.3. On the contrary, filtering ODT density and passing it back describes an "upscaling process", where information from small scales to larger scales is transferred. This is explained in Section 3.2.4.

Figure 3.3: LES and ODT time advancement.

Figure 3.4: LES-ODT time advancement including upscaling and downscaling.
3.2. LES-ODT Coupling

3.2.3 Correction Coupling

The pressure gradient is not accounted for in the ODT governing equations but it is present in the LES governing equations. Therefore, the ODT mean velocity must be corrected by the LES velocity, while maintaining the turbulent fluctuations from ODT, however.

The velocity correction consists of four consecutive steps numerically. (1) Filtering of the ODT velocity solution to the LES level, (2) subtracting LES and ODT velocity to obtain the correction velocity $\tilde{u}_{i,\text{COR}}$ at the LES level, (3) interpolating the correction velocity to the ODT level and (4) adding it to the ODT velocity to obtain the corrected value, while maintaining the subgrid fluctuations. These four steps are expressed mathematically as

\begin{align}
(1) \text{Filter ODT velocity} & \quad \tilde{u}_{i,\text{ODT}} = \tilde{u}_{i,\text{ODT}}^0 + \tilde{u}_{i,\text{ODT}}^0 \tag{3.20a} \\
(2) \text{Compute } \tilde{u}_{i,\text{COR}} & \quad \tilde{u}_{i,\text{COR}} = \tilde{u}_{i,\text{LES}} - \tilde{u}_{i,\text{ODT}} \tag{3.20b} \\
(3) \text{Interpolate } \tilde{u}_{i,\text{COR}} \text{ to ODT} & \quad \hat{\tilde{u}}_{i,\text{COR}} = \hat{\tilde{u}}_{i,\text{LES}} - \hat{\tilde{u}}_{i,\text{ODT}} \tag{3.20c} \\
(4) \text{Add } u_{i,\text{COR}} \text{ to ODT} & \quad u_{i,\text{ODT}} = u_{i,\text{ODT}}^0 + u_{i,\text{ODT}}^0 + \tilde{u}_{i,\text{ODT}}^0 + u''_{i,\text{ODT}}. \tag{3.20d}
\end{align}

where the ’$\hat{\sim}$’ (symbolizing interpolation) and the ’$\tilde{\sim}$’ (symbolizing filtering) cancel each other and can be neglected in the last step, so that finally the correction step returns for the new ODT velocity

\[ u_{i,\text{ODT}} = u_{i,\text{ODT}}^0 + u''_{i,\text{ODT}}. \tag{3.21} \]

Therefore, the adjustments of the ODT velocity field enforces the consistency of the velocity field between LES and ODT. This correction coupling operation is depicted in Figure 3.4 and symbolized in Figures 3.5 and 3.6, as the process reaching from LES to ODT, the downscaling process. A discussion about upscaling or filtering of the ODT density (the process reaching from ODT to LES) follows next. Filtering and interpolation operations are discussed and explained numerically in Sections 3.2.6 and 3.2.7.
3.2.4 Variable Density Coupling

For variable density flows, the filtered density from ODT is used in the LES governing equations. This is the process reaching from ODT to LES in Figures 3.4, 3.5 and 3.6. The ODT density field is calculated based on the equation of state (Eq. (2.115)) from the ODT temperature field

\[ p_0 = \rho \left( 1 + T \left( \frac{\alpha}{1 - \alpha} \right) \right), \]

and then filtered and passed to the LES solution. \( p_0 \) is the zeroth order pressure constant and \( \alpha \) the non-dimensional temperature.

Because the ODT density is considered constant across the LES interval, the density is also constant across the Runge-Kutta steps, such that the density gradients within the Runge-Kutta sub-steps become (recalling Eqs. (3.14a) to (3.14c))

\[
\begin{align*}
\frac{\delta \rho^1}{\delta t} &= 0 \quad (3.22a) \\
\frac{\delta \rho^2}{\delta t} &= 0 \quad (3.22b) \\
\frac{\delta \rho^3}{\delta t} &= 0, \quad (3.22c)
\end{align*}
\]

where the poisson equation for pressure reduces to

\[
\frac{\delta^2 p^k}{\delta x_i^2} = \frac{1}{\Delta t_k} \left[ \frac{\delta (p^k \bar{u}_i^*)}{\delta x_i} \right]. \quad (3.23)
\]

The numerical implementation of filtering is discussed in Section 3.2.6.

3.2.5 LES-ODT Solution Algorithm Summary

The following discussion is a summary of the findings from the previous sections about the coupled LES-ODT solution procedure.

The ODT solver is called from within the LES time loop. Passing velocities from LES
to ODT is termed downscaling, which is done in the correction coupling step. Information is transferred from large scales to subgrid scales. Passing density from ODT to LES is termed upscaling. Information is transferred from subgrid scales to large scales. The downscaling process is implemented as interpolation. The upscaling operation is implemented as filtering. The LES-ODT coupling concept is summarized and symbolized in Figure 3.5.

Figure 3.5: Downscaling and upscaling.

The downscaling process encompasses two separate processes in reality, one is the already mentioned correction coupling step, and the other one is downscaling the large scale advection velocity $\tilde{u}_{j,\text{LES}} = \tilde{u}_j$ as needed in the ODT node and intra-node advection equations, which are designed to be a "filtered" or a "mean" advection.

The ODT solution process consists of three events - advection, diffusion-reaction and stirring, which are physically parallel but numerically serial and alternating. These processes are solved with the operator splitting method as discussed in Section 2.3. Figure 3.6 illustrates the LES-ODT coupling and the ODT solution algorithm in principal.

Figure 3.7 depicts the ODT solution algorithm in greater detail. The parallel events advection, diffusion-reaction and stirring are picked based on the smallest value of their individual time. The ODT solution is advanced until the same time as in LES is reached, then the ODT procedure aborts and passes density to LES (Fig. 3.6).
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Figure 3.6: LES-ODT solution algorithm.
3.2. LES-ODT Coupling

Figure 3.7: ODT solution algorithm.
3.2.6 Filtering

The filtering operation used is done in physical space and already described in Cao [12]. For completeness, this operation is presented here again. Weighted averages of a function \( \varphi(x_j, t) \) are computed for all three physical orthogonal (Cartesian) directions \( x_j \) over a defined filter size \( \Delta \) (which represents a volume for a three-dimensional filter). Mathematically, the filter function is defined as the integral (Eq. (2.7))

\[
\overline{\varphi}(x_j, t) = \int_{\Delta} \varphi(x'_j, t) \cdot G(x_j - x'_j, \Delta) \, dx'_j,
\]

with the filter function \( G \) that has to satisfy the normalization condition

\[
\int G(x_j - x'_j, \Delta) \, dx'_j = 1. \tag{3.24}
\]

The most commonly used filter functions are the box filter, Gaussian filter and the spectral cut-off filter.

In the present LES-ODT formulation as proposed by Cao [12] and Cao & Echekki [13], the box filter is used. With the box filter, the filtered function \( \overline{\varphi}(x_j, t) \) is the box average of the original function \( \varphi(x_j) \) in the interval \( (x_j - \Delta/2) < x'_j < (x_j + \Delta/2) \). The box filter function can then be written as

\[
G(x') = \begin{cases} 
0 & \text{for } |x_j - x'_j| > \frac{\Delta}{2}, \\
\frac{1}{\Delta} & \text{for } |x_j - x'_j| < \frac{\Delta}{2}.
\end{cases} \tag{3.25}
\]

The illustration which shows the three-dimensional intersection of ODT domains with an overlaid LES cell is recalled here again (Fig. 2.2), this time with different labels in Figure 3.8. The intra-nodes are depicted in black, the ODT nodes are depicted in grey and the LES nodes are depicted in black. LES node coordinates are denoted with \((i,j,k)\) and ODT node coordinates are denoted with \((in,jn,Kn)\), the ODT index is denoted as \((i1d,j1d,k1d)\) respectively.

Practically speaking, in the present formulation, the filter width \( \Delta \), is the number of
3.2. LES-ODT Coupling

ODT intervals that fall within one LES interval, given as \( i_{ed} \)

\[
i_{ed} = \frac{N_{x_{ODT}} - 1}{N_{x_{LES}} - 1} = \frac{N_{y_{ODT}} - 1}{N_{y_{LES}} - 1} = \frac{N_{z_{ODT}} - 1}{N_{z_{LES}} - 1}
\]  

Then numerically, the filtered result \( \varphi \) at a location \((i,j,k)\) on the LES grid can be expressed as an average of the one-dimensional function \( \varphi \) on the ODT grid

\[
\varphi(i,j,k) = \frac{1}{3(i_{ed} + 1)} \left( \sum_{i_{1d} = (i - i_{ed}/2)}^{(i + i_{ed}/2)} \varphi(i_{1d}) + \sum_{j_{1d} = (j - i_{ed}/2)}^{(j + i_{ed}/2)} \varphi(j_{1d}) + \sum_{k_{1d} = (k - i_{ed}/2)}^{(k + i_{ed}/2)} \varphi(k_{1d}) \right).
\]

This average is taken over the box (cube) of width \( i_{ed} \), over all three ODT directions. The filtering operation from ODT to LES has to be done by taking into account contributions from all three ODT directions, to keep the values at the LES nodes consistent. This is because three independently filtered one-dimensional solutions will not intersect their function value at the node \((i,j,k)\). So, filtering needs to be a true three-dimensional operation. This is true whether the ODT domains are actually aligned with the LES.
cell boundaries or not. If the ODT domains are not aligned with the LES cell edges, interpolation from LES to ODT also needs to be a three-dimensional operation. On the contrary, the interpolation operation can be done one-dimensionally, if the ODT domains are aligned with the LES cell edges, this is addressed next.

### 3.2.7 Interpolation

Interpolation basically represents an inverse filtering operation. However, contrary to the three-dimensional filter, and for the special case of aligned ODT domains with the LES cell edges, the interpolation can be done one-dimensionally. This is because the intra-node values are being reconstructed based on the LES node values, which overlie physically with the ODT nodes.

Using linear interpolation, an expression can be written for an interpolated generic variable $\hat{\varphi}$ for all three directions at the ODT level as

\[
\hat{\varphi}(i1d) = (1 - \alpha(i1d))\varphi(i,j,k) + \alpha(i1d)\varphi(i+1,j,k) \tag{3.28a}
\]
\[
\hat{\varphi}(j1d) = (1 - \beta(j1d))\varphi(i,j,k) + \beta(j1d)\varphi(i,j+1,k) \tag{3.28b}
\]
\[
\hat{\varphi}(k1d) = (1 - \gamma(k1d))\varphi(i,j,k) + \gamma(k1d)\varphi(i,j,k+1), \tag{3.28c}
\]

with the interpolation factors

\[
\alpha(i1d) = \frac{x_{ODT}(i1d) - x_{LES}(i)}{x_{LES}(i+1) - x_{LES}(i)} \tag{3.29a}
\]
\[
\beta(j1d) = \frac{y_{ODT}(j1d) - y_{LES}(j)}{y_{LES}(j+1) - y_{LES}(j)} \tag{3.29b}
\]
\[
\gamma(k1d) = \frac{z_{ODT}(k1d) - z_{LES}(k)}{z_{LES}(k+1) - z_{LES}(k)}. \tag{3.29c}
\]

The interpolation operation must be three dimensional (tri-linear, for example) if the ODT domains are not aligned with the LES cells edges. Tri-linear interpolation is presented in Cao [12].

Alternatively, the present LES-ODT formulation has the option to use Lagrangian
interpolation. This is generally formulated as

$$\hat{\varphi}(x_j) = \sum_{k=0}^{N} \varphi_k(x_j) L_{j,k}(x_j), \quad L_{j,k}(x_j) = \prod_{l \neq k} \frac{x_j - x_{j,l}}{x_{j,k} - x_{j,l}},$$

(3.30)

with the generic quantity \( \varphi \) and \( N \) basis points, constituting an \( n = (N - 1) \)th order. With aid of Fig. 3.8, this can be written in discretized form as

$$\hat{\varphi}(i1d) = \sum_{k=0}^{N} \varphi_k(i1d) L_{\alpha,k}(i1d)$$

(3.31a)

$$\hat{\varphi}(j1d) = \sum_{k=0}^{N} \varphi_k(j1d) L_{\beta,k}(j1d)$$

(3.31b)

$$\hat{\varphi}(k1d) = \sum_{k=0}^{N} \varphi_k(k1d) L_{\gamma,k}(k1d)$$

(3.31c)

and with the interpolation factors

$$L_{\alpha,k}(i1d) = \prod_{l \neq k} \frac{x_{ODT}(i1d) - x_{LES,l}(i)}{x_{LES,k}(i) - x_{LES,l}(i)}$$

(3.32a)

$$L_{\beta,k}(j1d) = \prod_{l \neq k} \frac{y_{ODT}(j1d) - y_{LES,l}(j)}{y_{LES,k}(j) - y_{LES,l}(j)}$$

(3.32b)

$$L_{\gamma,k}(k1d) = \prod_{l \neq k} \frac{z_{ODT}(k1d) - z_{LES,l}(k)}{z_{LES,k}(k) - z_{LES,l}(k)}.$$  

(3.32c)

If reduced to first order \( (n = 1) \) polynomials, the Lagrangian interpolation becomes a linear interpolation, where \( N = 2 \) basis points are needed. This concludes the discussion of LES-ODT coupling, the numerical solution of the ODT governing equations is addressed in the following.
3.3 ODT Governing Equations

This section discusses the numerical integration of the ODT governing equations for the
nodes as given in Eqs. (2.118)-(2.120), and for the intra-nodes as given in Eqs. (2.121)-(2.123) with regards to the operator-splitting method employed. This section distinguishes
clearly between temporal advancement for advection, diffusion as well as stirring and
provides a summary for each of the event updates at the end of each subsection.

3.3.1 Advection Advancement

The ODT advection update is based on the operator splitting method as introduced in
the modeling section (Sec. 2.3). The update consists of two steps - node advection and
intra-node advection. The advection scheme is designed in such a way that the advection
direction is determined automatically. The ODT gradients are transported by the large
scale LES advection velocity, constituting a mean advection.

The advective transport of momentum, energy and temperature for the nodes is re-
peated here in discrete form

\[
\frac{\delta u_i}{\delta t} = -\tilde{u}_j \frac{\delta u_i}{\delta x_j}, \quad (3.33)
\]

\[
\frac{\delta T}{\delta t} = -\tilde{u}_j \frac{\delta T}{\delta x_j}, \quad (3.34)
\]

\[
\frac{\delta Y_k}{\delta t} = -\tilde{u}_j \frac{\delta Y_k}{\delta x_j}. \quad (3.35)
\]

and the discrete from for the intra-nodes

\[
\frac{\delta u_i}{\delta t} = \left[ -\tilde{u}_1 \frac{\delta u_i}{\delta x_1} \right] + \left\{ -\tilde{u}_2 \frac{\delta u_i}{\delta x_2} - \tilde{u}_3 \frac{\delta u_i}{\delta x_3} \right\}, \quad (3.36)
\]

\[
\frac{\delta T}{\delta t} = \left[ -\tilde{u}_1 \frac{\delta T}{\delta x_1} \right] + \left\{ -\tilde{u}_2 \frac{\delta T}{\delta x_2} - \tilde{u}_3 \frac{\delta T}{\delta x_3} \right\}, \quad (3.37)
\]

\[
\frac{\delta Y_k}{\delta t} = \left[ -\tilde{u}_1 \frac{\delta Y_k}{\delta x_1} \right] + \left\{ -\tilde{u}_2 \frac{\delta Y_k}{\delta x_2} - \tilde{u}_3 \frac{\delta Y_k}{\delta x_3} \right\}, \quad (3.38)
\]
3.3. ODT Governing Equations

with resolved terms inside brackets ’[ ]’ and modeled terms inside the braces ’\{\}’. Because of the similarity of Eqs. (3.33) - (3.35) and Eqs. (3.36) - (3.38), the two sets of three equations can be reduced to a set of two equations with the generic variable \( \varphi \), for the nodes

\[
\frac{\delta \varphi_i}{\delta t} = \left[ -\tilde{u}_1 \frac{\delta \varphi_i}{\delta x_1} - \tilde{u}_2 \frac{\delta \varphi_i}{\delta x_2} - \tilde{u}_3 \frac{\delta \varphi_i}{\delta x_3} \right], \tag{3.39}
\]

where the right hand side has been expanded, and for the intra-nodes

\[
\frac{\delta \varphi_i}{\delta t} = \left[ -\tilde{u}_1 \frac{\delta \varphi_i}{\delta x_1} \right] + \left\{ -\tilde{u}_2 \frac{\delta \varphi_i}{\delta x_2} - \tilde{u}_3 \frac{\delta \varphi_i}{\delta x_3} \right\}. \tag{3.40}
\]

3.3.1.1 Node Advection Scheme

First, the node advection update is executed, as given in Eq. (3.39). For the advection scheme to pick the advection direction automatically, each term on the right-hand-side of Eq. (3.39) is expressed as

\[
\tilde{u}_j \frac{\delta \varphi_i}{\delta x_j} = \left[ \tilde{u}_j^+ \left( \frac{\delta \varphi_i}{\delta x_j} \right)^- + \tilde{u}_j^- \left( \frac{\delta \varphi_i}{\delta x_j} \right)^+ \right]. \tag{3.41}
\]

with \((j = 1, 2, 3)\) and the convective velocities are obtained from

\[
\tilde{u}_j^+ = \frac{1}{2} (\bar{u}_j + |\bar{u}_j|) \quad \text{and} \quad \tilde{u}_j^- = \frac{1}{2} (\bar{u}_j - |\bar{u}_j|), \tag{3.42}
\]

such that for positive convection velocity \(\bar{u}_j > 0\) ("upwind"), Eq. (3.41) becomes

\[
\tilde{u}_j \frac{\delta \varphi_i}{\delta x_j} = \left[ \tilde{u}_j \left( \frac{\delta \varphi_i}{\delta x_j} \right)^- \right], \tag{3.43}
\]

where \((\delta \varphi_i/\delta x_j)^-\) is the upwind gradient, defined by a backward-difference operator, as given below.
For negative convection velocity $\tilde{u}_j < 0$ ("downwind"), Eq. (3.41) becomes

$$\tilde{u}_j \frac{\partial \phi_i}{\partial x_j} = \left[ -\tilde{u}_j \left( \frac{\partial \phi_i}{\partial x_j} \right)^+ \right], \quad (3.44)$$

where $(\partial \phi_i / \partial x_j)^+$ is the downwind gradient, defined by a forward-difference operator, as given below.

The gradients take the form of

$$\left( \frac{\partial \phi_i}{\partial x_1} \right)^- = \left( \frac{\phi_i(i1d) - \phi_i(i1d-1)}{\Delta x_{ODT}} \right) \quad (3.45a)$$

$$\left( \frac{\partial \phi_i}{\partial x_1} \right)^+ = \left( \frac{\phi_i(i1d+1) - \phi_i(i1d)}{\Delta x_{ODT}} \right) \quad (3.45b)$$

for the $x$ direction, and analogous for the $y$ and $z$ directions

$$\left( \frac{\partial \phi_i}{\partial x_2} \right)^- = \left( \frac{\phi_i(j1d) - \phi_i(j1d-1)}{\Delta y_{ODT}} \right) \quad (3.46a)$$

$$\left( \frac{\partial \phi_i}{\partial x_2} \right)^+ = \left( \frac{\phi_i(j1d+1) - \phi_i(j1d)}{\Delta y_{ODT}} \right) \quad (3.46b)$$

$$\left( \frac{\partial \phi_i}{\partial x_3} \right)^- = \left( \frac{\phi_i(k1d) - \phi_i(k1d-1)}{\Delta z_{ODT}} \right) \quad (3.47a)$$

$$\left( \frac{\partial \phi_i}{\partial x_3} \right)^+ = \left( \frac{\phi_i(k1d+1) - \phi_i(k1d)}{\Delta z_{ODT}} \right). \quad (3.47b)$$

First order finite-difference operators have been chosen, as that scheme basically behaves like a total variable diminishing (TVD) scheme, as proposed by Cao [12]. The finite-difference operators are formulated based on constant grid spacing (homogeneous grid). In case of a stretched grid, the general form of the finite difference operators are given in Section 3.4.2.

A scheme is basically TVD, when the fluxes are limited, to avoid oscillations around
strong or abrupt gradients,

\[
\left( \sum_i |\varphi_{i+1} - \varphi_i| \right)^{n+1} \leq \left( \sum_i |\varphi_{i+1} - \varphi_i| \right)^n ,
\]

(3.48)

where \( n \) stands for the time step. A thorough discussion about total variation diminishing is given in Tannehill [120].

The temporal update is then finally obtained by a simple forward-Euler finite-difference time-integration of Eq. (3.39)

\[
\varphi_i^{n+1} = \varphi_i^n + \Delta t_a \cdot \left[ -\bar{u}_1 \frac{\delta \varphi_i}{\delta x_1} - \bar{u}_2 \frac{\delta \varphi_i}{\delta x_2} - \bar{u}_3 \frac{\delta \varphi_i}{\delta x_3} \right],
\]

(3.49)

where \( \Delta t_a \) is the advection time step.

### 3.3.1.2 Intra-Node Advection Scheme

The intra-node advection update follows the node advection update. The numerical scheme for the intra-nodes is considered here. The resolved part of Eq. (3.40) is updated according to the advection scheme as given in Eq. (3.41), whereas the unresolved terms are reconstructed based on the nodal values, which is discussed here.

In the present formulation, this reconstruction is done with a linear interpolation, as described in Section 3.2.7, such that with the aid of Fig. 3.8 and Eqs. (3.28), for the unresolved convective velocities, one can write

\[
\tilde{\bar{u}}_2(i1d) = (1 - \alpha(i1d)) \bar{u}_2(jn) + \alpha(i1d) \bar{u}_2(jn+Ny_{ODT})
\]

(3.50a)

\[
\tilde{\bar{u}}_3(i1d) = (1 - \alpha(i1d)) \bar{u}_3(kn) + \alpha(i1d) \bar{u}_3(kn+Nz_{ODT})
\]

(3.50b)

and for the unresolved gradients

\[
\frac{\tilde{\delta \varphi}_i}{\delta x_2}(i1d) = (1 - \alpha(i1d)) \frac{\delta \varphi_i}{\delta x_2}(jn) + \alpha(i1d) \frac{\delta \varphi_i}{\delta x_2}(jn+Ny_{ODT})
\]

(3.51a)

\[
\frac{\tilde{\delta \varphi}_i}{\delta x_3}(i1d) = (1 - \alpha(i1d)) \frac{\delta \varphi_i}{\delta x_3}(kn) + \alpha(i1d) \frac{\delta \varphi_i}{\delta x_3}(kn+Nz_{ODT}).
\]

(3.51b)
With this information, one can write for the temporal update for the intra-nodes

\[ \varphi_i^{n+1} = \varphi_i^n + \Delta t \cdot \left\{ -\tilde{u}_1 \frac{\delta \varphi_i}{\delta x_1} + \left\{ -\tilde{u}_2 \frac{\delta \varphi_i}{\delta x_2} - \tilde{u}_3 \frac{\delta \varphi_i}{\delta x_3} \right\} \right\}. \tag{3.52} \]

This procedure is analogous for the intra-node update in the second \((x_2)\) and third \((x_3)\) direction.

### 3.3.1.3 Advection Advancement Algorithm Summary

Figure 3.10 summarizes the advection advancement as discussed in the previous subsections. First, the node advection is executed. The node advection step includes computing the derivatives (see Section 3.4.2), initializing the convective velocities ("upwind", "downwind"), the temporal node update and the check for scalar boundness. Numerically, scalar boundness has to be maintained, in order to avoid scalar quantities to be larger than 1 or less than 0.

The intra-node advection update is second, which includes computing the derivatives in the entire domain based on the already updated nodal information. Then, as a second sub-step, interpolating the unresolved nodal information onto the one-dimensional domain under consideration. The advection direction is determined, followed by an intra-node advection update. The scalar boundness has to be checked again.

The boundary condition update concludes the advection step. After the advection step is complete, the next ODT event is determined based on the smallest time condition as illustrated in Figure 3.7.
Figure 3.9: ODT advection algorithm.
3.3.2 Diffusion-Reaction Advancement

3.3.2.1 Node and Intra-Node Diffusion-Reaction

Like the advection advancement, the diffusion-reaction advancement consists of two steps, the node update and the intra-node update. The diffusive transport of momentum, energy and temperature for the nodes is repeated here in discrete form

\[
\frac{\delta u_i}{\delta t} = \left[ \frac{1}{\rho \text{Re}} \left( \frac{\delta^2 u_i}{\delta x_1^2} \right) \right] \quad (3.53)
\]

\[
\frac{\delta T}{\delta t} = \left[ \frac{1}{\rho \text{RePr}} \left( \frac{\delta^2 T}{\delta x_1^2} \right) + \dot{s} \right] \quad (3.54)
\]

\[
\frac{\delta Y_k}{\delta t} = \left[ \frac{1}{\rho \text{RePrLe}} \left( \frac{\delta^2 Y_k}{\delta x_1^2} \right) - \dot{s} \right], \quad (3.55)
\]

and the discrete form of the intra-node diffusion becomes

\[
\frac{\delta u_i}{\delta t} = \left[ \frac{1}{\rho \text{Re}} \left( \frac{\delta^2 u_i}{\delta x_1^2} \right) \right] + \left\{ \frac{1}{\rho \text{Re}} \left( \frac{\delta^2 u_i}{\delta x_2^2} + \frac{\delta^2 u_i}{\delta x_3^2} \right) \right\} \quad (3.56)
\]

\[
\frac{\delta T}{\delta t} = \left[ \frac{1}{\rho \text{RePr}} \left( \frac{\delta^2 T}{\delta x_1^2} \right) + \dot{s} \right] + \left\{ \frac{1}{\rho \text{RePr}} \left( \frac{\delta^2 T}{\delta x_2^2} + \frac{\delta^2 T}{\delta x_3^2} \right) \right\} \quad (3.57)
\]

\[
\frac{\delta Y_k}{\delta t} = \left[ \frac{1}{\rho \text{RePrLe}} \left( \frac{\delta^2 Y_k}{\delta x_1^2} \right) - \dot{s} \right] + \left\{ \frac{1}{\rho \text{RePrLe}} \left( \frac{\delta^2 Y_k}{\delta x_2^2} + \frac{\delta^2 Y_k}{\delta x_3^2} \right) \right\}, \quad (3.58)
\]

where in the current formulation, the 1/3-term, as well as the term \(\chi\) (defined in Eq. (2.42)) in the momentum diffusion have been neglected. A second-order centered-difference approximation is used to express the second derivative, which with the generic variable \(\varphi\), can directly be written as (Hoffmann [35])

\[
\left( \frac{\delta^2 \varphi_i}{\delta x_1^2} \right) = \frac{\varphi(i1d - 1) - 2\varphi(i1d) + \varphi(i1d + 1)}{\Delta x_{\text{ODT}}^2} \quad (3.59)
\]

for the \(x_1\) direction, where constant grid spacing (homogeneous grid) has been assumed. For variable grid sizes (stretched grids for example), a generic form of the finite-difference
3.3. ODT Governing Equations

operator is needed. This is discussed in Section 3.4.2.

As in the advection advancement step, in the diffusion advancement also, unresolved contributions are reconstructed based on the resolved nodal values by utilizing a linear interpolation

\[
\left( \frac{\partial^2 \varphi_i}{\partial x_2^2} \right)_{i1d} = (1 - \alpha(i1d)) \left( \frac{\partial^2 \varphi_i}{\partial x_2^2} \right)_{jn} + \alpha(i1d) \left( \frac{\partial^2 \varphi_i}{\partial x_2^2} \right)_{jn+Ny_{\text{ODT}}} \quad (3.60a)
\]

\[
\left( \frac{\partial^2 \varphi_i}{\partial x_3^2} \right)_{i1d} = (1 - \alpha(i1d)) \left( \frac{\partial^2 \varphi_i}{\partial x_3^2} \right)_{kn} + \alpha(i1d) \left( \frac{\partial^2 \varphi_i}{\partial x_3^2} \right)_{kn+Nz_{\text{ODT}}}. \quad (3.60b)
\]

Finite-difference as well as linear interpolation operations are done analogously for the \(x_2\) and \(x_3\) directions. The solution at the next time step is obtained by using a first order forward-Euler time integration, analogous to the convection step. The density is computed by using the equation of state (Eq. (2.115))

\[p_0 = \rho \left(1 + T \left(\frac{\alpha}{1 - \alpha}\right)\right)\]

and the reaction rate is given by Eq. (2.66)

\[\dot{s} = D_a \rho Y_F Y_O \cdot \exp \left(\frac{-\beta(1 - T)}{1 - \alpha(1 - T)}\right).\]

3.3.2.2 Diffusion-Reaction Advancement Algorithm Summary

The flow chart in Fig. 3.10, summarizes the diffusion-reaction event in ODT schematically. First, within the nodal update, the derivatives are computed for the entire domain. Density and reaction rates are given by equations as discussed previously and updated for nodes as well as for intra-nodes. The node diffusion temporal update concludes the first sub-step.

In the second sub-step the diffusion-reaction advancement is done on the intra-nodes. The unresolved terms are interpolated as discussed in previous sub-sections, while resolved terms can be integrated directly. After the intra-nodes have been updated in time, the boundary conditions are updated as well and the next ODT sub-step is determined.
Figure 3.10: ODT diffusion-reaction algorithm.
3.3.3 Stirring Advancement

3.3.3.1 General Overview of the Stirring Event

The stirring event (stirring advancement), introduced in Section 2.3.3, models the turbulent transport in ODT. The ODT governing equations (Eqs. (2.118) - (2.120)) and (Eqs. (2.121) - (2.123)) introduce them with the idea of the operator splitting method and denote the stirring event with $\Omega$, for momentum, energy and species

$$\frac{\delta u_i}{\delta t} = \Omega u_i$$

$$\frac{\delta T}{\delta t} = \Omega T$$

$$\frac{\delta Y_k}{\delta t} = \Omega Y_k,$$

where in fact however, the stirring event consists of several sub-steps. This has been explained thoroughly in Section 2.3.3 from a physical standpoint and shall now be also addressed from the numerical standpoint.

The triplet map can only be executed on a one-dimensional domain. Therefore, the three-dimensional solution needs to be converted to a one-dimensional solution and after the triplet map is complete, it needs to be converted back. Computing the average at the nodes concludes the grid conversion steps. Grid conversion and node-averaging is one of three major numerical sub-steps in the stirring event. The eddy sampling procedure is the second major step, and, in the case of a variable mesh, mapping the eddy profile from a stretched to a homogeneous grid and back is necessary. This mapping procedure is done over the numerical eddy size ($se$) and discussed further in Section 3.4.3.

Figure 3.11 depicts the flow chart for the stirring event, including the three major sub-steps of grid conversion, eddy sampling and variable mesh map, as just discussed. The "eddy sampling" step includes the "eddy rejection tests", as introduced in Section 2.3.3.4. The flow chart for the rejection tests is given in Figure 3.12.

After the stirring event is complete, the next ODT event is chosen based on the ODT time step selection procedure shown in Figure 3.7.
3.3. ODT Governing Equations

Figure 3.11: ODT stirring algorithm.
3.3.3.2 Eddy Sampling Procedure

The eddy sampling procedure determines the size, location, likelihood and "maturity" of an accepted eddy. Once the eddy is accepted, the eddy event takes place and the eddy time step is adjusted, if necessary. At the beginning of the sampling procedure (as depicted in Fig. 3.12), the "eddy flag", the signal that an eddy can be executed is set to \( \text{eddy-flag}=1 \).

**Eddy Size Selection**

Given the integrated eddy size probability density function in discrete form,

\[
    f = \frac{1}{3} \cdot \frac{s_{\text{min}}}{1 - \text{rand()} \cdot \left(1 - \frac{s_{\text{min}}}{s_{\text{max}}}ight)},
\]

one can compute the index eddy size

\[
    s_{\text{e}} = 3 \cdot \text{nint}(f).
\]

If the eddy is smaller than a minimum eddy size \( s_{\text{min}} \) or larger than a maximum eddy size \( s_{\text{max}} \), the eddy will be rejected (\( \text{eddy-flag}=0 \)) and a new one will be sampled again by determining a new random number \( \text{rand()} \), which is a uniform distribution in the interval of \([0; 1]\). The physical eddy length can be recovered as

\[
    l_{\text{e}} = \text{real}(s_{\text{e}}) \cdot \Delta x_{j,\text{ODT}}.
\]

**Eddy Location Selection**

The discrete integrated eddy location probability distributions function is given by

\[
    i_{\text{le}} = 1 + \text{int} \left[ \text{rand()} \cdot \text{real}(N_{x,j,\text{ODT}} - 1) \right],
\]

where \( i_{\text{le}} \) is the left starting index of the eddy. The eddy location has to follow the boundary conditions. This is addressed in Section 4.2.1.
3.3. ODT Governing Equations

First Rejection Test: Radicand of the Eddy Distribution Function

With this, the radicand of the eddy rate distribution function can be computed. The analytic expression has been developed in Section 2.3.3.2 and shall be repeated here (Eq. 2.104)

\[
\text{rad}(\lambda_e) = \left( \frac{u_i K l_e}{\nu} \right)^2 + \alpha_e \sum_{j} T_{i,j} \left( \frac{u_j K l_e}{\nu} \right)^2 - Z.
\]

If the radicand of the eddy rate is smaller than zero (Eq. 2.107),

\[
\text{rad}(\lambda_e) < 0,
\]

the eddy is rejected (\text{eddy-flag}=0). In order to save simulation time however, it is beneficial to re-sample the eddy right away. This addition to the eddy selection process is called "intensified sampling". If however, after \text{N}_{\text{max}} trials, the eddy could still not be sampled, then the sampling procedure is aborted and the flow advanced.

Second Rejection Test: Acceptance Probability

Next, the eddy rate distribution, eddy size and location distributions are computed with

\[
\lambda_e = \frac{C}{l_e^2} \sqrt{\text{rad}(\lambda_e)} \quad (3.68)
\]

\[
f = \frac{s_{\text{min}} \cdot s_{\text{max}}}{s_{\text{min}} - s_{\text{max}}} \cdot \Delta x_{j,\text{ODT}} \quad (3.69)
\]

\[
g = \frac{\Delta x_{j,\text{ODT}}}{N_{\text{ODT}}} \quad (3.70)
\]

such that for the acceptance probability one can write Eq. (2.105)

\[
P_e = \frac{\lambda_e \Delta t_s}{f \cdot g},
\]

where \(\Delta t_s\) is the stirring time step. If the acceptance probability of an eddy is less than a random number trial in the interval of \([0;1]\),

\[
P_e < \text{rand}(),
\]
as already mentioned in Eq. (2.109) the eddy is rejected (eddy-flag=0).

**Third Rejection Test: Maturity Condition**

With the elapsed time (Eq. (2.110)) and the characteristic eddy turn over time (Eq. (2.111))

\[
t_{\text{elap}} = \frac{x_{j,0}}{U_m}, \quad \text{where} \quad U_m = \frac{1}{2} (u_{i,\text{max}} + u_{i,\text{min}})
\]
\[
\tau_e = \frac{C}{l_e^2 \lambda_e}
\]

one can determine, whether the eddy is mature. If the elapsed time is less than the characteristic eddy turn over time \( \tau_e \)

\[
t_{\text{elap}} < \beta_m \tau_e,
\]

as mentioned in (Eq. (2.112)), then the eddy is rejected (eddy-flag=0).

**Pressure Scrambling and Triplet Map**

With the constants for the pressure scrambling model (Eq. (2.98))

\[
c_i = \frac{27}{4l} \left[ -u_{i,K} + \text{sgn}(u_{i,K}) \sqrt{u_{i,K}^2 + \alpha_e \sum_j T_{i,j} u_{j,K}^2} \right]
\]

and the discrete form of the triplet map (Eq. 3.71)

\[
M(i) = i_0 + \begin{cases} 
3(i - i_0) & \text{if } i_0 \leq i \leq i_0 + 1/3se \\
2l - 3(i - i_0) & \text{if } i_0 + 1/3se \leq i \leq i_0 + 2/3se \\
3(i - i_0) - 2se & \text{if } i_0 + 2/3se \leq i \leq i_0 + se \\
(i - i_0) & \text{otherwise}
\end{cases}
\]

The triplet mapping procedure for velocities and scalars is complete, and summarized by
3.3. ODT Governing Equations

Eqs. (2.86a) and (2.86b)

\[
\begin{align*}
    u_i(x_j) & \rightarrow u_i[M(x_j)] + c_i \cdot (x_j - M(x_j)), \\
    \phi_i(x_j) & \rightarrow \phi_i[M(x_j)],
\end{align*}
\]

where Eq. (2.89) has been used to substitute the kernel transformation.

Stirring Time Step Adjustment

The time step is adjusted following Eq. (2.113) based on a predefined target probability \( P_{\text{targ}} \), which defines a mean probability for the simulation and the actual acceptance probability, as given in Eq. (2.105)

\[
\Delta t_s^{\text{new}} = \Delta t_s^{\text{old}} \frac{P_{\text{targ}}}{P_e},
\]

A range for \( P_{\text{targ}} \) of 0.1 to 0.4 is reasonable, to be conservative and to avoid oversampling. The algorithm for the stirring time step adjustment (which basically is a sampling period controller) is given in Tab. 3.1, which is called after a certain amount of trials \( n_{\text{trials}} \).

<table>
<thead>
<tr>
<th>Table 3.1: Stirring time step adjustment.</th>
</tr>
</thead>
<tbody>
<tr>
<td>1: ( n_{\text{trials}} = n_{\text{trials}} + 1 )</td>
</tr>
<tr>
<td>2: \textbf{if} { \text{mod} [n_{\text{trials}}, \text{nint}(\Delta t_{\text{ODT}}/\Delta t_s)].eq.0 } \textbf{then}</td>
</tr>
<tr>
<td>3: \hspace{1em} \text{ratio} = P_{\text{targ}}/P_e</td>
</tr>
<tr>
<td>4: \hspace{1em} \Delta t_s = \max (\Delta t_s \cdot \text{ratio}, \Delta t_{s,\text{min}})</td>
</tr>
<tr>
<td>5: \hspace{1em} \Delta t_s = \min (\Delta t_s, \Delta t_{s,\text{max}})</td>
</tr>
<tr>
<td>6: \textbf{endif}</td>
</tr>
</tbody>
</table>
Figure 3.12: Eddy sampling algorithm.
3.4 Spatial Discretization

As already introduced in Section 2.1 and illustrated in Figure 2.2, the computational domain is discretized by the LES and the ODT grid, where the one-dimensional ODT domains are aligned with the LES cell edges. The intersection point of three orthogonal ODT domains is defined as ODT node coincides with the LES node.

To illustrate this better, and explain the data setup of the model, Figure 3.13 shows an assembly of eight LES cells for any arbitrary domain, while only one LES cell is highlighted. For any real problem, the grid extents beyond the LES cells as shown. LES and ODT nodes coincide, where ODT intra-nodes basically resolve the edges of the LES cells.

![Figure 3.13: LES-ODT grid.](image)

The three-dimensional ordering of the ODT domains parallel to the $x, y$ and $z$ directions, but along LES cell edges, suggest a data structure that is set-up accordingly, such that the arrays will look like

\[
\begin{align*}
\varphi_x[M, N_{ODT}, N_{Y_{LES}}, N_{Z_{LES}}] \\
\varphi_y[M, N_{LES}, N_{Y_{ODT}}, N_{Z_{LES}}] \\
\varphi_z[M, N_{X_{LES}}, N_{Y_{LES}}, N_{Z_{ODT}}]
\end{align*}
\] (3.72)
for the generic variable $\varphi$, where $M$ is the number of components (velocities, scalars) for that array. The decomposition of the ODT data (and thus the ODT grid) into three sets is depicted in Figures 3.14 - 3.16.

For example, for the case depicted in Figure 3.14, the array size in $y$ and $z$ corresponds to the LES resolution, while the array size in $x$ corresponds to the ODT resolution. Discretizing the ODT domain like this makes one-dimensional DNS-like resolutions possible while saving enormous computational cost and memory. This is because the resolution does not scale as $(N_x,\text{DNS} \times N_y,\text{DNS} \times N_z,\text{DNS})$ but rather $(N_y,\text{LES} \times N_z,\text{LES} \times N_x,\text{ODT}) + (N_x,\text{LES} \times N_z,\text{LES} \times N_y,\text{ODT}) + (N_x,\text{LES} \times N_y,\text{LES} \times N_z,\text{ODT})$.

A similar method to discretize the domain has been chosen for a finite-volume LES formulation as introduced by Kerstein [51]. This method refers to the incremental ODT control-volumes as "wafers" and has been continuously used in subsequent works (Gonzalez-Juez [29]).

### 3.4.1 Grid Geometry

A structured, orthogonal, non-staggered grid for ODT as well as for LES is used to discretize the domain. In non-staggered grids, all dependent variables (velocities and scalars) are located at the same position, this means that continuity cells and momentum cells coincide.
The problem considered in this work is the spatially developing turbulent reacting shear layer. In a shear layer, the largest gradients are in the center of the domain, it is beneficial that the grid is finer in those regions. Therefore, the grid is "stretched" in the \((y)\)-direction.

Figure 3.17 illustrates the LES grid in the \((x, y)\)-plane with uniform \((x)\)-direction and non-uniform (stretched) \((y)\)-direction. The dependent variables are stored at the grid nodes. The continuity and transport equations are solved by considering a continuity cell of size \((\Delta x_i, \Delta y_j)\), associated with LES node \((i,j)\).

For grid stretching a sine wave function is utilized with a stretch factor, or stretch-ratio of \(sr=4\), meaning that the ratio of the largest grid spacing to the smallest grid spacing is 4. The ODT grid is stretched in a likewise manner to the LES grid. The stretching factor is the same. The ODT nodes coincide with the LES nodes and the edges defined by the LES "grid spacing cell" (the distances between the nodes, not the
continuity cell), is resolved by additional ODT intra-node points. The stretching function for the \((y)\)-direction is given as (Mason [69])

\[
f(j) = \sin \left[ \pi \cdot \left( \frac{j - \frac{1}{2}}{Ny - 1} \right) - \pi \right],
\]

(3.73)

with \(Ny\) the number of grid points in the \((y)\)-direction for the LES or the ODT grid, where for the ODT grid \(j\) is substituted with \(j1d\).

A stretching algorithm (pseudo code) to scale the grid can then be written as

<table>
<thead>
<tr>
<th>Table 3.2: Grid stretching algorithm (pseudo code), Mason [69].</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 : fac = min((f))</td>
</tr>
<tr>
<td>2 : (f = f \cdot \text{fac})</td>
</tr>
<tr>
<td>3 : fac = (\frac{1}{\max(f)})</td>
</tr>
<tr>
<td>4 : (f = f \cdot \text{fac} (\text{sr}-1)+1)</td>
</tr>
<tr>
<td>5 : sum = 0</td>
</tr>
<tr>
<td>6 : do (j = 1, Ny-1)</td>
</tr>
<tr>
<td>7 : sum = sum + f((j))</td>
</tr>
<tr>
<td>8 : enddo</td>
</tr>
<tr>
<td>9 : fac = (\frac{L_y}{\text{sum}})</td>
</tr>
<tr>
<td>10 : (f = \text{fac} \cdot f)</td>
</tr>
</tbody>
</table>

The stretch ratio can be recovered with

\[
\text{sr} = \frac{\max(f)}{\min(f)}
\]

(3.74)

And the new grid can then be simply constructed by Algorithm 3.3
3.4. Spatial Discretization

Table 3.3: Grid construction algorithm (pseudo code).

<p>| | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>y(1)=0</td>
</tr>
<tr>
<td>2</td>
<td>do j=1,Ny-1</td>
</tr>
<tr>
<td>3</td>
<td>y(j+1) = y(j)+f(j)</td>
</tr>
<tr>
<td>4</td>
<td>enddo</td>
</tr>
</tbody>
</table>

### 3.4.2 Finite-Difference Schemes

Mason [69], presents an approach of constructing finite-difference operators to solve the governing equations directly on a stretched grid, without employing transformation or mapping operations between computational and physical domain (Hoffmann [36]). The fundamentals to this approach is also found in literature, for example in Tannehill [120].

The approach of constructing finite-difference operators, is based on the generic expression of a finite difference approximation

\[ \frac{\delta^n \varphi}{\delta x^n_i} = C^n_i \varphi, \]  

with \( \varphi \) the already introduced generic variable (a column vector of size \( N \)), \( n \) the order of the differentiation and \( C^n_i \) a \( N \times N \) matrix, which has units \( 1/l^n \), if \( l \) is a length. Terms in the \( i \)th row of \( C^n_i \), constitute the stencil for the derivative at node \( i \).

The coefficients are obtained via the approach of canceling truncation errors associated with Taylor series expansions, which involves solving a system of linear equations. The procedure is illustrated for constructing simple first and second order finite difference operators for the first and second derivative, as needed in the ODT advection and ODT diffusion-reaction advancement.

The Taylor series expansion for node \( i \) of function \( \varphi \) for the neighboring nodes, takes the form

\[ \varphi_{i-1} = \varphi_i + \frac{\delta \varphi}{\delta x}_i \mid (x_{i-1} - x_i) + \frac{\delta^2 \varphi}{\delta x^2}_i \mid \frac{(x_{i-1} - x_i)^2}{2!} + \ldots \]  

\[ \varphi_{i+1} = \varphi_i + \frac{\delta \varphi}{\delta x}_i \mid (x_{i+1} - x_i) + \frac{\delta^2 \varphi}{\delta x^2}_i \mid \frac{(x_{i+1} - x_i)^2}{2!} + \ldots. \]
For a first order, upwind operator, only \( \varphi_i \) and \( \varphi_{i-1} \) are needed, therefore Eq. (3.76a) is multiplied by the coefficient \( c_{i-1} \)

\[
c_{i-1} \cdot \left[ \varphi_{i-1} = \varphi_i + \frac{\delta \varphi}{\delta x_i} (x_{i-1} - x_i) + \frac{\delta^2 \varphi}{\delta x^2_i} \frac{(x_{i-1} - x_i)^2}{2!} + \ldots \right]. \tag{3.77}
\]

To construct a first-order first derivative operator, \( c_{i-1} \) must be calculated such that the terms multiplying \( \frac{\delta \varphi}{\delta x} \) sum to one and the terms multiplying \( \frac{\delta^2 \varphi}{\delta x^2} \) sum to zero, which can be expressed as

\[
\begin{bmatrix}
(x_{i-1} - x_i) & 0 \\
\frac{(x_{i-1} - x_i)^2}{2!} & 0 \\
\end{bmatrix} \cdot \begin{pmatrix} c_{i-1} \\ 0 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \tag{3.78}
\]

or as

\[
(x_{i-1} - x_i) \cdot c_{i-1} = 1 \tag{3.79a}
\]

\[
\frac{(x_{i-1} - x_i)^2}{2!} \cdot c_{i-1} = 0 \tag{3.79b}
\]

so that

\[
c_{i-1} = \frac{1}{(x_{i-1} - x_i)}, \tag{3.80}
\]

but Eq. (3.77) also states

\[
\frac{\delta \varphi}{\delta x_i} \mid_i = c_{i-1} (\varphi_{i-1} - \varphi_i). \tag{3.81}
\]

By substituting the constant one obtains finally for the upwind, first-order, first derivative operator at location \( i \),

\[
\left( \frac{\delta \varphi}{\delta x_i} \right)^- = \frac{\varphi_i - \varphi_{i-1}}{x_i - x_{i-1}} \tag{3.82}
\]

as has been pre-defined in Eqs. (3.45a), (3.46a) and (3.47a). The first-order, first-derivative downwind operator at location \( i \) in the grid, as predefined in Eqs. (3.45b), (3.46b) and (3.47b), is obtained analogously and is repeated here as

\[
\left( \frac{\delta \varphi}{\delta x_i} \right)^+ = \frac{\varphi_{i+1} - \varphi_i}{x_{i+1} - x_i} \tag{3.83}
\]
A first-order second derivative operator can be obtained by the same method. In this case however, $\varphi_{i-1}$ and $\varphi_{i+1}$ are needed and terms multiplying $\frac{\delta \varphi}{\delta x}$ sum to zero and the terms multiplying $\frac{\delta^2 \varphi}{\delta x^2}$ sum to one, such that for the linear equation system one can write

$$
\begin{bmatrix}
\frac{(x_{i-1} - x_i)}{2!} & \frac{(x_{i+1} - x_i)}{2!}
\end{bmatrix}
\begin{bmatrix}
c_{i-1} \\
c_{i+1}
\end{bmatrix} =
\begin{bmatrix}
0 \\
1
\end{bmatrix}
$$

(3.84)

and the derivative stencil is given by adding Eqs. (3.76a) and (3.76b) after multiplying with $c_{i-1}$ and $c_{i+1}$

$$
\frac{\delta^2 \varphi}{\delta x^2} \bigg|_{i} = c_{i-1} \varphi_{i-1} - \left(c_{i-1} + c_{i+1}\right) \varphi_{i} + c_{i+1} \varphi_{i+1},
$$

(3.85)

with

$$
c_{i-1} = \frac{2}{x_{i-1}^2 - x_i x_{i-1} - x_{i-1} x_{i+1} + x_i x_{i+1}} \quad \text{and} \quad c_{i+1} = \frac{2}{x_{i+1}^2 - x_i x_{i+1} - x_{i-1} x_{i+1} + x_i x_{i-1}},
$$

(3.86)

which for a uniform grid become second order accurate and reduces to $c_{i-1} = c_{i+1} = 1/\Delta x^2$. The number of nodes required for a second derivative stencil at location $i$, can be expressed by $n = m + 2$, while $m$ being the order of accuracy of the stencil. For uniform grid and even $m$, a special case exists, because then the number of nodes required for a second derivative is given by $n = m + 1$, as a result of extra cancelation in the truncation errors, so that the FD-operator result for the homogeneous grid (Eq. (3.59)) can be recovered here as

$$
\frac{\delta^2 \varphi}{\delta x^2} \bigg|_{i} = \frac{\varphi_{i+1} - 2 \varphi_{i} + \varphi_{i-1}}{\Delta x^2}.
$$

(3.87)

The procedure as described above has been implemented in the LES code by Mason [69], and is automated. The $C$ matrix can be calculated for uniform as well as for non-uniform grids. In the present work, the generic finite difference operators are for ODT.
3.4.3 Triplet Map on Stretched Grids

The key motivation for mesh stretching is to resolve localized flow structures and to save computational effort where high resolutions of the flow field are not needed. If static stretched meshes are used, which is a viable alternative, it has to be known a-priori where and how to stretch the mesh. Another disadvantage of static stretched grids is that the turbulent region of interest may migrate as the flow evolves. For statistically stationary flows like a spatially developing shear layer however, a static stretched mesh will be sufficient.

Executing an eddy event on a stretched grid has physical and mathematical implications on the triplet map and requires special attention. On fixed, non-uniform grids, triplet maps cannot be implemented non-dissipatively, if momentum and scalars are to be conserved, as discussed in Lignell [64].

A discrete triplet map acting on a variable mesh may not fully obey the conservation laws, as it will alter velocity or scalar profiles and locally swap unequal control volumes. Each discrete grid-point is encompassed by a fluid volume (or control volume), with a mass associated with it. Swapping control volumes of different size (volume or mass) with the triplet map operation will violate mass conservation. Reaction-diffusion processes and large scale advection processes do not have these issues and can be implemented straightforwardly on a variable grid size by utilizing generic finite-difference operators, as has been shown in Section 3.4.2. The only constraints on advective and diffusive-reactive advancement is that the CFL condition has to be met when dealing with smaller grid spacings.

The problem concerning mass conservation when triplet mapping a property profile can be avoided, if the triplet map acts on a uniform grid. Therefore, interpolating the stretched property profile onto a uniform grid, will avoid such problems. This is the approach that has been chosen in the present work. From an implementation standpoint, the mapping procedure from a stretched to a homogeneous grid can happen after the eddy-size and location selection process, as illustrated in Fig. 3.11. However, the property profile needs to be mapped back to the stretched grid, which is done after the triplet map has been executed, such that the profile can be advanced in time by advection or diffusion after stirring is complete.
The mapping process is accomplished by means of linear interpolation, as discussed in Section 3.2.7, where the interpolation itself only happens over the size of the eddy in the domain.

There have also been efforts to implement a variable triplet mesh map on adaptive grids. This new triplet map for control volumes will take into account variable mesh sizes automatically and does not require additional mapping or interpolation. These aspects have been studied by Ricks et. al. [106] and Krishnamoorthy [59] in cylindrical coordinates and later by Lignell [64] for shear flows and boyant stratified flows of a two-dimensional lagrangian stand-alone ODT formulation as has been under development by Kerstein [49].
Chapter 4

Numerical Simulation

Steps remaining to find an explicit numerical solution to the governing equations introduced in Chapter 2 and solved in Chapter 3, are the definition of a computational domain (the geometrical setup), initial and boundary conditions governing that domain and finally the definition of simulation parameters used.

The problem at hand considers a shear layer. After definition of the geometrical dimensions, inlet and outlet in the streamwise directions are defined, periodicity in the spanwise and slip walls in the transverse direction. A more detailed discussion about domain size choices and the reasoning behind it can be found in Section 4.3.1, as well as a brief discussion on numerical stability for each of the methods involved DNS, LES and ODT.

The inlet boundary conditions for the streamwise and transverse velocities include forcing of the subharmonic modes by randomly walked phases. This approach is adopted from linear inviscid stability theory, while for scalars a constant profile is applied at the inlet. The boundary conditions are discussed in great detail and their implications for the pressure solution as well as for the ODT eddy selection processes.

The chapter concludes on a discussion about code performance and scalability. The LES-ODT code performance for a detail-problem like a spatially developing reacting shear layer is quite reasonable with regards to achieved turn-around times, where DNS simulations remain very expensive.
4.1 Geometrical Setup

The computational domain is depicted in Figure 4.1. It is of size $L_x, L_y, L_z$, with an inlet at the $x = 0$ plane, outlet at $x = L_x$ plane, friction-less (slip) walls at $y = 0$ and $y = L_y$, and periodicity in the $z$ direction. Slip walls indicate that there is no boundary layer growth.

![Figure 4.1: Computational domain.](image)

The initial and boundary conditions for DNS and LES as well as for ODT are analogous, and therefore no distinction needs to be made, however if there is a difference it will be pointed out. There are however several steps in the solution procedure, where great care has to be taken when considering the boundary conditions in ODT.

In the velocity correction step (see Sec. 3.2.3: ”Correction Coupling”) for example, there is no correction at the inlet plane. The ODT velocities are basically replaced with the LES values, such that the ODT velocity inlet condition is identical with that from LES. Further, outlet, zero gradient and periodic boundary conditions in ODT must be updated after each deterministic (advection and diffusion) event is complete, as discussed in Sections 3.3.1 and 3.3.2. The inlet boundary condition does not require such an update.
and different rules apply for the stochastic stirring events in ODT, as will be discussed later in this chapter. Also in ODT, the boundary conditions are implemented with the aid of ghost points, which are held by the solution arrays, but actually lie outside the computational domain.

This chapter first presents the initial conditions and boundary conditions treatment for the deterministic velocities and scalar solution simultaneously, where boundary conditions for pressure and the ODT boundary conditions for the stochastic stirring event are discussed separately toward the end of this chapter.

4.2 Initial and Boundary Conditions

4.2.1 Inlet Boundary and Initial Conditions

The initial conditions for velocities as well as for scalars are basically the inlet conditions for these dependent variables. Therefore, the initial and inlet conditions are discussed simultaneously. The initial conditions are defined throughout the entire, three-dimensional computational domain in all three coordinate directions \((x,y,z)\), whereas the inlet conditions are defined at the inlet plane, the \((y,z)\)-plane at \(x = 0\).

For the velocities at the inlet plane however, the inlet boundary condition for \(u_1\) and \(u_2\) \((u,v)\) are superimposed with inlet perturbations, which are realized with randomly walked phases of the fundamental mode and subharmonics of the velocity inlet profile. Those inlet perturbations enable the formation of streamwise vortices.

4.2.1.1 Velocities

The inlet and initial profile of the streamwise \((x)\)-component is defined by a hyperbolic tangent profile, which defines a high- and a low-speed air stream, whereas the profiles for the transverse \((y)\)- and spanwise \((z)\)-components are given by pairs of counter-rotating vortices. The superposition of the inlet profiles will contribute to the formation of downstream rollers.
Streamwise Velocity

The initial and inlet condition for the streamwise velocity component $u_1 = u$ is specified with the non-dimensional hyperbolic tangent profile

$$U = U_m + \frac{\Delta U}{2} \tanh \left( \frac{y - L_y/2}{\sigma} \right),$$

(4.1)

which basically constitutes a high-speed air stream ($U_1$) in the upper half of the domain (Fig. 4.1) and a low-speed air stream ($U_2 < U_1$) in the lower half of the domain, which is incorporated in Eq. (4.1) as $\Delta U = (U_2 - U_1)$ and $U_m = (U_1 + U_2)/2$, $\sigma$ is the steepness of the profile.

Velocity Inlet Perturbations

Mason [69] presents a method to force the inlet velocities, which enables formation of streamwise vortices. Formation of these rollers can be accelerated by forcing the inlet plane velocities with two-dimensional, time-dependent, randomly-walked perturbations calculated from linear inviscid stability theory for incompressible flow. The perturbations correspond to the fundamental (most unstable) mode of the base profile as given in Eq. (4.1). The fundamental mode is also known as Kelvin-Helmholtz mode. Further, subsequent pairing is enabled by adding perturbations corresponding to the subharmonics of the fundamental mode.

The perturbations are obtained from solving the Rayleigh equation in the $(x, y)$-plane

$$\left( U - \frac{\omega}{\eta} \right) \cdot (\Phi'' - \eta^2 \Phi) - U'' \Phi = 0.$$  

(4.2)

$U(y)$ is the base velocity profile as given in Eq. (4.1) and $\Phi(y)$ is the stability mode, which is a complex number. The stability variables $\eta (\eta = \eta_r + i\eta_i)$ and $\omega (\omega = \omega_r + i\omega_i)$ are complex variables, too, where $\eta_r$ and $\omega_r$ are wave number and frequency and $\eta_i$ and $\omega_i$ are spatial and temporal growth rates. In this work, the spatial growth rate is more important than the temporal growth rate and thus, $\omega_i = 0$. Instability is characterized by eigenvalues of $\eta_i < 0$.

The solution to the Rayleigh equation is an eigenvalue problem to either temporally
or spatially developing disturbances. The velocity perturbations for spatially developing disturbances are given as (Mason [69])

\[ u_p = \Phi'_r \cos(-\omega t) - \Phi'_i \sin(-\omega t) \]  
\[ v_p = (\eta_i \Phi_r + \eta_r \Phi_i) \cos(-\omega t) + (\eta_r \Phi_r + \eta_i \Phi_i) \sin(-\omega t). \]

\( \eta \) is the eigenvalue and \( \Phi \) is the eigenfunction. Details to solve the eigenvalue problem numerically, are given in Mason [69] in short and in Michalke [77] in greater depth.

The code as provided by Mason includes the complete solution procedure for the Rayleigh equation. The procedure first determines the minimum value of the spatial growth rate \( \eta_i \) and its corresponding wave number \( \eta_r \) as well as frequency \( \omega \), which involves solving a Ricatti differential equation for \( \Phi \). For \( u_m = 1, \Delta U = 1 \) and \( \sigma = 0.5 \), the most unstable mode is found as \( \eta_i = 0.8758 - 0.1969i \) at \( \omega = 0.8774 \).

With the eigenvalues \( \eta \), one can calculate the eigenfunction \( \Phi \) by integrating the Raleigh Equation (Eq. (4.2)). Then the subharmonic modes are identified and in turn, their eigenfunctions. The subharmonic modes can be determined with \( \eta_r/2^i \), with \( \eta_r \) the growth rate of the fundamental mode and \( i \) the number of the subharmonic. Table 4.1 summarizes the results for the fundamental mode and the first, second and third subharmonics. The eigenfunctions are plotted in Fig. 4.2, showing the fundamental mode (a) and first three subharmonics (b-d).

<table>
<thead>
<tr>
<th>Mode</th>
<th>Eigenvalue ( \eta )</th>
<th>Angular Velocity ( \omega )</th>
<th>Wavelength ( \lambda = 2\pi/\eta_r )</th>
<th>Period ( \tau = 2\pi/\omega )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fundamental</td>
<td>0.8758</td>
<td>-0.1969</td>
<td>0.8774</td>
<td>7.17</td>
</tr>
<tr>
<td>1st Subharmonic</td>
<td>0.4073</td>
<td>-0.1470</td>
<td>0.4387</td>
<td>15.42</td>
</tr>
<tr>
<td>2nd Subharmonic</td>
<td>0.1905</td>
<td>-0.0827</td>
<td>0.2194</td>
<td>32.98</td>
</tr>
<tr>
<td>3rd Subharmonic</td>
<td>0.0915</td>
<td>-0.0430</td>
<td>0.1097</td>
<td>68.67</td>
</tr>
</tbody>
</table>
The transverse and spanwise velocities can then be assembled as

\[ u = U + \varepsilon_p \sum_{n=1}^{N_{\text{modes}}} u_p \]  \hspace{1cm} (4.5) \\
\[ v = \varepsilon_p \sum_{n=1}^{N_{\text{modes}}} v_p \]  \hspace{1cm} (4.6)

\( N_{\text{modes}} \) is the total number of modes, \( \varepsilon_p \) is the magnitude of the forcing perturbations.
The growth rate of shear layers depends on vortex pairing, which occurs randomly. In an attempt to mimic this shear layer behavior as it occurs in nature, randomly-walked phases are added to each of the subharmonics. This has been studied by Sandham and Reynolds [112].

The randomly-walked phase is termed $\Theta_r$ and the modified subharmonic will take the form of $\exp [i(\omega t + \Theta_r)]$. $\Theta_r$ is sampled from a random but uniform distribution bound by a positive and negative maximum value. The first subharmonic mode with the randomly-walked phase compared to a constant phase is shown in Figure 4.3, with values of $\Theta_r = 20$ and $N_r = 100$, such that the randomly-walked phase changes 100 times during one period. As Mason [69] summarizes, the combination of $\Theta_r$ and $N_r$ were chosen, such that the time-averaged growth-rates of the shear layer corresponds to reported values in literature. Combinations that yield very discontinuous changes cause numerical difficulties and combinations that produce too few changes in time do not result in sufficient number of vortex pairings for statistical averaging.
Spanwise and Transverse Velocity

For spatially developing shear layers it is common to initialize spanwise variation by superimposing pairs of counter-rotating streamwise vortices with the inlet profile, as suggested by Lowery and Reynolds [65] as well as Buell [10]. Superposition of such vortices and of the inlet flow will create streamwise ("rib") vortices.

Mason [69] uses so-called Oseen vortices (also called Lamb vortices) to express the transverse ($u_2 = v$) and spanwise ($u_3 = w$) velocities in the $(y,z)$-plane, which are constant along the $(x)$-direction. The vortex pair spacing in the $(z)$-direction is chosen such that the distance between the same-sense-rotation-vortices is two-thirds of the wavelength of the spanwise instability fundamental mode. This value of two-thirds has been suggested in experimental work by Huang and Ho [33], Tung and Kleis [121], and theoretical work of Pierrehumbert and Widnall [97].

Mathematically, the Oseen vortices are expressed as

$$
v = -\frac{\Gamma (z - z_c)}{(y - y_c)^2 + (z - z_c)^2} \left\{ 1 - \exp \left[ -\frac{\left( (y - y_c)^2 + (z - z_c)^2 \right)}{\xi} \right] \right\} \quad (4.7)
$$

$$
w = -\frac{\Gamma (y - y_c)}{(y - y_c)^2 + (z - z_c)^2} \left\{ 1 - \exp \left[ -\frac{\left( (y - y_c)^2 + (z - z_c)^2 \right)}{\xi} \right] \right\}. \quad (4.8)
$$

$\Gamma$ is the magnitude, $\xi$ is the size and $y_c$ and $x_c$ are the center of the vortex. The expressions can be found in Panton [89] for example. The relative location of these vortices is depicted in Fig. 4.4, with solid lines indicating clockwise rotation and dashed lines indicating counter-clockwise rotation. The contours show streamwise vorticity. The wavelength of the fundamental mode is given in Table 4.1 as 7.17, which determines the distance between a vortex pair to 4.78. Using four vortex pairs, this determines the minimum value of $L_z$ to 19.13. A summary of the parameters for the eight Oseen vortices is given in Table 4.2.
4.2. Initial and Boundary Conditions

Figure 4.4: Vorticity iso lines of initial/inlet Oseen vortices.

Table 4.2: Parameter summary for Oseen vortices

<table>
<thead>
<tr>
<th>Vortex</th>
<th>Magnitude $\Gamma$</th>
<th>Size $\xi$</th>
<th>Center $y_c$</th>
<th>Center $z_c$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.01</td>
<td>8.0</td>
<td>30.0</td>
<td>1.20</td>
</tr>
<tr>
<td>2</td>
<td>-0.01</td>
<td>8.0</td>
<td>30.0</td>
<td>3.59</td>
</tr>
<tr>
<td>3</td>
<td>0.01</td>
<td>8.0</td>
<td>30.0</td>
<td>5.98</td>
</tr>
<tr>
<td>4</td>
<td>-0.01</td>
<td>8.0</td>
<td>30.0</td>
<td>8.37</td>
</tr>
<tr>
<td>5</td>
<td>0.01</td>
<td>8.0</td>
<td>30.0</td>
<td>10.76</td>
</tr>
<tr>
<td>6</td>
<td>-0.01</td>
<td>8.0</td>
<td>30.0</td>
<td>13.15</td>
</tr>
<tr>
<td>7</td>
<td>0.01</td>
<td>8.0</td>
<td>30.0</td>
<td>15.54</td>
</tr>
<tr>
<td>8</td>
<td>-0.01</td>
<td>8.0</td>
<td>30.0</td>
<td>17.93</td>
</tr>
</tbody>
</table>
4.2. Initial and Boundary Conditions

4.2.1.2 Scalars

The initial and inlet condition for temperature is given by imposing a thin region of high temperature in the center of the domain. This is accomplished by means of a Gaussian distribution, given by

\[ T = T_{\text{ign}} \cdot \exp \left[ -\frac{(y - L_y/2)^2}{2\sigma^2} \right]. \]  
(4.9)

\( T_{\text{ign}} \) is the ignition temperature, which corresponds to the normalized adiabatic flame temperature, such that \( T_{\text{ign}} = 1 \). An initial reactant premixing is achieved by slightly overlapping hyperbolic tangent profiles of fuel and oxidizer mass fractions \( Y_k \)

\[ Y_F = \frac{Y_{F,\text{in}}}{2} \cdot \left[ 1 - \tanh \left( \frac{y - L_y/2}{\sigma} \right) \right], \]  
(4.10)

\[ Y_O = \frac{Y_{O,\text{in}}}{2} \cdot \left[ 1 + \tanh \left( \frac{y - L_y/2}{\sigma} \right) \right], \]  
(4.11)

where \( Y_{F,\text{in}} = 1 \) on the fuel side, which overlaps with the low-speed stream and \( Y_{O,\text{in}} = 1 \) on the oxidizer side, which overlaps with the high-speed stream. The initial and inlet profiles for scalars are plotted in Figure 4.5. Reactant premixing and high temperature in the inlet plane has the functionality of a "numeric flame holder"; without it, the flame will convect out of the domain and extinguish.

4.2.2 Outlet Boundary Condition

As presented in Mason [69], the outflow boundary conditions for DNS are based on the convection technique by Lowery and Reynolds [65] and Rutland et al. [110]. This formulation has been adopted for the present LES formulation. For the LES velocities, this condition is given as

\[ \text{LES} \ x = L_x : \ \frac{\delta \tilde{u}_i}{\delta t} + \tilde{u} \frac{\delta \tilde{u}_i}{\delta x} - \frac{\delta}{\delta x} (\tilde{u}_i \tilde{u} - \tilde{u}_i \tilde{u}) = 0, \]  
(4.12)

with \( \tilde{u} \) the mean advection velocity over the outlet plane and \( \tilde{u}_i \) the velocity components \( \tilde{u}, \tilde{v}, \tilde{w} \). On the ODT subgrid, both, advective and diffusive outlets are implemented for velocities and scalars. The ODT grid point at the outlet will always be a nodal point.
4.2. Initial and Boundary Conditions

Figure 4.5: Scalar initial and inlet profile.

For the advective outlet, the instantaneous streamwise LES large-scale velocity is the advective velocity at the outlet

\[
\text{ODT } x = L_x : \quad \frac{\delta \varphi_i}{\delta t} + \bar{u} \frac{\delta \varphi_i}{\delta x} = 0,
\]

where \( \varphi_i \) stands for velocities or scalars. For the diffusive outlet, one obtains

\[
\text{ODT } x = L_x : \quad \frac{\delta \varphi_i}{\delta t} - \kappa_i \frac{\delta^2 \varphi_i}{\delta x^2} = 0,
\]

where \( \varphi_i \) stands for velocities and scalars, and \( \kappa_i \) is a constant, which takes different forms for different dependent variables. So, for

\[
\kappa_i = \begin{cases} 
\frac{1}{\rho \text{Re}}; & \text{for } i = 1, 2, 3 \\
\frac{1}{\rho \text{RePr}}; & \text{for } i = 4 \\
\frac{1}{\rho \text{RePrLe}}; & \text{for } i = 5, 6
\end{cases}
\]
where \( \varphi_{1,2,3} = u, v, w, \varphi_4 = T \) and \( \varphi_{5,6} = Y_F, Y_O \). This is just a simplified analytical expression for the diffusive transport at the outlet. Numerically, the outlet boundary conditions have been implemented as a zeroth-order extrapolation, which basically entails copying the values onto the ghost points, but is physically equivalent with the equations given above.

### 4.2.3 Transverse and Spanwise Boundary Conditions

#### 4.2.3.1 Transverse Direction

In the transverse \((y)\)-direction the domain is bounded by slip walls. For velocities, the boundary condition constraint becomes for the LES part

\[
\text{LES } y = 0 \text{ \& } y = L_y : \frac{\delta u}{\delta y} = v = \frac{\delta w}{\delta y} = 0, \tag{4.16}
\]

and for ODT

\[
\text{ODT } y = 0 \text{ \& } y = L_y : \frac{\delta u}{\delta y} = \frac{\delta v}{\delta y} = \frac{\delta w}{\delta y} = 0. \tag{4.17}
\]

The additional constraint of \( v = 0 \) in the LES portion of the code guarantees that the fluid does not flow through the walls, out of the domain. This specific condition has not been adopted for the ODT part, as the shear layer will not interact with the slip walls; in other words, \( L_y \) is chosen large enough, that the constraints do not influence the interior solution. The zero-gradient condition models the friction-less (slip) walls, which is identical for temperature and species (for LES and ODT)

\[
\text{LES and ODT } y = 0 \text{ \& } y = L_y : \frac{\delta T}{\delta y} = \frac{\delta Y_F}{\delta y} = \frac{\delta Y_O}{\delta y} = 0. \tag{4.18}
\]

Zero temperature gradient implies that the walls are adiabatic.

#### 4.2.3.2 Spanwise Direction

The spanwise \((z)\)-direction is periodic, which provides a homogeneous direction for statistical averaging

\[
\text{LES } \varphi_i(z = 0) = \varphi_i(z = L_z), \tag{4.19}
\]
In ODT, for the spanwise as well as for all other boundary conditions, the method of ghost points has been adopted, which expresses the periodic boundary condition as

\[ \text{ODT } z = 0 : \quad \varphi_{z}GP[i,:,:0] = \varphi_{z}GP[i,:,:N_{z,\text{ODT}}] \]  \hspace{1cm} (4.20)

with \( \varphi_{j}GP[i,:,::] \) the solution matrix \( \varphi_{i} \) as introduced in Eq. (3.72), including the ghost points outside of the computational domain.

Eq. (4.20) illustrates the periodicity for the first ghost point 0 of the lower boundary in the \( (z) \)-direction, there are \( (3 \cdot (i_{ed}) + 1) \) ghost points for the lower as well as for the upper boundary, however. The same principle applies for the upper bound

\[ \text{ODT } z = L_{z} : \quad \varphi_{z}GP[i,:,:N_{z,\text{ODT}}+1] = \varphi_{z}GP[i,:,:1], \]  \hspace{1cm} (4.21)

which again illustrates the principle for the first ghost point \( (N_{z,\text{ODT}} + 1) \) on the upper boundary.

### 4.2.4 Pressure Boundary Conditions

Pressure only exists at the LES level. Pressure and velocities at the LES level drive the large-scale (LES) flow, which in turn drives the subgrid ODT flow, via the velocity correction step and large scale advective transport.

The source code as provided by Mason [69] implements a collocated (non-staggered) grid, therefore boundary conditions for the pressure in the non-periodic directions need to be specified. For the present case of the spatially developing shear layer geometry readily available boundary conditions can be used.

For the outflow, the same convective condition is used as for the velocities

\[ \text{LES } x = L_{x} : \quad \frac{\delta p}{\delta t} + \vec{u} \frac{\delta p}{\delta x} = 0. \]  \hspace{1cm} (4.22)

Miyauchi [80] shows that such a boundary condition is suitable for spatially developing shear layers. This specifies a Dirichlet boundary condition for the Poisson equation for pressure, which result in faster convergence.
4.2. Initial and Boundary Conditions

For the transverse direction, a zero-gradient condition is given by

\[
\text{LES } y = 0 \& \ y = L_y : \frac{\delta p}{\delta y} = 0, \tag{4.23}
\]

which is basically a von-Neumann boundary condition. This is analogous to the pressure at the inlet

\[
\text{LES } x = 0 : \frac{\delta p}{\delta x} = 0. \tag{4.24}
\]

This is similar to specifying a free stream condition, however the gradient definition provides greater flexibility in its ability to respond to the velocity perturbations imposed at the inlet. To avoid drift of the pressure field, the pressure can be specified in the corner of the domain.

4.2.5 Stirring Boundary Conditions

The stochastic eddy emulation mechanism on the ODT subgrid, termed "stirring event" in the present work, behaves fundamentally different from the deterministic advection and diffusion-reaction events. This has been discussed in previous sections (Sec. 2.3.3 and Sec. 3.3.3). Therefore, implementation of the boundary conditions require different consideration.

Boundary conditions need to be defined based on the location of an eddy on the subgrid. After sampling the eddy, the eddy index start location is given by Eq. (3.67)

\[
\text{ile} = 1 + \text{int} [\text{rand()} \cdot \text{real}(N_{x_{ODT}} - 1)],
\]

where \( \text{ile} \) describes the start location in the \((x)\)-direction, and \( j_{le}, k_{le} \) accordingly the start locations in the \((y)\) and \((z)\)-direction. The eddy size is given by Eq. (3.65)

\[
\text{se} = 3 \cdot \text{nint} \left[ \frac{1}{3} \cdot s_{\text{min}} \cdot \frac{1 - \text{rand()} \cdot \left( 1 - \frac{s_{\text{min}}}{s_{\text{max}}} \right)}{1 - \text{rand()} \cdot \left( 1 - \frac{s_{\text{min}}}{s_{\text{max}}} \right)} \right].
\]
4.2. Initial and Boundary Conditions

With this, the right index of the eddy $ire$ can be found

$$ire = ile + se$$  \hspace{1cm} (4.25)

and $jre$, $kre$ analogously. $jle$, $kle$, $(jre, kre)$ have been introduced to make explanations easier. As the stirring subroutines in the code only deal with one-dimensional domains and act on one domain at a time, the code only uses one variable $ile$ for all three directions.

With regards to triplet mapping and computing the eddy rate distribution in the stirring event, only periodic versus non-periodic boundary distinctions need to made. If a boundary is periodic, the eddy is allowed to reach over the boundary. If the boundary however is non-periodic, proper conditions need to be set that the eddy is not allowed to reach over the physical (i.e. numerical) boundary.

4.2.5.1 Streamwise Eddies

The streamwise boundaries, both, the inflow and the outflow, are non-periodic boundary conditions, which can then be formulated as

$$\begin{align*}
x = 0 & \quad ile \leq 1 \\
x = L_x & \quad ire \geq Nx_{GDT}
\end{align*}$$

or as pseudo code the boundary condition can be formulated as

Table 4.3: Streamwise eddy boundary conditions.

```plaintext
1: if [(ile .le. 1) .or. (ire .ge. Nx_{GDT})] then (select new ile)
```

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4.2.5.2 Transverse Eddies

The transverse boundaries in the \((y)\)-direction are non-periodic as well, follow the same condition and can be formulated here analogously

\[
\begin{align*}
    y &= 0 & \text{\(jle \leq 1\)} \\
    y &= L_y & \text{\(jre \geq Ny_{ODT}\)}
\end{align*}
\]

or as pseudo code the boundary condition can be formulated as

\begin{table}
\centering
\begin{tabular}{|c|}
\hline
1: if \([(jle \leq 1) \text{ or } (jre \geq Ny_{ODT})]\) then (select new \(jle\)) \\
\hline
\end{tabular}
\caption{Transverse eddy boundary conditions.}
\end{table}

4.2.5.3 Spanwise Eddies

The spanwise \((z)\)-direction is periodic and the eddy is allowed to reach across the numerical domain boundary. This is important for procedures where the eddy rate distribution function is computed as well as when pressure scrambling and the triplet map is executed. The implementation of this boundary condition is illustrated in the pseudo-code in Table 4.5. Operations of pressure scrambling usually only reach over the size of the eddy, with index range of \([kle,kle+se]=[kle,kre]\), where \(k\) indicates the \((z)\)-direction. \(k1\) defines the index location at the lower bound of the one-dimensional domain, which can be used in operations concerning pressure scrambling and triplet mapping.
4.2.5.4 Exception on Inlet Plane

On the inlet plane, no eddies are allowed. This concerns all ODT domains in transverse and spanwise direction at \( x=0 \), and is accomplished by letting \( \text{eddy-flag}=0 \), such that the eddy-sampling procedure is aborted and the next ODT event is selected. This exception at the inlet can mathematically be expressed as

\[
\begin{align*}
  x_j &= y \quad \text{and} \quad x = 0 \\
  x_j &= z \quad \text{and} \quad x = 0 \\
\end{align*}
\]

\( (\text{eddy-flag}=0) \) \tag{4.28}

4.3 Simulation Parameters

In this work, five different cases are studied. The two benchmark cases of constant density, reacting and the variable density non-reacting case with density as passive scalar, then three variable density, reacting cases, where the Lewis number is varied from 0.5, to 1.0 and to 2.0.

This section elaborates on the parameters used in these simulations. If the parameter value is not given in previous sections, this section shall serve to complete the parameter set by discussing the missing parameter choices in detail. This section also serves as an overview over all parameters, a summary is given in Table 4.6.

The non-reacting and constant density cases are preliminary studies to find suitable ODT eddy sampling parameter settings for the full reacting, variable density runs. The preliminary parameter studies involve utilizing empirical values from previous ODT studies, but also trial and error approaches and educated guesses. Previous ODT studies considered were among others, auto-ignition in decaying homogeneous isentropic turbulence.
by Cao [12] and a study on free shear flows by Kerstein [52]. For parameters concerning DNS and shear layers, Mason [69] is consulted.

A Lewis number parameter study is performed to demonstrate non-equilibrium effects between thermal and mass diffusiveness, as the Lewis number relates thermal diffusivity to mass diffusivity. The Lewis number is defined as given in Eq. (2.77)

\[
Le = \frac{\lambda}{\rho_{ref}c_pD}.
\]

It appears in the species conservation equations. For Le numbers smaller 1, mass diffusivity overrules thermal diffusivity and vice versa for Le numbers greater than 1. For Le numbers equal to unity mass and thermal diffusivity happen at equal rates. The ability to simulate different Le number effects for practical flows, demonstrates the capabilities of the present LES-ODT model formulation, as other model need major adjustments in order to be able to account for non-unity Le number effects.

The results of these studies are then summarized in Chapter 5, which presents the comparison of first and second order statistics as well as growth rates of LES-ODT against DNS simulations. The DNS simulations results are used as benchmark values to validate the LES-ODT model. Before presenting the results however, a discussion to complete the parameter set follows next.

### 4.3.1 Domain Size, Spatial and Temporal Resolution

According to the specifications given in Mason [69], the length \((L_x)\) of the domain (streamwise \((x)\)-direction), is set such that at least two vortex pairs can interact within the domain, without chemical reaction. The height \((L_y)\) of the domain (transverse \((y)\)-direction) is set high enough such that under consideration of the velocity inlet condition, the influence of the slip walls is negligible. From previous simulations, ratios of \(L_y/L_x\) around 0.5 have been found satisfactory. The limiting factor for the width \((L_z)\) of the domain in the spanwise \((z)\)-direction, has to be set so that the desired number of counter-rotating streamwise vortices can be incorporated, as discussed earlier in this chapter in Section 4.2.1.1.

Time step and grid resolution were chosen such that all fluid and chemical scales are
4.3. Simulation Parameters

properly resolved. The more important criteria for time step and resolution are stability considerations. A constant and equal grid spacing is used in streamwise and spanwise directions of $\Delta x = \Delta z = 0.25$. As discussed in Section 3.4.1, the grid in the transverse direction is stretched and denser in the center region of the computational domain ($y=30$-plane), where the highest gradients occur. The stretch ratio $sr=\frac{(\Delta y)_{\max}}{(\Delta y)_{\min}}$ is 4, such that the average grid spacing in the $(y)$-direction turns out to be $\Delta y = 0.25$ as well.

Mason [69] has undertaken a simple von Neumann stability analysis of a one-dimensional convection-diffusion equation, which can serve as guideline for setting the time step for non-reacting simulations of DNS as well as ODT

$$
\frac{\partial u}{\partial t} + a \frac{\partial u}{\partial x} - b \frac{\partial^2 u}{\partial x^2} = 0.
$$

(4.29)

For this equation, the convective (advective) and diffusive stability limits are given by the following Courant-Friedrich-Lewy (CFL) conditions

$$
\text{CFL}_a \geq \frac{a\Delta t}{\Delta x},
$$

(4.30)

$$
\text{CFL}_d \geq \frac{b\Delta t}{\Delta x^2}.
$$

(4.31)

With this and with upwinded, as well as downwinded convection operators and $a \geq 0$, one can determine the stability limits by plotting CFL$_a$ over CFL$_d$ where the region of stability is under the curve. A representative set of CFL parameters is found as CFL$_a = 0.52$ and CFL$_d = 0.002$, which is stable for low wave numbers as the spectral analysis for $|G(\Theta)|$ has shown. This combination of CFL parameters is also stable for two and three-dimensional reacting shear layers. The stability limits for the reaction rate term depend most likely on the Damköhler number. Parameter variation studies show that for moderate Damköhler numbers ($Da<50$), the time step needs to be about half the time step for the reacting case. One can obtain a rough estimate for the time step ($\Delta t$) with $\overline{\Delta x} = 0.25$ and by letting $a = \max(u_i) = U_1 = 1.5$ and $b = 1/Re = 1/200$, as given in Section 4.3.2, such that $\Delta t_c = 0.13$ and $\Delta t_d = 0.025$. Meaning the time step for DNS has to be between

$$
0.025 \leq \Delta t \leq 0.13.
$$

(4.32)
4.3. Simulation Parameters

For the non-reacting and constant density case, a time step of $\Delta t = 0.1$ returns stable solutions and for the reacting case a time step of $\Delta t = 0.05$ was determined.

For LES, the resolution is reduced by a factor of four compared to DNS, resulting in an average grid spacing of $\Delta x_j = 1.0$. The grid for LES in the transverse direction is stretched by the same factor of $sr = 4.0$, like for the DNS grid. For the reacting case and for this grid, the LES time step is set to $\Delta t = 0.05$, identical to the DNS value.

For ODT, the same value for grid stretching is adopted, however, the resolution is doubled to that of the DNS value, resulting in an average grid spacing of $\Delta x_j = 0.125$. This step is necessary to keep the LES value at a reasonable resolution while at the same time achieving a high enough ratio between ODT and LES resolution. Using an LES time step of $\Delta t = 0.05$, the advection time step for ODT is chosen to $\Delta t_a = 0.005$, such that ten advection events fit into one LES time step. Other limitations for the ODT advection time step are given by the numerical scheme used. This can be found out by trial- and error, using a von Neumann Stability analysis or by simple rule-of-thumb relations as

$$\Delta t_a \leq \text{CFL}_a \cdot \left\{ \frac{\min(\Delta x, \Delta y, \Delta z)}{\max(|u|, |v|, |w|)} \right\},$$

which, with a generous CFL$_a$ number of 1.0, returns a value of 0.0428, where the scheme was still stable for values of $\Delta t = 0.05$. The time step for the diffusion advancement is chosen to a value of $\Delta t = 0.05$, such that it is similar and at the same order of the advection time step, but different. The centered finite-difference operators used for ODT diffusion advancement are more stable than the up- and down-wind one-sided finite-difference operators used for ODT advection advancement. A proper choice for the stirring time step $\Delta t_s$ is discussed in Section 4.3.4.

4.3.2 Non-dimensional Parameters

In this work, the reference velocity $U_{ref}$ is set as the velocity difference $\Delta U = U_1 - U_2$, with $U_1$ and $U_2$ the high- and low-speed free-stream velocities. The reference length $L_{ref}$ is the vorticity thickness at the inlet $\delta_{\omega 0}$, where in general, the vorticity thickness is defined as

$$\delta_\omega = \frac{\Delta U}{[d\tilde{u}/dy]_{\text{max}}},$$

which, with a generous CFL$_a$ number of 1.0, returns a value of 0.0428, where the scheme was still stable for values of $\Delta t = 0.05$. The time step for the diffusion advancement is chosen to a value of $\Delta t = 0.05$, such that it is similar and at the same order of the advection time step, but different. The centered finite-difference operators used for ODT diffusion advancement are more stable than the up- and down-wind one-sided finite-difference operators used for ODT advection advancement. A proper choice for the stirring time step $\Delta t_s$ is discussed in Section 4.3.4.
4.3. Simulation Parameters

which depends on the inlet velocity profile, as discussed in Section 4.2.1.1. By letting $L_{\text{ref}} = \delta_{\omega_0}$ and $U_{\text{ref}} = \Delta U$, the Reynolds number as defined in Eq. (2.16) becomes

$$Re = \frac{\rho_{\text{ref}} \delta_{\omega_0} \Delta U}{\mu},$$

(4.35)

and the Damköhler number, defined in Eq. (2.70) becomes

$$Da = \frac{\delta_{\omega_0} / \Delta U}{\left[ \frac{b}{M} \rho_{\text{ref}} \cdot \exp \left( -\frac{\beta}{\alpha} \right) \right]^{-1}}.$$  

(4.36)

With a vorticity thickness at the inlet of $\delta_{\omega_0} = 1.0$ and free-stream velocities of $U_1 = 1.5$ and $U_2 = 0.5$, such that $\Delta U = 1.0$, the Reynolds number at the inlet was set to a value of $Re = 200.0$. Given the Reynolds number and the definition of the kinematic viscosity

$$\nu = \frac{\mu}{\rho_{\text{ref}}}$$

(4.37)

the kinematic viscosity can be determined as $\nu = 1/Re = 5 \cdot 10^{-3}$.

The value for the non-dimensional heat release $\alpha$, the Schwab-Zeldovich number $\beta$ and Damköhler number $Da$, were chosen based on the results from parameter studies performed by Mason [69] for a two-dimensional reacting shear layer case. $Da$ and $\alpha$ can be determined by keeping one parameter constant and varying the other, while looking at the shear layer development in the stream-wise direction. In general, the higher the reaction-rate, the greater the suppression of the shear layer downstream growth rate. The outcome was to set $\alpha = 0.85$, which corresponds to an adiabatic flame temperature of about $T_{\text{ad}} = 2000K$ and $Da = 25$, which represents a reaction rate that is fast to the mixing rates of the fluid. The two-dimensional shear layer studies can be applied to three-dimensional shear layers, because three-dimensional simulations are quasi two-dimensional, as they are dominated by two-dimensional flow structures.

The value for the non-dimensional activation energy (or Schwab-Zeldovich number) $\beta$, was determined to be $\beta = 1.5$ (Mason [69]), which is lower than in practical cases. For propane-air and methane-air combustion, $\beta$ is 5.7 and 5.9. However, in the case at hand, a value of 1.5 ensures that the heat generated downstream is two or three times greater than
4.3. Simulation Parameters

the flame holder influx heat. Consequently, this measure overcomes the limitations given by the one-step reaction, simple chemistry assumption, which leads to only moderate temperature rises downstream. In typical hydrocarbon combustion, radical production and chain reaction yield much higher heat release rates. Therefore, a lower value of $\beta$ results in higher heat release rates downstream as observed in reality. This then allows a proper numerical study of the effects of heat release on turbulence transport.

The standard Prandtl number of $Pr = 0.7$ is chosen and the Lewis number ($Le$) as subject of a parameter study is varied from 0.5 to 1.0 and 2.0, as indicated at the beginning of this section.

4.3.3 Statistical Data Sampling Procedure and Parameters

For model validation purposes of LES-ODT against DNS, the post-processing flow analysis is statistical and based on first and second order RANS and Favre time averaged statistics. For that purpose, attention needs to be paid that the flow statistics are not influenced by initial conditions and that statistics are only accumulated over times where the flow is deemed statistically stationary.

Therefore, statistical data accumulation starts at the third convective flush, where the first two convective flushes are needed to reach a statistically steady-state solution. Then, eight convective flushes are used to accumulate statistical data, summing to ten convective flushes of simulation time. A convective flush is defined as the time required for a fluid particle to travel (convect) through the computational domain in the streamwise direction, based on the mean velocity at the inlet. The mean velocity at the inlet is defined in Section 4.2.1.1, such that for the time of one convective flush, one can write

$$t_f = \frac{L_x}{U_m}.$$  \hspace{1cm} (4.38)

Figure 4.6 illustrates the data sampling procedure for DNS as well as for LES-ODT graphically. The procedure for LES-ODT is slightly different than that for DNS. LES is initialized by the initial DNS filed. This is to ensure that the LES initial conditions are identical to the DNS initial conditions. LES is then run for one convective flush, which is when the ODT simulation is started. This is mainly done to save simulation
After another convective flush of LES-ODT, statistical flow data (first and second order statistics) are accumulated over eight convective flushes, summing to a total of ten convective flushes.

One convective flush corresponds to $t_f = 120$ time units. With a time step of $\Delta t = 0.05$ for both, DNS and LES, this is equivalent to $n = t_f/\Delta t = 24000$ iterations. The total sampling time ($t_{samp}$) of eight convective flushes corresponds to 960 time units or 19200 iterations.

In the case of DNS runs, 24 flow samples per flush (SPF), or flow realizations per flush are sampled, corresponding to sampling a flow realization every 5 time units or 100 iterations. These 192 data sets are used to calculate the second order statistics, which are the root-mean squared (RMS) of the fluctuating quantities, which in the case of turbulent flow in literature are denoted as the turbulent intensities and basically represent...
the standard deviation from the mean. The actual mean quantities in the DNS case are calculated "on-board" (or "on-the-fly"), meaning the means are computed as the simulation progresses.

In the case of the LES-ODT runs, both means and turbulent intensities are computed on-board. This allows the flow field to be sampled at every time step and produces the most accurate result. The LES-ODT code however, has the capability to define an interval in which the data is to be accumulated, such that the data accumulation can be adjusted to the frequency of the DNS accumulation procedure.

As indicated above, the total sampling time of $t_{\text{samp}} = 960$ time units, over which data is sampled and statistically averaged is chosen such that a sufficient number of large turbulent structures (eddies), convect through the domain, in this case about 30 vortex pairings. This can also be estimated based on the mean velocity at the inlet and and the size of the large structures, approximated by the wavelength of the second subharmonic perturbation (see Section 4.2.1.1).

Ultimately, the computational resources available limit sampling time, sampling rate, grid resolution and domain size. The codes (DNS and LES-ODT) were run as shared memory (OpenMP) processes on one node of Dr. Frank Mueller’s ARC cluster at NCSU’s Computer Science Department, with 16 AMD Opteron 1.8 GHz and 32 GB RAM. The total wall-clock-time for DNS sums up to 30 days and for LES-ODT sums up to 8 days. Section 4.4 looks into code performance considerations in greater detail.

### 4.3.4 Eddy Sampling Parameters for ODT

The eddy sampling process is an essential part within the ODT model, as the stochastic contributions from the triplet map (Sec. 2.3.3.2), which simulates an eddy turnover event, account for under-resolved flow structures. For the Eulerian LES-ODT case, the ODT resolution is comparable to the DNS resolution only along specific ODT domains, parallel to the orthogonal coordinate directions, but not at any arbitrary point in the domain.

Fundamental parameters for the eddy selection (or sampling) process are given by the minimum and maximum eddy sizes ($s_{\text{min}}$, $s_{\text{max}}$), the shape of the eddy size ($f$) and location ($g$) PDF’s, the eddy rate constant ($C$), viscous penalty ($Z$), degree of energy exchange between velocity components ($\alpha_{e}$), ODT resolution ($\Delta x_j$), stirring time step
4.3. Simulation Parameters

(\Delta t_s) and stirring time step boundaries (\Delta t_{s,\text{min}}, \Delta t_{s,\text{max}}) and eddy target acceptance probability \( P_{\text{targ}} \), as well as the eddy maturing parameter (\( \beta_m \)).

The reasoning and thoughts behind the choices for all of these parameters is discussed in the following in greater detail. Although the parameter listed above are the primary parameters that influence the number, frequency and size of eddies sampled, secondary parameters are domain size, and simulation time or total statistics sampling time (\( t_{\text{samp}} \), see Section 4.3.3), over which statistics are accumulated.

4.3.4.1 Minimum and Maximum Eddy Size

Minimum and maximum eddy size (\( s_{\text{min}}, s_{\text{max}} \)), define the number of intervals involved in the triplet map. The minimum necessary eddy size in order to be able to execute a triplet map is \( s_{\text{min}} = 6 \). The maximum recommended eddy size usually is the size of an LES interval (Cao, [12]), which represents the LES filter size. As the current ratio of ODT to LES intervals is \( \text{ied} = 8 \), and the eddy event simulated by the triplet map can only be a multiple of three, a maximum eddy size of \( s_{\text{max}} = 15 \) is allowed, which means that an eddy can reach over two LES cells, allowing eddy sizes of 6, 9, 12 and 15.

4.3.4.2 Eddy Size and Location PDF’s, Intensified Sampling

The shape of the probability density functions for size and location are given in Kerstein [49] and Echekki [21]. These PDF’s however, allow only little control over where on the physical one-dimensional ODT domain the eddy is sampled. This may not be important for homogeneous isotropic turbulence cases, but for more general flows however, it may be beneficial to incorporate more control parameter into these equations. This has not been attempted in this work, but is recommended for future work. For example in the case of the turbulent shear layer, one goal would be to have as many eddy sampling successes as possible within the shear layer region and not outside of it. However, in the current work, this disadvantage is compensated by a so-called ”intensified sampling” loop in the eddy sampling algorithm, as presented in Fig. 3.12. In case an eddy is rejected, the code tries, \( N_{\text{max}} \) number of times again, until a valid eddy was found, and, if not, the eddy sampling procedure is revisited the next time stirring advancement is executed. For the work at hand, a value of \( N_{\text{max}} = 100 \) was found to provide the best results. It should be
noted at this point however, that a too high value of $N_{\text{max}} = 100$, will result in poor code performance.

### 4.3.4.3 Eddy Rate Constant and Viscous Penalty

The eddy rate constant ($C$), as introduced in Section 2.3.3.2, scales the speed of the kinetic energy cascade as discovered by Kolmogorov down to viscosity, whereas the the viscous penalty parameter ($Z$), suppresses the formation of small vortices by introducing an artificial viscosity. High values of $C$ increase turbulent intensity, but also increase the dissipation of turbulent kinetic energy down to smaller scales. A reasonable range for $C$ is at the order of $10^0$ to $10^1$, where on the other hand, typical values for $Z$ are on the order of $10^{-3}$ to $10^{-2}$, depending on the flow under investigation. A parameter combination of $C = 4.0$, and $Z = 0.001$, was found for the present studies. These values are comparable to the values found in previous investigated cases in literature [12, 13, 44–46, 49, 50, 52].

As for the maximum number of trials for the intensified sampling algorithm, a high value of $C$ increases the chance of an accepted eddy and therefore increases the computational cost. Too high values of $C$ may result in oversampling and too low values of $C$ may result in undersampling. Undersampling is less desirable because it will produce incorrect results, whereas oversampling mainly influences computational cost. The most adequate parameter combination of $C$ and $Z$ can be found by computing the turbulent kinetic energy spectrum over the homogeneous ($z$)-direction at several locations. This allows to match the slopes and the region of the LES and the ODT energy spectra, such that overlaps and gaps can be avoided and by doing so, find the correct setting for $C$, $Z$ and $s_{\text{max}}$.

### 4.3.4.4 Equi-partition of Kinetic Energy and Grid Resolution

An equi-redistribution of kinetic energy among the ODT velocity components is desired, such that $\alpha_e$ has been set to $2/3$, or 0.667. Like the grid for LES and DNS, the ODT grid is stretched in the transverse direction by the same factor of $s_{\text{fr}} = 4$, resulting in an average grid spacing of $\overline{\Delta x_j} = 0.125$, as already discussed in Section 4.3.1.
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4.3.4.5 Target Acceptance Probability, Time Step, Maturing Condition

The target acceptance probability is another important parameter to "steer" the solution through adjusting the stirring time step. The time step adjustment relation is defined in Eq. (2.113) and presented in Section 2.3.3.4. The target acceptance probability therefore represents a mean acceptance probability, around which the actual computed eddy acceptance probability will fluctuate, as the computed acceptance probability is based on the time step (Eq. (2.105)).

The algorithm shown in Table 3.1 shows how the time step adjustment is accomplished. A predefined target probability is related to the computed eddy acceptance probability and the ratio is then used to multiply to the old stirring time step, such that a new stirring time step is obtained. However, the values of the new time step is limited by $\Delta t_{s,\text{min}}$ and $\Delta t_{s,\text{max}}$. This procedure is called every certain amount of trials.

The target acceptance probability, just as the time step have severe impacts on whether the flow is over- or undersampled. As suggested in Section 3.3.3.2, a range of $P_{\text{targ}} = 0.1$ to 0.4 is reasonable. Therefore, for the current flow configuration, a target acceptance probability of 0.3 was chosen, where a stirring time step of $\Delta t_s = 0.004$ and boundaries of $\Delta t_{s,\text{min}} = 0.003$ and $\Delta t_{s,\text{max}} = 0.01$ were determined.

In ODT, eddies are sampled over nine convective flushes of $t = 1080$ time units. Typical values for acquired eddies are about 2,000,000 for eddy size 6, 1,750,000 for $se = 9$, 1,000,000 for $se = 12$ and for $se = 15$, 500,000, in total about 5,250,000 eddy turnover events. These values can strongly vary, depending on the input parameters, but the values listed here are a good representation of the simulations undertaken in the work at hand.

4.3.5 Simulation Parameters Summary

Table 4.6 summarizes all of the discussed parameter settings and presents them in a structured form. The table is organized into five sections grouping together parameters relevant for geometry and numerical solver, non-dimensional parameters, ODT specific parameters, LES specific parameters as well as data sampling parameters combined with simulation realtime values. Whenever necessary distinction between DNS, LES and ODT values have been made.
Parameters with the greatest difference between the three methods (DNS, LES, ODT) are grid resolution, relative magnitude of forcing perturbations $\varepsilon_p$, time steps and simulation time.

Trial-and-error test have shown that a value of $\varepsilon_p = 0.15$ needs to be chosen for LES inlet velocity forcing. This is twice the value of DNS at 0.075. The difference in resolution however is a factor of four in each direction, and on the inlet plane this would mean a factor of 16 difference.

The biggest advantage of LES-ODT over DNS can be seen when comparing the real simulation times. DNS averages at a time of 30 days (one month!), while LES-ODT simulations need only one week, or 7 days to complete. This is a factor 4 improvement.
4.3. Simulation Parameters

Table 4.6: Simulation parameter summary.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Geometry and Numerics</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Grid</td>
<td>Domain size</td>
<td>$120 \times 60 \times 20$</td>
</tr>
<tr>
<td>$L_x \times L_y \times L_z$</td>
<td>DNS resolution</td>
<td>$481 \times 241 \times 81$</td>
</tr>
<tr>
<td>DNS $-N_x \times N_y \times N_z$</td>
<td>LES resolution</td>
<td>$121 \times 61 \times 21$</td>
</tr>
<tr>
<td>LES $-N_x \times N_y \times N_z$</td>
<td>ODT resolution</td>
<td>$961 \times 481 \times 161$</td>
</tr>
<tr>
<td>ODT $-N_x \times N_y \times N_z$</td>
<td>ODT intervals per LES interval</td>
<td>8</td>
</tr>
<tr>
<td>sr</td>
<td>Grid stretch ratio (DNS, LES, ODT)</td>
<td>4</td>
</tr>
<tr>
<td>nxo $\times$ nyo $\times$ nzo</td>
<td>ODT domains in $(x, y, z)$-direction</td>
<td>$121 \times 61 \times 21$</td>
</tr>
<tr>
<td><strong>Velocities</strong></td>
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<td></td>
</tr>
<tr>
<td>$U_1, U_2$</td>
<td>High- and low-speed velocities</td>
<td>1.5, 0.5</td>
</tr>
<tr>
<td>$\Delta U$</td>
<td>Velocity difference</td>
<td>1.0</td>
</tr>
<tr>
<td>$U_m$</td>
<td>Mean velocity</td>
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</tr>
<tr>
<td>$\sigma$</td>
<td>Hyperbolic and gaussian shape function</td>
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</tr>
<tr>
<td>$N_{\text{modes}}$</td>
<td>Number of forced modes</td>
<td>3</td>
</tr>
<tr>
<td>DNS $-\varepsilon_p$</td>
<td>DNS magnitude of perturbations</td>
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</tr>
<tr>
<td>LES $-\varepsilon_p$</td>
<td>LES magnitude of perturbations</td>
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</tr>
<tr>
<td>$\Theta_{\text{max}}, N_r$</td>
<td>Random-walk parameters</td>
<td>20, 100</td>
</tr>
<tr>
<td>$N_{\text{Oseen}}$</td>
<td>Number of Oseen vortex pairs</td>
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<tr>
<td>$\Gamma, \xi$</td>
<td>Magnitude and size of Oseen vortex</td>
<td>8.3, 2.0</td>
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<td><strong>Scalars</strong></td>
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<tr>
<td>$Y_{F,\text{in}}$</td>
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<tr>
<td>$Y_{O,\text{in}}$</td>
<td>Inlet oxidizer stream</td>
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<td>$T_{\text{ign}}$</td>
<td>Ignition temperature</td>
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<td><strong>Solver</strong></td>
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<td>$\Delta t_{\text{DNS}}$</td>
<td>DNS time step</td>
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<td>$\Delta t_{\text{LES}}$</td>
<td>LES time step</td>
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<td>$\omega_{\text{SOR}}$</td>
<td>Successive over-relaxation parameter</td>
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<td>$\varepsilon_{\text{SOR, max}}$</td>
<td>Upper tolerance limit for pressure solver</td>
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<tr>
<td>$\varepsilon_{\text{SOR, min}}$</td>
<td>Lower tolerance limit for pressure solver</td>
<td>$2.4 \cdot 10^{-4}$</td>
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4.3. Simulation Parameters

Table 4.6 continued

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<tr>
<td>$p_0$</td>
<td>Zeroth order pressure</td>
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<tr>
<td>$Re$</td>
<td>Reynolds number at inlet</td>
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<tr>
<td>$Pr$</td>
<td>Prandtl number</td>
</tr>
<tr>
<td>$Le$</td>
<td>Lewis number</td>
</tr>
<tr>
<td>$Da$</td>
<td>Damköhler number</td>
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<tr>
<td>$\alpha$</td>
<td>Non-dimensional temperature</td>
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<tr>
<td>$\beta$</td>
<td>Schwab-Zeldovich number</td>
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<table>
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<tbody>
<tr>
<td>$\Delta t_a$</td>
<td>ODT advection time step</td>
</tr>
<tr>
<td>$\Delta t_d$</td>
<td>ODT diffusion-reaction time step</td>
</tr>
<tr>
<td>$\Delta t_s$</td>
<td>ODT stirring time step</td>
</tr>
<tr>
<td>$\Delta t_{s,\text{min}}$</td>
<td>Minimum stirring time step</td>
</tr>
<tr>
<td>$\Delta t_{s,\text{max}}$</td>
<td>Maximum stirring time step</td>
</tr>
<tr>
<td>$\text{smin}$</td>
<td>Minimum eddy size</td>
</tr>
<tr>
<td>$\text{smax}$</td>
<td>Maximum eddy size</td>
</tr>
<tr>
<td>$C$</td>
<td>Constant for eddy rate distribution function</td>
</tr>
<tr>
<td>$Z$</td>
<td>Viscous penalty parameter</td>
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<tr>
<td>$P_{\text{targ}}$</td>
<td>Target probability</td>
</tr>
<tr>
<td>$N_{\text{max}}$</td>
<td>Maximum count for intensified sampling</td>
</tr>
<tr>
<td>$\beta_m$</td>
<td>Beta for eddy maturing condition</td>
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<tr>
<td>$\alpha_e$</td>
<td>Degree of kinetic energy redistribution among ODT velocities</td>
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</table>

<table>
<thead>
<tr>
<th>LES Parameters</th>
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</tr>
</thead>
<tbody>
<tr>
<td>$C_S$</td>
<td>Smagorinsky constant</td>
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</table>

<table>
<thead>
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<th>Sampling Parameters, Simulation Time</th>
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</thead>
<tbody>
<tr>
<td>$t_{\text{samp}}$</td>
<td>Total sampling time</td>
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<tr>
<td>$N_f$</td>
<td>Number of flushes</td>
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<tr>
<td>DNS - $SP_{\text{mean}}$</td>
<td>DNS samples per flush for mean quantities</td>
</tr>
<tr>
<td>DNS - $SP_{\text{fluct}}$</td>
<td>DNS samples per flush for fluctuating quantities</td>
</tr>
<tr>
<td>ODT - $SP_{\text{mean}}$</td>
<td>ODT samples per flush for mean quantities</td>
</tr>
<tr>
<td>ODT - $SP_{\text{fluct}}$</td>
<td>ODT samples per flush for fluctuating quantities</td>
</tr>
<tr>
<td>DNS - $t_{\text{real}}$</td>
<td>Real simulation time for DNS</td>
</tr>
<tr>
<td>ODT - $t_{\text{real}}$</td>
<td>Real simulation time for LES-ODT</td>
</tr>
</tbody>
</table>
4.4 Performance Considerations and Scalability

All of the simulations (DNS and LES-ODT) have been executed on the ARC cluster at the NCSU Computer Science Department, as shared memory (OpenMP) runs. Each node is equipped with 16 AMD Opteron processors, with 1.8 GHz and 32 GB RAM. As the DNS code is based on Mason’s work [69], the bulk of the code development, optimization and parallelization is related to the LES-ODT code.

During code development, great care has been taken that passing vectors to subroutines is kept to a minimum. Also, for best parallelization performance, the largest array dimension was put at the outermost loop. That way, added OpenMP pragmas yield the best speed-up.

LES-ODT code optimization has been conducted over 4 iteration steps to keep code improvement cycles efficient. PGI's profiler is used to identify the slowest subroutine at a time. Fig. 4.7 illustrates the code execution time of 4 LES-ODT iterations over the

![Figure 4.7: Execution time over number of processors.](image)
number of processors used \( t = f(P) \). As can be seen, the greatest gain in reducing execution time is achieved with 8 processors, as adding more processors only marginally decreases execution time further. The time saving ratio is about 3:2.

Code acceleration is better represented by the formal definition of the parallel speedup factor, which relates serial execution time \( t_s \) with a single processor to parallel execution time \( t_p \) with several processors

\[
S_p = \frac{t_s}{t_p}.
\] (4.39)

The speedup factor over the numbers of processors used is plotted in Fig. 4.8. The maximum speedup achieved is \( 1.59 \approx 1.6 \).

![Figure 4.8: Parallel speedup.](image)

Another important performance number in parallel computing is the parallel efficiency, defined as the ratio of the speedup over the number of processors

\[
\varepsilon_p = \frac{S_p}{P}
\] (4.40)
The parallel efficiency over the number of processors is plotted in Fig. 4.9. With 8 processors the parallel efficiency is at about 20%, where with 16 processors the parallel efficiency drops down to 10%.

Ideally, the efficiency would be a straight line with slope zero as the number of processors increase. This would mean that adding more processors equates to performing more useful work. Unfortunately, this is not the case here. If the amount of work and the amount of communication is modelled correctly in this type of iso-efficiency analysis, parallel codes often reveal a natural limit, when it comes to speed-up.

It is therefore very likely that with the current code, the hardware limitations with regards to memory usage are being hit. There is a bandwidth limitation on shared memory CPUs that define how quickly memory is made accessible to the CPUs. Even for multi-core systems, there is only one connection to memory, which creates a bottle neck. These observations have also been made by Barker et al. [4] as well as Alam et al. [2].

The best approach to scale a code is to find the optimum number of CPUs per node.
and then scaling the code across multiple nodes using the Message Passing Interface (MPI). Code parallelization as distributed memory with the MPI has not been attempted in this work, but is recommended for future work.
Chapter 5

Results

This chapter summarizes the findings from the three-dimensional turbulent reacting shear layer simulations with LES-ODT as well as with DNS. The DNS results are used for model validation purposes. The DNS governing equations and solution algorithm is discussed in the following in Section 5.1 as well as in Appendix A.

Two benchmark cases have been examined, in order to determine the appropriate ODT parameters. The first one is a constant density ($\rho=1$), but reacting case and the second one is a variable density, but non-reacting case. Both of the cases are not entirely physical as for the constant density case, the heat release due to chemical reaction is decoupled from the fluid mechanics, and for the non-reacting case, density is treated as a passive scalar and not changing as the temperature is a passive scalar for that case as well. Both effects are examined to isolate LES-ODT modeling aspects that are either related to chemistry or variable-density coupling. With the ODT parameters obtained, a combustion parameter study with three different Le numbers (Eq. (2.77) and Sec. 4.3) is then carried out.

The LES-ODT results are evaluated qualitatively with regards to flow field visualizations of temperature, product mass fraction, reaction rate and the shape of the three-dimensional flame front. A quantitative evaluation of the LES-ODT model performance against DNS is done by comparing shear layer growth rate in the streamwise direction as well as by comparing first and second order statistics of the random turbulent velocity and scalar variables. The first order statistic corresponds to the mean and the second
order statistic corresponds to the root-mean-squared (RMS, or standard deviation) of a random variable. The statistical spatial and temporal means are sampled as discussed in Section 4.3.3, and the mathematical definition is given below in Section 5.2.

The chapter concludes with a direct comparison of shear layer growth rates and scalar flow statistics for the Lewis number parameter study of the variable density, reacting shear layer cases. Qualitative and quantitative Lewis number effects are made visible for LES-ODT and are validated against DNS.

5.1 DNS Governing Equations

The unfiltered, non-dimensionalized and incompressible DNS governing equations can be found in Mason [69] for example and are presented here as momentum, energy and species conservation equations in differential form

DNS Momentum

\[
\frac{\partial u_i}{\partial t} + \frac{1}{2} \frac{\delta u_j u_j}{\delta x_i} - u_j \left( \frac{\delta u_j}{\delta x_i} - \frac{\partial u_i}{\partial x_j} \right) = -\frac{1}{\rho} \frac{\partial p}{\partial x_i} + \frac{1}{\rho \text{Re}} \left[ \frac{\partial^2 u_i}{\partial x_j^2} + \frac{1}{3} \frac{\partial}{\partial x_i} \left( \frac{\partial u_j}{\partial x_j} \right) \right]
\]

(5.1)

DNS Energy

\[
\frac{\partial T}{\partial t} + u_j \frac{\partial T}{\partial x_j} = \frac{1}{\rho \text{RePr}} \frac{\partial^2 T}{\partial x_j^2} + \dot{s}
\]

(5.2)

DNS Species

\[
\frac{\partial Y_k}{\partial t} + u_j \frac{\partial Y_k}{\partial x_j} = \frac{1}{\rho \text{RePrLe}} \frac{\partial^2 Y_k}{\partial x_j^2} - \dot{s}
\]

(5.3)

The reaction rate and the equation of state close the system of governing equations. These are given in Eq. (2.66) and Eq. (2.115) respectively.

Reactor Rate

\[
\dot{s} = D a p Y_F Y_O \cdot \exp \left( \frac{-\beta(1 - T)}{1 - \alpha(1 - T)} \right)
\]
5.2. Flow Statistics

Equation of State

\[ p_o = \rho \left( 1 + T \left( \frac{\alpha}{1 - \alpha} \right) \right) \]

The DNS momentum equations are integrated by applying the fractional step method with aid of Runge-Kutta time-stepping, as discussed in Section 3.1, analogous to the LES momentum equations. The only difference is that for the DNS momentum equations the residual (or closure) term due to Favre averaging is not present.

The transport equations for temperature and mass fractions are not solved for LES, but they are solved for DNS. The solution procedure to solve the DNS scalar equations is presented in Appendix A.

5.2 Flow Statistics

First and second order flow statistics are sampled from the simulations according to the sampling procedure given in the parameter discussion in Section 4.3.3, to compare the LES-ODT model performance against DNS for validation purposes. First order statistics are mean quantities and second order statistics are the root-mean-squared (RMS) of the fluctuating quantities, which represents a standard deviation from the mean, and in the case of turbulent flow are often referred to as turbulence intensities.

As introduced in Section 2.2, a turbulent flow quantity (random variable) is decomposed into a mean part and into a fluctuating quantity. In the case of Reynolds-averaging and for an arbitrary flow quantity \( \varphi \) this is given as

\[ \varphi = \bar{\varphi} + \varphi', \quad (5.4) \]

and for Favre-averaging this is expressed as

\[ \varphi = \bar{\varphi} + \varphi'', \]

as given in Eq. (2.9) and displayed in Fig. 2.1. The Reynolds-averaged mean is simply
the time average of a flow quantity within that time interval

\[ \bar{\varphi} = \frac{1}{\Delta t} \int_{\Delta t} \varphi(t) dt. \]  

(5.5)

A different method to time-average flow quantities is the Favre average, based on the density, and therefore used for variable density flows, which is given as

\[ \tilde{\varphi} = \frac{1}{\bar{\rho} \Delta t} \int_{\Delta t} \rho(t) \varphi(t) dt, \]  

(5.6)

or by using Eq. (5.5), can be rewritten as Eq. (2.8)

\[ \tilde{\varphi} = \frac{\bar{\rho} \varphi}{\bar{\rho}}, \]

where the "\( \sim \)" also often indicates LES filtered quantities.

It needs to be noted however, that the statistical average in this work is performed in the homogeneous, periodic (\( z \))-direction first, before the variable is accumulated over time. This means that the resulting average quantities have a spatial dependency on the (\( x \)) and the (\( y \))-directions. Numerically, this average can be expressed as

\[ \bar{\varphi}(x_i, y_j) = \frac{1}{t_{\text{samp}}} \sum_{n=2t_f}^{t_{\text{samp}}} \frac{1}{N_z} \sum_{k=1}^{N_z} \varphi(x_i, y_j, z_k, t_n), \]  

(5.7)

where \( N_z \) in this equation stands either for DNS or ODT resolution in the (\( z \))-direction. LES-ODT statistics are extracted from the ODT subgrid to have a comparable resolution to the DNS case.

The RMS or, turbulence intensities of a quantity for the Reynolds-averaged case is defined as

\[ \varphi_{\text{RMS}} = \sqrt{(\varphi')^2}, \]  

(5.8)

and for the Favre-averaged case is defined as

\[ \varphi_{\text{RMS}} = \sqrt{(\tilde{\varphi}'')^2}. \]  

(5.9)
5. RESULTS

Are the turbulence intensities to be computed during the simulation time, as has been done in the LES-ODT code, the RMS quantity can be reconstructed from the mean of the instantaneous flow quantity by first squaring Eqs. (5.4) or (2.9), then averaging and finally taking the square-root, which will result in

\[
\varphi_{\text{RMS}} = \left( \overline{\varphi^2} - \overline{\varphi}^2 \right)^{1/2}
\]

(5.10)

for the RANS case, and for the FAVRE case

\[
\varphi_{\text{RMS}} = \left[ \frac{1}{\rho} \left( \rho \overline{\varphi^2} - \overline{\rho \varphi^2} \right) \right]^{1/2}.
\]

(5.11)

The mean and the RMS statistics are accumulated and recorded at three different downstream locations of \( x = 30, 60 \) and 90 (non-dimensional), corresponding to three different local Reynolds numbers. The statistics are presented in this chapter as profiles in the transverse direction.

5.3 Shear Layer Growth Rate

Typically, three different methods can be used to determine the thickness of a shear layer, which when plotted as a downstream function are a measure of the shear layer growth rate. The first option has already been mentioned in Section 4.3.2, Eq. (4.34)

\[
\delta_\omega = \frac{\Delta U}{[d\tilde{u}/dy]_{\text{max}}}
\]

The second option is to compute the shear layer thickness based on the momentum thickness, as proposed by Oster and Wygnanski [88],

\[
\theta = \int_{y=0}^{y=L_y} \frac{\tilde{u} - U_2}{U_1 - U_2} \left( 1 - \frac{\tilde{u} - U_2}{U_1 - U_2} \right) dy,
\]

(5.12)

and the third method is to use the definition of the 1% thickness \( \delta \), which can also be determined based on the mean streamwise velocity, \( \tilde{u} \). \( \delta \) is defined as the location outside
of the shear layer, where the velocity is 99% of the free stream value, where the 1% change is based on the velocity difference \( \Delta U = U_2 - U_1 \). Defining the 99% velocities as \( u_{99}^- = U_1 - 0.01 \cdot \Delta U \) for the upper edge and as \( u_{99}^+ = U_2 + 0.01 \cdot \Delta U \) for the lower edge, one can develop a logic to find the 1% thickness for each location \( x \) as

\[
\text{if } \bar{u} > u_{99}^- : \quad \text{find } y_1(u_{99}^-) \\
\text{if } \bar{u} < u_{99}^+ : \quad \text{find } y_2(u_{99}^+) \tag{5.13a-b}
\]

such that

\[
\delta = y_1 - y_2. \tag{5.14}
\]

Finding locations \( y_1 \) and \( y_2 \) can be realized by a linear interpolation.

The Favre-averaged streamwise velocity component \( \bar{u} \) is a function of the streamwise \((x)\) and transverse \((y)\) coordinates only and spatially and temporally averaged over the homogeneous spanwise \((z)\)-direction. As indicated by Eqs. (2.8) and (5.7), the Favre-averaging reduces to Reynolds-averaging for the constant density case.

Mason [69], compares all three thicknesses in his work. The momentum thickness in general is an order of magnitude less than both, the vorticity and the 1% thickness and the vorticity thickness is approximately half the 1% thickness. Since the vorticity thickness is a non-integral method, it shows sensitivity to local changes of the mean quantity. In the following discussion of this work, the 1% thickness \( \delta \) is used to compare LES-ODT results against those from DNS.

## 5.4 Constant Density Reacting Shear Layer

This chapter summarizes the results from the three-dimensional simulations of the constant density, reacting shear layer of LES-ODT and DNS. The constant density case shear layer present the first of two benchmark cases. Constant density decouples chemical reaction from fluid dynamics in that the density will not change due to heat release. This is done in order to isolate physical effects for model development, but also to narrow down correct parameter settings.

In the following, Section 5.4.1, presents several different two-dimensional visualiza-
tions of the flow field of temperature, product mass fraction, reaction rate and three-dimensional flame surface. Section 5.4.2 discusses the growth rate behavior and Section 5.4.3 presents first and second order statistics at three different downstream locations.

5.4.1 Flow Field

The visualizations of the flow field discussed here are instantaneous depictions of the flow at the end of the simulation time at \( t = 1200 \), a "snapshot" in time. These are two-dimensional views in the \((x, y)\)-plane of the three-dimensional simulation at location \( z = 20 \). However, because of the homogeneity in the spanwise \( z \)-direction, any location can be chosen. The structures observed at this particular simulation time are representative of the processes that occur in shear layers, and they are also representative of the flow evolvement during the eight steady-state flushes used for statistical data sampling.

The visualizations compare LES-ODT filtered data to DNS filtered data. In either case, the information is filtered from a fine grid to a coarser and identical LES resolution size grid. The LES-ODT filtered field basically represents filtering information from the ODT-level subgrid to the LES-level grid. Principally, one could refer to the depicted flow field as a filtered ODT field. However, since the ODT solution is comprised of LES large scale as well as of ODT subgrid information, in the following it will be referred to as filtered LES-ODT fields.

Figure 5.1 compares filtered temperature fields of LES-ODT (top) and DNS (bottom). Downstream turbulent structures in the temperature field reveal that the shear layer is well beyond the laminar region and well into the mixing transition. It is clearly visible how the shear layer develops and forms spanwise vortices, for both LES-ODT and DNS.

For DNS, spanwise vortex roll-up (Kelvin-Helmholtz instability) begins at about \( x \approx 5 \). Between \( x \approx 5 \) and \( x \approx 30 \), three distinct and fully developed spanwise vortices ("rollers") are visible, indicating that roll-up is completed at \( x \approx 30 \). At this location, entrainment from the high-speed fluid stream combined with vortex pairing takes place, which grows to larger and larger vortices downstream. Another vortex pairing combined with fluid entrainment occurs at \( x \approx 50 \). After this location, the randomly forced subharmonic modes introduced considerable amount of three-dimensionality in the flow, which goes along with a loss of symmetry of the flow in the spanwise direction. Spanwise vortices
5.4. Constant Density Reacting Shear Layer

loose their structure and identification of vortex pairing is more difficult. Spanwise and streamwise vortices interact in the region between $60 < x < 90$ and produce small-scale three-dimensional turbulent structures downstream of $x \approx 90$.

For LES-ODT, vortex roll-up also starts at $x \approx 5$. Between $x \approx 5$ and $x \approx 30$, two distinct and fully developed spanwise vortices are visible. Vortex pairing occurs at $x \approx 30$ and $x \approx 50$, analogous to DNS. Vortex paring goes along with fluid entrainment from the high-speed fluid stream, a strong increase in shear layer growth and loss of symmetry beyond $x \approx 90$. The formation of small scale turbulent structures is not as

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Figure 5.1: Instantaneous $\tilde{T}$-field of ODT and DNS ($z=20$, $t=1200$, $\rho=1$).

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prevalent as in DNS. The reason is that those are not resolved by the grid, rather, they are emulated by ODT stirring events (see Section 2.3.3), which will not be visible as small scale structures in a filtered field.

The small-scale turbulence in ODT simulations can be obtained by introducing more ODT domains per LES cell. Essentially, if the ODT resolution goes to the DNS resolution, in the limit, ODT becomes a DNS, and with stirring events turned off, the ODT flow field should look more similar to the DNS flow field.

For both simulations, the temperature fields show a small deflection toward the low-
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speed side. This is consistent with many previous numerical and experimental findings, as discussed under the non-reacting shear layer case in the introductory parts of this work in Section 1.3.2. The discussion also applies to the constant density reacting case, as chemistry is decoupled from fluid dynamics.

The spanwise turbulent shear layer structures and general behavior can also be made visible by looking at the filtered fields of product mass fractions, $\tilde{Y}_P$, displayed in Figure 5.2. The largest mass fraction of product occurs in the cores of the spanwise vortices, which is where mixing is the greatest also. For values of $\tilde{Y}_P \approx 1$, reaction is completed.
and the reaction rate $\tilde{s}$ is zero, as illustrated in Figure 5.3, which is where temperature is the largest however. The reaction zone is thickest near the top and bottom of the cores and thinner between the cores due to flame stretching. The high Damköhler number conditions a thin reaction zone (fast chemistry) compared to flow times. The reaction rate at the inlet is high due to the flame holder.
5.4. Constant Density Reacting Shear Layer

Figure 5.4 depicts the three dimensional flame front compared between LES-ODT and DNS. The flame front is defined where \( Y_F = Y_O \), meaning zero mixture fraction and zero product mass fraction. The flame front shows contours of the filtered streamwise vorticity \( \tilde{\omega}_x \). One can see that the overall development of the shear layer is dominated by two-dimensional streamwise vortices, as the smoothness of the flame front shows despite regions of high streamwise vorticity.

5.4.2 Growth Rate

Figure 5.5 compares LES-ODT and DNS growth rates, computed based on the 1% thickness, as defined in Eqs. (5.13a - 5.14) and plotted over the streamwise direction \( x \). The one-percent thickness is based on the Favre-averaged streamwise component (see Section 5.2).

![Figure 5.5: Shear layer growth rate of LES-ODT and DNS, \( \rho=1 \).](image)

The growth rate is monotonic and close to linear. This is an indication that the vortex pairings are evenly distributed downstream as a result of the randomly-walked
phases imposed on the subharmonic modes. The convergence of the growth rate can be
determined by computing it after several different sampling times. The obtained growth
rates will be rough and the tendency is to converge to the same overall shape as time
increases, indicating that a sufficient number of large-scale structures have been sampled.
The Reynolds number at the exit \((x = 120)\) based on the one-percent thickness is \(Re_\delta \approx 5300\).

Previous studies (Mason [68, 69], Dimotakis [19]) have shown the growth rate to be
linear for non-reacting shear layers, and Dimotakis proposed a growth rate expression as

\[
\frac{\delta}{x} = C_\delta \frac{1 - r}{1 + r},
\]

with the 1% thickness \(\delta\), the velocity ratio \(r = U_2/U_1\) and growth rate constant \(C_\delta\),
\(0.25 < C_\delta < 0.45\). For a value of \(r = 1/3\), \(C_\delta = 0.42\) can be found from a linear curve
fit. These results from Mason [69] agree with findings from Brown and Roshko [8] and
Pickett [95].

The state of the shear layer can be characterized as fully turbulent, where the local
Reynolds number based on the one-percent thickness is given by \(Re_\delta > 10^4\) (Dimotakis
[19]). The ”pairing parameter” in conjunction with the Reynolds number may be a better
method to describe the state of the layer, which is defined as

\[
\frac{Rx}{\lambda_0}; \quad R = \frac{1 - r}{1 + r}
\]

\(\lambda_0\) is the wavelength of the initial (fundamental) instability. Experimentally, transition
was observed for \(Rx/\lambda_0 \approx 22\) (Karasso and Mungal [41]) and \(Rx/\lambda_0 \approx 8\) (Huang and Ho
[37]).

As discussed above, the shear layer in the present study is in the early stages of
mixing transition near a fully developed state, with a local Reynolds number at the end
of the computational domain of \(Re_\delta \approx 5300\), and an estimated pairing parameter of
\(Rx/\lambda_0 \approx 8.4\), as determined by Mason [69], Pickett [95] and others.
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5.4.3 First and Second Order Statistics

In order to validate the LES-ODT model at a detailed quantitative level, first and second order statistics have been evaluated at three downstream locations $x = 30, 60, 90$ according to Eqs. (2.8, 5.7, 5.11) and for the sampling period specified in Section 4.3.3. For the constant density case, Favre-averaging automatically reduces to Reynolds-averaging.

5.4.3.1 Velocities

The means and turbulence intensities of the $u, v$ and $w$ velocity component are given in Figs. 5.6 - 5.8. The mean profile for $u$ shows the typical hyperbolic tangent shape with a value of 0.5 in the low speed stream and a value of 1.5 for the high-speed stream. As the spread of the shear layer increases downstream, so does the slope of the profile. LES-ODT and DNS show excellent agreement at all of the three locations. This is also true for the $v$ mean component, with small values between -0.05 and 0.05 only. The mean of $w$ is zero and it indicates the homogeneity in the $z$-direction, with increasing non-symmetry due to increase in small-scale turbulence toward the exit of the domain. LES-ODT is able to capture this phenomena.

The turbulence intensities for each $u, v$ and $w$ show a similar dome-like shape, but they are different in magnitude. The RMS values also visualize the spread of the shear layer along the downstream direction. The agreements between LES-ODT are again excellent, and agree with other studies under similar conditions from literature, such as Oster and Wygnanski [88] as well as Lowery and Reynolds [65]. The difference of the $w$ RMS peak value is most likely due to a small difference in initial conditions and interaction with forcing. The ODT initial condition is generated by interpolating DNS onto ODT.

For LES-ODT, the $u$-velocity RMS values show a small "cup" (non-smootheness) in the peak-region on the low-speed side. Lowery and Reynolds note that the "cup" is a consequence of forcing. In certain regions, vortices rotate and convect downstream without much movement in the transverse direction. Profiles without this cup therefore indicate a shear layer that behaves similar to an unforced layer, as is desired.
5.4. Constant Density Reacting Shear Layer

5.4.3.2 Scalars

Mean and RMS values of temperature as well as fuel and mass fractions are given in Figures 5.9 - 5.11.

The mean temperature profile resembles the gaussian profile, as defined at the inlet. The peak value decreases downstream as the shear layer spreads. The mean profiles for fuel and oxidizer mass fractions are like the streamwise velocity component hyperbolic tangent profiles with $Y_F = 0, Y_O = 1$ on the high-speed side and $Y_F = 1, Y_O = 0$ on the low-speed side.

RMS values for temperature reveal the double-hump, as the turbulent intensities are highest at the edge of the shear layer, this is also confirmed by the fuel and oxidizer mass fractions with a hump on the low- and the high-speed side respectively.

LES-ODT is able to match mean and RMS of the DNS values perfectly, with slightly overpredicting fuel mass fraction at $x = 90$. 
5.4. Constant Density Reacting Shear Layer

Figure 5.6: Streamwise velocity first and second order statistics, $\rho=1$.

Figure 5.7: Transverse velocity first and second order statistics, $\rho=1$. 
Figure 5.8: Spanwise velocity first and second order statistics, $\rho=1$.

Figure 5.9: Temperature first and second order statistics, $\rho=1$. 

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Figure 5.10: Fuel mass fraction first and second order statistics, \( \rho=1 \).

Figure 5.11: Oxidizer mass fraction first and second order statistics, \( \rho=1 \).
5.5 Variable Density Non-Reacting Shear Layer

The second benchmark case is the non-reacting, "variable" density case. The density is considered variable, because it is initialized as a gaussian distribution according to the temperature distribution, following the equation of state as given in Eq. (2.115) and therefore transported as a passive scalar. As the reaction is disabled (reaction rate $\dot{s}$ is set to zero), the temperature is a passive scalar also and does not change due to heat release. Because the temperature does not change, the density will not change due to heat release. However, the density appears as a denominator in the pressure term, as well as in the denominator of the diffusive terms of the transport equations, as given in Eqs. (2.116 - 2.117) for LES and in Eqs. (2.118 - 2.123) for ODT. Density also appears in the pressure solver of the LES poisson equation, given in Eq. (3.13) and discussed in Section 3.1.2. Due to these influences of density (although treated as a passive scalar), the solution will be different from a constant density non-reacting case. The method of how the ODT computed density is coupled with LES is discussed in Section 3.2.4.

In the following, the flow field structures of filtered temperature, fuel mass fraction and density (Section 5.5.1), as well as growth rate (Section 5.5.2) and first and second order statistics (Section 5.5.3) are discussed.

5.5.1 Flow Field

As in the previous case, the flow visualizations are two-dimensional instantaneous depictions of the three-dimensional flow field at the end of the simulation time, after ten convective flushes at $t = 1200$, in the $(x,y)$-plane at $z = 20$. They compare ODT and DNS data filtered to an LES size grid. The turbulent flow structures visible at this time are representative for the flow during each of the eight convective flushes over which the flow has been statistically averaged.

The effect of passive scalar mixing is made visible by looking at the temperature field, as seen in Figure 5.12. The temperature is high in the region of the flame holder where it cools down downstream. Red indicates high values of temperature, green moderate and blue low temperature values. The LES-ODT flow field shows earlier vortex roll-up as compared to DNS, with vortex roll-up starting at $x = 10$ and vortex pairing with
entainment tongues occurring as early as $x = 20$. For DNS, vortex roll-up starts at $x = 20$ followed by vortex-interactions at 40. Two single large vortex interactions are visible at $x = 60$ and $x = 90$. Interacting vortex structures are due to encasement of pockets of high-speed fluid forming entrainment tongues.

When looking at fields of fuel mass fraction and density in Figures 5.13 and 5.14 respectively, the rollers at locations $x = 60$ and $x = 90$ are stronger pronounced. Both structures are clearly visible for LES-ODT as well as DNS. In general, the flow appears to be less three-dimensional compared to the constant density case. Vortex structures are
clearly visible until the end of the domain, although the last vortex at \( x = 110 \) appears to break down into smaller three-dimensional turbulent structures, as visible in Figure 5.13, the flow is clearly dominated by two-dimensional spanwise structures.

When looking at the LES-ODT fields as displayed in Figures 5.13 and 5.14 more closely, that for the case considered ODT tends to break down into more smaller structures when compared to DNS.
5.5. Variable Density Non-Reacting Shear Layer

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5.5.2 Growth Rate

The growth rate for the non-reacting case is displayed in Figure 5.15 for LES-ODT and DNS. It is computed based on the one-percent thickness and plotted over the streamwise direction $x$. As for the previous case, the shear layer one-percent thickness is based on evaluation of the spatially and temporally averaged streamwise velocity component $\tilde{u}$, at chosen downstream increments, defined by the grid resolution $\Delta x$.

Initially, the growth rate shows non-linear growth up until $x \approx 50$ and then the shear layer growth becomes monotonic and linear as for the previous constant density case. The
Figure 5.15: Shear layer growth rate of LES-ODT and DNS, \( \dot{s} = 0 \).

The near linear behavior indicates that the vortex pairing are evenly distributed downstream. Since the one-percent thickness is an integral quantity, the growth rate curve is smooth. LES-ODT and DNS show reasonable well agreement.

Besides the shape of the curve, the total increase in the thickness is also comparable between LES-ODT and DNS. At the end of the domain, the thickness has increased by a factor of 9.3.

Looking at the growth rate at several different sampling times, one can see that the curve will converge to the same overall shape by consecutively increasing the sampling times up to eight flushes, indicating that a sufficient number of large-scale structures have been sampled.

### 5.5.3 First and Second Order Statistics

As discussed in Section 5.2 mean and turbulence intensities are extracted from the flow and displayed at three different downstream locations \((x = 30, 60, 90)\). The profiles are analyzed with regards to overall trend, shape, magnitude and spread of the quantities as they progress downstream. This is done for velocities as well as for scalars.
5.5. Variable Density Non-Reacting Shear Layer

5.5.3.1 Velocities

Mean and turbulence intensity of velocities for the non-reacting case are given in Figures 5.16 - 5.18. The top rows show the averaged mean profiles and the bottom rows show the averaged RMS profiles at $x = 30, 60$ and $90$ respectively.

The mean streamwise velocity profile looks very typical for a shear layer, showing the hyperbolic tangent shape profile, with different degree of flatness while moving downstream. The flatter the profile gets, the greater the spread of the shear layer. The mean transverse velocity reveals the typical up-and-down profile, which is caused by forcing the layer. The overall $\tilde{v}$ shape is not as steep as for the constant density case however. The mean spanwise velocity is zero, showing slight disturbances of symmetry and therefore showing effects of three-dimensionality when moving downstream.

All of the velocity turbulence intensity plots show, like in the constant density case, a dome-like shape with the greatest magnitude for the streamwise velocity, followed by the transverse velocity and then the spanwise velocity. The LES-ODT $\tilde{u}_{RMS}$ (or $\langle u \rangle_{RMS}$) curves seem to be deflected toward the high-speed stream, while also showing the cup shape near the peak, typical for a forcing dominated layer. There are also discrepancies between the LES-ODT and DNS predicted $\tilde{w}_{RMS}$ values at $x = 60$ and $90$. These discrepancies can be attributed to small differences in the initial conditions, the LES-ODT initial condition is obtained by interpolating from DNS.

5.5.3.2 Scalars

Mean and turbulence intensity for the scalars are summarized in Figures 5.19 - 5.21. The mean temperature velocity profile of both LES-ODT and DNS are closely overlapped, both predicting the same values while moving downstream and showing the effects of passive scalar mixing. Mean profiles for fuel and oxidizer mass fractions are very close as well, both showing slight discrepancy however, at the $x = 90$ location. The behavior of the RMS profiles is analogous, with excellent agreement for temperature, but slight disagreements for the fuel and oxidizer mass fractions. DNS predicts a wide and round to flat velocity profile, while the LES-ODT shapes are both leaning toward the low-speed side.
5.5. Variable Density Non-Reacting Shear Layer

Figure 5.16: Streamwise velocity first and second order statistics, $\dot{s}=0$.

Figure 5.17: Transverse velocity first and second order statistics, $\dot{s}=0$. 

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Figure 5.18: Spanwise velocity first and second order statistics, $\dot{s}=0$.

Figure 5.19: Temperature first and second order statistics, $\dot{s}=0$. 
5.5. Variable Density Non-Reacting Shear Layer

Figure 5.20: Fuel mass fraction first and second order statistics, \( \dot{s}=0 \).

Figure 5.21: Oxidizer mass fraction first and second order statistics, \( \dot{s}=0 \).
5.6 Variable Density Reacting Shear Layer

This section presents findings of the reacting and variable density shear layer case. All of the effects simulated here are closer to physical reality, as the effects of heat release due to combustion are coupled with the fluid mechanics through the equation of state by changes in pressure.

This section also includes a Lewis number parameter study, where the Lewis number is varied from 0.5, to 1.0 and 2.0. The Lewis number appears in the denominator of the diffusive contributions of the species transport equations, as given in Eqs. (2.120) and (2.123). The Lewis number is defined in Eq. (2.77) and relates thermal diffusivity to mass diffusivity. For Lewis numbers smaller than one (Le<1), the flow is dominated by mass diffusion and for Lewis numbers greater than one (Le>1) the flow is dominated by thermal diffusion. Since the Prandtl number relates viscous diffusion to thermal diffusion, and the Schmidt number relates viscous diffusion to mass diffusion, the Lewis number can also be expressed as ratio of Schmidt over Prandtl number

\[ \text{Le} = \frac{\text{Sc}}{\text{Pr}}. \]  

5.6.1 Le=0.5 Shear Layer

This section summarizes the results for the variable density, reacting shear layer for Le=0.5. The results discussion includes again, the flow field visualizations, downstream shear layer development (growth rate), as well as mean and turbulence intensity of velocities and scalars.

5.6.1.1 Flow Field

In the following, filtered fields of temperature, product mass fraction, reaction rate and flame surface are presented and compared between LES-ODT and DNS. The flow fields are two-dimensional snapshots in the \((x,y)\)-plane at the end of the simulation time \((t = 1200)\), at \(z = 20\). All of the contour plots show that the flow development is very different from the benchmark cases of constant density or the non-reacting case.
5.6. Variable Density Reacting Shear Layer

Figure 5.22: Instantaneous $\tilde{T}$-field of ODT and DNS ($z=20$, $t=1200$, $Le=0.5$).

Heat release due to chemical reaction suppresses the shear layer growth, as discussed in Section 1.3.3. This is modeled by a variable density with the equation of state and coupling with the governing equations and poisson equation for pressure. The suppressed shear layer growth can be seen by looking at the temperature flow field as given in Figure 5.22. The shear layer growth is much less developed as compared to the previous benchmark cases of constant density and non-reacting flow and dominated by two-dimensional vortices in the entire domain. Although the initial growth rate is similar, the vortices do not roll up but are convected downstream while the wavelength is stretched. Also, there
is no vortex pairing observable.

The emergence of the first developed vortex is visible at about $x \approx 30$ and $x \approx 40$, when looking at temperature and product mass fraction flow fields as given in Figures 5.22 and 5.23, respectively. Vortices continue to roll up downstream, however without pairing. Pairing would emerge, if the domain was long enough.

Density changes due to heat release reduce the formation of streamwise vorticity. In addition to that, less interaction between streamwise and spanwise vortices lead to suppression of three-dimensional small-scale turbulent structures. The entrainment tongues
are less deep and less pronounced and therefore yield a growth rate that is much smaller compared to the constant density and non-reacting shear layer. This is true for LES-ODT as well as DNS simulation. The LES-ODT simulation however, shows more entrainment of high-speed fluid than the DNS case. The fact that the ODT shear layer looks like it is forced at a higher amplitude could be due to the fact that the ODT density changes across the Runge-Kutta steps are held constant (Section 3.2.4), this might be a crude approximation.

The product mass fractions are visible in Figure 5.23. The largest mass fraction occurs
in the cores of the spanwise vortices, which is were mixing has progressed the most. Values of $Y_P$ near 1, suggest that the reaction is nearly completed, as the reactants are consumed.

This is confirmed by looking at the reaction rate, given in Figure 5.24. As can be seen by the visualization the reaction rate is close to zero which indicates a completed reaction. The reaction rate is thickest at the top and bottom of the vortices. Between the vortices
the reaction zone is thinner due to flame stretching. High Damköhler numbers condition a thin reaction zone (fast chemistry compared to flow times).

The three-dimensional flame front for the discussed case is computed for $Y_F = Y_O$ and shown in Figure 5.25. The surface is colored by streamwise vorticity. Low vorticity values, a smooth and continuous flame surface indicate that the flow is dominated by two-dimensional effects. This illustrates again, how the variable density case is less developed than the constant density case.

### 5.6.1.2 Growth Rate

As for the previously discussed cases, the one-percent thickness is used to quantify the shear layer growth as a function of downstream distance. Again, the 1% thickness is evaluated based on the Favre-averaged streamwise velocity component $\tilde{u}$, accumulated over eight convective flushed, as explained in Section 4.3.3. Figure 5.26 shows the growth rate for the variable density case of Le=0.5.

![Figure 5.26: Shear layer growth rate of LES-ODT and DNS, Le=0.5.](image-url)

Figure 5.26: Shear layer growth rate of LES-ODT and DNS, Le=0.5.
The initially highly non-linear growth of the shear layer flattens out at about $30 \leq x \leq 40$, which is when the first fully developed vortex occurs. The thickness for this case is about two-thirds or almost 70% of the thickness of the previously discussed cases. This emphasizes again that the shear layer growth is significantly reduced by coupled heat release and the connected reduction in large-scale vortex pairings.

The convergence of the growth rate can be determined by computing the growth rate at different sampling times. In doing so, one can observe a convergence to the same overall shape, indicating that a sufficient number of large scale structures have been sampled and that the shear layer is in a statistically steady-state condition.

5.6.1.3 First and Second Order Statistics

Mean and turbulence intensities of velocities and scalars are extracted from the subgrid according to the discussions in Sections 5.2 and 4.3.3, plotted in the transverse direction at three different locations at $x = 30, 60, 90$ for direct comparison with DNS. These are discussed in the following.

Velocities

Figures 5.27 - 5.29 show mean and RMS of the streamwise, transverse and spanwise velocity component. The profiles are very similar to the previous cases, however they are more slender as they reflect the smaller growth rate. The mean values for $\bar{v}$ and $\bar{w}$ are small (less than 1%) of $\Delta U$, which confirm that the shear layer is dominated by two-dimensional vortices.

The suppressed growth rate is also visible in the smaller width of the RMS profiles of the velocities. The magnitudes are also less than compared to the previous cases, at $x = 90$, they are at 10% ($\bar{u}_{\text{RMS}}$), 5% ($\bar{v}_{\text{RMS}}$) and 2.5% ($\bar{w}_{\text{RMS}}$), which is 10%, 15% and 7.5% less than the constant density case. Generally however, the turbulence intensities decline in the downstream direction.

For variable density cases based on heat release, LES-ODT tends to overpredict the fluctuations of $\bar{v}$ and the RMS values of all three velocity components. Most likely this is attributed to the fact that the ODT filtered density is kept constant across the Runge-Kutta steps for integration of the LES governing equations, as given in Eq. (3.1), also
the ODT filtered density may not be directly comparable to DNS filtered density. This aspect of LES-ODT coupling needs more work.

**Scalars**

Scalar means and RMS are shown in Figures 5.30 - 5.32. The mean temperature at $x = 90$ show a value of approximately 0.5, which, given a dimensional adiabatic flame temperature of 2000K, corresponds to 1000K. At a 50\% drop in temperature the density drops by about 75\%, to a value of $\bar{\rho} = 0.25$, using the equation of state and a value of $\alpha = 0.85$. For adiabatic flame temperatures ($\tilde{T} = 1$), the density corresponds to $\bar{\rho} = 0.15$, a 85\% drop.

For temperature and mass fractions, and for the oxidizer mass fraction especially, LES-ODT predicts wider profiles, when moving further downstream, as well as higher peak values. The deflection toward the low-speed side is more pronounced.
Figure 5.27: Streamwise velocity first and second order statistics, $Le=0.5$.

Figure 5.28: Transverse velocity first and second order statistics, $Le=0.5$. 
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Figure 5.29: Spanwise velocity first and second order statistics, Le=0.5.

Figure 5.30: Temperature first and second order statistics, Le=0.5.
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Figure 5.31: Fuel mass fraction first and second order statistics, $Le=0.5$.

Figure 5.32: Oxidizer mass fraction first and second order statistics, $Le=0.5$.
5.6.2 Le=1.0 Shear Layer

The Le=1.0 variable density reacting shear layer case is discussed next. Unity Lewis number implies that mass and thermal diffusion effects are in equilibrium. As in the previous cases, the shear layer is evaluated based on the flow fields, growth rate and mean quantities as well as turbulence intensities.

5.6.2.1 Flow Field

Two-dimensional instantaneous filtered fields of temperature, product mass fraction, reaction rate as well as flame surface are shown at the end of the simulation. The contour plots in Figs. 5.33 - 5.34, show that the flow develops very different from the first two benchmark cases, but is only slightly different from the previous Le = 0.5 case.

Filtered temperature of LES-ODT and DNS are shown in Figure 5.33. Both simulations show a more distinct formation of streamwise vortices. The shear layer appears thinner over the first third of the downstream distance and also the temperature distribution seems thinner between the vortices as the mass diffusivity is decreased and the thermal diffusivity increased compared to the previously discussed case. Therefore, it appears as if the vortices are able to complete their roll-up. As for the Le = 0.5 case, there is no vortex pairing noticeable. However, different, from the Le = 0.5 case, the first developed streamwise vortex appears earlier, at $x \approx 20$ and larger vortices continue to roll-up further downstream. As in the previous case, heat release leads to formation of streamwise vortices and less interaction between streamwise and spanwise vortices lead to lesser formation of vortex pairing small scale turbulence.

These observations are confirmed when looking at the filtered product mass fraction distribution, as given in Figure 5.34. As in all of the previous reacting cases, the highest product mass fraction occurs in the center of the vortices, where mixing is the highest.

The reaction rate is lowest where the product mass fraction is highest (Figure 5.35), as the reaction tends toward completeness in the cores. As in the previous case, the reaction zone is thickest at the top and bottom of the rollers and thins out in between the rollers due to flame stretching. As the Damkohler number has not changed, the reaction zone remains thin compared to flow scales (fast chemistry).

The three-dimensional flame front ($Y_F = Y_O$) is given in Figure 5.36. As in the pre-
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**Figure 5.33:** Instantaneous $\tilde{T}$-field of ODT and DNS ($z=20$, $t=1200$, $Le=1.0$).

In previous case, the flame front is smoother than for the variable density case, indicating less three-dimensional, small-scale turbulence effects. The two-dimensional behavior is confirmed by the numbers of streamwise vorticity. The flame front also reveals the tendency for streamwise vortices to complete the roll-up process as discussed above. Although there are regions of high streamwise vorticity, the flame front in the DNS case stays smooth and continuous. This however is not the case for LES-ODT.

The behavior of LES-ODT compared to DNS is like in the previously discussed reacting, variable density case different in that the flow seems more forcing dominated rather
5.6. Variable Density Reacting Shear Layer

Figure 5.34: Instantaneous $\bar{Y}_P$-field of ODT and DNS ($z=20$, $t=1200$, $Le=1.0$).

than mixing dominated. The flame front also exhibits that the flow shows more three-dimensional effects compared to the $Le = 0.5$ case, as the flame front is less smooth. This can be attributed to the zeroth order approximation of variable density coupling between ODT and LES and should be studied further and in greater detail in future work.

5.6.2.2 Growth Rate

The Favre-averaged streamwise velocity component $\bar{u}$, which has been spatially and temporally averaged over the sampling period of eight convective flushes as illustrated in
Figure 5.35: Instantaneous $\tilde{s}$-field of ODT and DNS ($z=20$, $t=1200$, $Le=1.0$).

Section 4.3.3 and according to the formulation in Section 5.2 is used to quantify shear layer growth. In this work, the 1% thickness has been used to visualize the growth rate quantitatively. The way in which the 1% thickness is determined from the $\tilde{u}$ distribution, is elaborated in Section 5.3. Figure 5.37 shows the shear layer downstream growth development for the case of $Le = 1.0$.

As it seems typical for the variable density, reacting shear layer, the shear layer growth is non-linear over the first part of the domain, after which the slope of the curve becomes flat and monotonic. However the flattening, monotonic behavior happens earlier than in
the previous case, namely at $x \approx 20$, and not in the range of $30 \leq x \leq 40$, which was observed for Le = 0.5. The thickness at the end of the domain is comparable to the Le = 0.5 case, but not identical. It is however reduced by 30% compared to the thickness of the constant density and non-reacting case. Comparing the final value of $\delta = 15$ for Le = 1.0 and $\delta = 16$ in the case of Le = 0.5, may indicate that increased thermal diffusivity leads
to increased suppression of shear layer growth. Indeed, this fits in the picture of general growth suppression for reacting, variable density shear layers. The parameter discussion about the Lewis number dependency is given in Section 5.6.4 and in fact confirms the findings as discussed here.

5.6.2.3 First and Second Order Statistics

A discussion about first and second order statistics of velocities and scalars for the case of $Le = 1.0$ follows next. Mean profiles between LES-ODT and DNS portray a better understanding of how the simulation progresses over time in overall trends and magnitudes. Therefore comparisons at several downstream locations is reasonable, where locations of $x = 30, 60, 90$ have been chosen.

Velocities

Figures 5.38 - 5.39 plot mean and turbulence intensities of the three velocity components in the transverse direction at the three chosen downstream distances. The mean profiles for $\tilde{u}$ and $\tilde{w}$ agree perfectly between LES-ODT and DNS, for $\tilde{v}$ however, the discrepancy
is similar as in the $Le = 0.5$ case, however somewhat improved, as the curves are closer. Again, this discrepancy is attributed to the variable density coupling method, which seems to be a crude approximation to advance the solution.

This issue also seems to be translated into the second order statistics, where LES-ODT tends to overpredict the DNS value. While the DNS RMS peaks decrease when moving downstream, the LES-ODT values increase for $\tilde{u}_{\text{RMS}}$, $\tilde{v}_{\text{RMS}}$, while $\tilde{w}_{\text{RMS}}$ does seem to follow the DNS trend here. Due to the overpredicted RMS values, there also seems to be an overprediction in the spread of the layer by the ODT values.

**Scalars**

The overprediction in peak and spread for the case discussed can also be seen when looking at the scalar RMS values of temperature, as well as fuel and oxidizer mass fraction, given in Figures 5.41 - 5.43. The scalars also show that the LES-ODT solution tends to lean toward the low-speed stream, while the means of the scalars agree fairly well with DNS. At the location of $x = 90$, the temperature mean shows a small drop, revealing that the thermal diffusion is increased compared to mass diffusivity, also the spread of the scalars seems increased compared to the $Le = 0.5$ case while the spread of the velocities seems decreased.
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Figure 5.38: Streamwise velocity first and second order statistics, Le=1.0.

Figure 5.39: Transverse velocity first and second order statistics, Le=1.0.
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Figure 5.40: Spanwise velocity first and second order statistics, Le=1.0.

Figure 5.41: Temperature first and second order statistics, Le=1.0.
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Figure 5.42: Fuel mass fraction first and second order statistics, Le=1.0.

Figure 5.43: Oxidizer mass fraction first and second order statistics, Le=1.0.
5.6.3 **Le=2.0 Shear Layer**

The third case of the Lewis number parameter study includes a reacting shear layer which is dominated by thermal diffusion, at $\text{Le} = 2.0$. For this case, a skinnier shear layer, more and further developed vortices are to be expected, when following the argumentation of reducing mass diffusivity and increasing thermal diffusivity. For that reason instantaneous filtered fields are examined as well as spread rate and flow statistics to evaluate flow physical phenomena due to Lewis number changes.

5.6.3.1 **Flow Field**

When looking at the DNS filtered temperature field, depicted in Figure 5.44, it is visible how roll-up is completed closer toward the inlet. A distinct vortex is visible at approximately as early as $x \approx 5$. For LES-ODT, the first spanwise roll-up is completed at $x \approx 30$. Comparing the spread of the shear layer to the previous case of $\text{Le} = 0.5$, one can see how the shear layer appears wider, while flow structures are skinnier and more stretched. This is due to the fact that the spanwise vortices are able to rotate further as compared to the previous case, as the mass diffusivity is reduced compared to the thermal diffusivity. Increasing the Lewis number increases the wavelength between of the spanwise vortices. An increasing spread in the thermal field does not condition an increase in growth rate, which is based on the streamwise velocity. Vortex pairing as mentioned for $\text{Le} = 0.5$ and $\text{Le} = 1.0$ is still suppressed due to heat release coupled with the governing through the equation of state.

The filtered product mass fraction (Figure 5.45) shows the same flow features as discussed for the temperature field, with the product mass fraction the highest in the center of the vortex cores, which is were mixing is the greatest and therefore the reaction has progressed the furthest. This means that the reaction rate at the centers of the streamwise vortices will be close to zero, as is displayed in Figure 5.46.

As initially discussed, the vortices are stretched out further as compared to the previous cases ($\text{Le} = 0.5, 1.0$) and thus the flame stretching effect in the DNS case, is better visible between the vortices. The typical phenomena of thick reaction zones on either the top or the bottom of the vortices is visible as well, however they remain thin compared to flow structures as the fast chemistry assumption ($\text{Da} \gg 1$) shows its effect.
The flame front, defined by $Y_F = Y_O$, is plotted in Figure 5.47. It is smooth and homogenous in the $(z)$-direction, and shows that the streamwise vortices manage to advance the roll-up effect. The filtered streamwise vorticity is monotone as well, indicating only little three-dimensionality.

The behavior of the LES-ODT simulation for $Le = 2.0$ and $Le = 0.5$, is dominated by two-dimensional flow structures also, where in the case of $Le = 1.0$, this has not been observed. All of the three LES-ODT simulations however exhibit stark excitation, which leads to the conclusion that the shear layer is forcing dominated instead of mixing.
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Figure 5.45: Instantaneous $\bar{Y}_p$-field of ODT and DNS ($z=20$, $t=1200$, $Le=2.0$).

dominated. The reasons gain, can be attributed to the constant ODT density approximation across the Runge-Kutta steps, when evaluating the LES governing equations of momentum, pressure and continuity.

5.6.3.2 Growth Rate

The shear layer thickness as a function of downstream distance for the $Le = 2.0$ case is given in Figure 5.48. This growth rate is evaluated as explained in Section 5.3 and resembles the same overall shape as the previously discussed cases of $Le = 0.5$ and $Le =$
Figure 5.46: Instantaneous $\bar{s}$-field of ODT and DNS ($z=20$, $t=1200$, $Le=2.0$).
growth rate based on Favre-averaged velocity is decreasing. A detailed discussion and direct comparison of the growth rates is given in Section 5.6.4.

LES-ODT follows the same overall trend, shows however exponential growth of the shear layer thickness toward the domain exit, which again, must be attributed to the forcing dominated nature by variable density.
5.6. Variable Density Reacting Shear Layer

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The growth rate has converged, when the overall shape does not change after probing the values at several different sampling times.

5.6.3.3 First and Second Order Statistics

Flow statistics help to understand the flow behavior over a timely averaged fashion. For engineering solutions necessary to dimension machinery, RANS (FAVRE) averages are most important at critical design points. In the present case, the means provide an understanding of the shear layer shape, while the turbulent intensities give an understanding of how turbulent the flow is. Due to the non-dimensional governing equations, they represent a "relative intensity" with respect to $\Delta U = 1.0$.

To validate the LES-ODT model assumptions, statistics extracted from the ODT subgrid (according to Sections 4.3.3 and 5.3) are evaluated at three different downstream locations at $x = 30, 60, 90$ and compared to DNS.

Velocities

Figures 5.49 - 5.51 show mean and RMS values of the velocities along the transverse
(y)-direction at three different downstream distances $x$. The mean profiles of $\tilde{u}$ and $\tilde{w}$ agree perfectly with DNS, but also the profile of $\tilde{v}$ agrees much better with DNS for the present case as in the previous ones for $Le = 0.5$ and 1.0.

The intensity values are the typical dome-shaped functions for $\tilde{u}_{\text{RMS}}$ and $\tilde{v}_{\text{RMS}}$, with a less pronounced dome for $\tilde{w}_{\text{RMS}}$. The magnitudes at $x = 90$, are at 15%, 12% and 5% for $u, v, w$ respectively, a 5%, 8% and 5% drop compared to the constant density case.

However, as for the previous cases of variable density and reacting shear layer, LES-ODT tends to generally overpredict RMS values for the velocities. As mentioned earlier, this can be attributed to the simplifications done in the variable density coupling (Section 3.2.4).

**Scalars**

The mean profiles for scalars, as given in Figures 5.52 - 5.54, show good agreement between LES-ODT and DNS. LES-ODT tends to overpredict the widening of the shear layer when moving downstream. The magnitudes of the scalar RMS values are close to the DNS value. Like in the previous cases, LES-ODT shows a shift of the shear layer toward the low-speed stream.
5.6. Variable Density Reacting Shear Layer

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Figure 5.49: Streamwise velocity first and second order statistics, Le=2.0.

Figure 5.50: Transverse velocity first and second order statistics, Le=2.0.
5.6. Variable Density Reacting Shear Layer

Figure 5.51: Spanwise velocity first and second order statistics, Le=2.0.

Figure 5.52: Temperature first and second order statistics, Le=2.0.
Figure 5.53: Fuel mass fraction first and second order statistics, Le=2.0.

Figure 5.54: Oxidizer mass fraction first and second order statistics, Le=2.0.
5.6.4 Influence of Lewis Number

Direct comparisons of growth rates as well as first and second order statistics using Lewis number as parameter, help to quantify changes in the flow field due to changes of the Lewis number. These parametric studies of DNS and LES-ODT are compared to each other.

5.6.4.1 Shear Layer Growth Rate

The shear layer growth rate is evaluated as 1% thickness based on the dominant mean streamwise velocity component $\bar{u}$. It is defined where the velocity is 99% of the free stream velocity, as explained in Section 5.3. The mean velocity component $\bar{u}$ is found as outlined in Section 4.3.3. After plotting the shear layer thickness as a function of downstream distance, it provides a quantification of the growth rate.

Figure 5.55 compares Le number parametric studies of the shear layer growth rates between LES-ODT and DNS. It is immediately visible that increasing the Le number leads to slower growth rates, or growth at a suppressed rate, while thicknesses achieved at the exit of the domain are at a comparable value.

![Figure 5.55: Shear layer growth rates for Le=0.5, 1.0, 2.0.](image-url)
This is explainable because the Lewis number relates thermal diffusion to mass diffusion. Increased Le number relates to increased thermal diffusion, which has the effect of increased heat release. When comparing constant density growth rates of LES-ODT as well as DNS (Figure 5.5) to the growth rate displayed in Figure 5.55, one can see the dramatic drop in growth due to heat release. For the constant density case, heat release is decoupled from fluid mechanics, as density is set to one and not evaluated based on the equation of state, as given in Eq. (2.115).

When looking at the shear layer region in greater detail, one can see how the $\bar{u}$ velocity profiles downstream reduce the shear layer spread, or thickness over the first two-thirds of the domain, while when progressing downstream, the spread coincides. Figure 5.56, shows a zoom view of the shear layer region with $\bar{u}$ as a function of the transverse direction $y$, at several downstream locations $x = 30, 60, 90$. The initial suppressed shear layer spread (growth) is almost identical toward the exit of the domain. This is supported by Figure 5.55 also.
5.6. Variable Density Reacting Shear Layer

5.6.4.2 First Order Statistics

Figure 5.57 - 5.62 compare LES-ODT and DNS mean values of velocities and scalars with Lewis number as parameter.

The only other mean quantity which supports the trends observed about the growth rate and discussed in the previous section (Section 5.6.4.1) is the mean of the temperature, as plotted in Fig. 5.60, displaying a suppressed shear layer growth over the first two thirds of the domain and almost identical spread toward the exit of the domain. Increased thermal diffusion has the effect of lowering the mean temperature.

All other mean quantities, $\bar{v}, \bar{Y}_F$ and $\bar{Y}_O$ show inverted behavior with increased shear layer spread.

5.6.4.3 Second Order Statistics

Figure 5.63 - 5.68 compare LES-ODT and DNS rms values of velocities and scalars with Lewis number as parameter.

All of the turbulent intensities except temperature show an increase in magnitude and spread, when the Lewis number is increased. This applies to $u_{\text{RMS}}, v_{\text{RMS}}, w_{\text{RMS}}, Y_{F,\text{RMS}}, Y_{O,\text{RMS}}$. For the temperature turbulence intensity $T_{\text{RMS}}$ however, the magnitude decreases while the spread increases also.
Figure 5.57: Mean streamwise velocity for different Le.

Figure 5.58: Mean transverse velocity for different Le.
Figure 5.59: Mean spanwise velocity for different Le.

Figure 5.60: Mean temperature for different Le.
Figure 5.61: Mean fuel mass fraction for different Le.

Figure 5.62: Mean oxidizer mass fraction for different Le.
5. RESULTS

Figure 5.63: Turbulence intensity of streamwise velocity for different Le.

Figure 5.64: Turbulence intensity of transverse velocity for different Le.
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Figure 5.65: Turbulence intensity of spanwise velocity for different Le.

Figure 5.66: Turbulence intensity of temperature for different Le.
5.6. Variable Density Reacting Shear Layer

Figure 5.67: Turbulence intensity of fuel mass fraction for different Le.

Figure 5.68: Turbulence intensity of oxidizer mass fraction for different Le.
Chapter 6

Conclusions and Recommendations

Spatially developing turbulent reacting shear layers are analyzed with large eddy simulation (LES) in conjunction with the one-dimensional turbulence (ODT) model and with direct numerical simulation (DNS). Direct comparison of flow fields and characteristic flow quantities are used to validate and advance the LES-ODT concept.

While momentum and pressure is solved on the coarse LES grid, reacting scalars and momentum are solved on the ODT subgrid. The chemical reaction is simulated as a global single-step, second-order equilibrium reaction with an Arrhenius reaction rate. Reduction in resolution compared to DNS is compensated by introducing a one-dimensional triplet map, which emulates eddy turn-over events allowing for different eddy sizes on the subgrid level. The LES turbulence closure is accomplished with the Smagorinsky model. The LES-ODT model therefore aims to resemble the turbulent energy cascade down to the Kolmogorov dissipation scales. The governing equations are non-dimensionalized and follow a low Mach number approximation. The effects of heat release are accounted for through variable density with the equation of state. Density is evaluated at the subgrid level, filtered and passed to LES. The LES governing equations are integrated with a third-order Runge-Kutta time-integration, and the ODT governing equations are integrated with an explicit Forward-Euler method. Spatial discretization for LES as well as for ODT are accomplished through generic finite difference operators of third and first order, respectively that allow three-dimensional structured but stretched meshes. A fully consistent fractional step method at the LES level concludes the solution algorithm.
6.1 Conclusions

Physical-numerical LES-ODT modeling aspects are summarized and advancements compared to Cao and Echekki [12, 13] are highlighted and explained in greater detail, whenever different to this previous work. Flow-physical aspects are also discussed which expose other current model limitations. These need attention for ongoing future work.

6.1.1 Physical-Numerical LES-ODT Model Advancements

The LES-ODT model as introduced by Cao and Echekki [12, 13] is applied to a more practical flow type relevant for engineering problems for the first time. Choosing the turbulent reactive shear layer means a flow regime generalization to statistically stationary, inhomogeneous, anisotropic turbulence. In the course of doing so, several limitations are overcome.

Major restructuring of the model was found necessary with regards to three-dimensional coupling of the one-dimensional ODT subgrid domains. The three-dimensional intersection points of ODT domains, defined as nodes are governed by different governing equations as the intra-nodes, ODT points that lie in-between nodes. The region around an ODT node is fully resolved by the grid in all three directions and thus, no modeling is necessary. The ODT subgrid used for this work is set up in such a way that the ODT nodes coincide with the LES grid points. Due to the nature of triplet maps and the allowance for the ODT eddies to reach across the length of an LES cell however, a stochastic term needs to be added to the ODT nodal governing equations. The temporal advancement for the intra-nodes follows a different method. While the given direction is resolved fully and does not need modeling, information from the second and third unresolved directions are modeled by interpolation of the three-dimensional information available at the nodes. This principle is applied to advection and diffusion-reaction advancements. Stirring advancement is defined by executing triplet maps, simulating one-dimensional eddy profiles on the ODT domains. These eddies are selected in location and size based on a probability density function distributions and defined eddy input parameters, that control shape and turbulent cascade, which are eddy size definitions ”smin” and ”smax” as well as eddy rate constant, viscous penalty, eddy-maturing parameter and maximum
count for intensified sampling cycling \((C, Z, P_{\text{targ}}, \beta_m, N_{\text{max}})\), respectively. Those values were found to be \(C = 4.0, Z = 0.001, P_{\text{targ}} = 0.3\) from the benchmark cases. These values are comparable to the values reported in literature [12, 13, 44–46, 49, 50, 52]. For the present study, best results are achieved with values of \(\beta_m = 1.0\) and \(N_{\text{max}} = 100\). There can be the case of two or three intersecting eddies at a node and it is unclear what the stochastic contribution \((\Omega)\) at the node should be. This dilemma however, has a very simple solution. The value at the node can be determined by averaging the value originating from three different updates with a simple arithmetic mean. This is considered valid as the eddy turnover event follows a stochastic process. The argument is that a stochastic contribution altered by averaging is still a stochastic contribution. At this point it shall be noted that this averaging is not valid for evaluating momentum and scalar fluxes across ODT nodes. An averaging operation on deterministic equations will in fact result in incorrect results. In the special case of homogeneous isotropic turbulence, it is allowed for diffusive advancement to consider only the resolved direction multiplied by a factor of three, as the value of the second and third orthogonal directions will coincide with the value of the direction under consideration (isotropy principle).

Numerically, advection and diffusion advancement follow the same procedures. As the intra-nodes values are node-dependent, the nodal updated is executed first. In the node update, the derivatives are evaluated. Then, for advection, the advection direction is determined, followed by the temporal advancement of the nodal values. Scalar boundness is checked before proceeding to the intra-node update. Then again, the derivatives are computed based on the nodal update wherever accessed, then the three-dimensional information is interpolated onto one-dimensional information, after which the advection direction can be determined and the intra-node temporal update follows with a check for scalar boundness. It is important that before leaving advection or diffusion events, the boundary conditions stored in ghost cells, need to be updated based on the new flow information. One further difference between advection and diffusion updates is that the density and reaction rates are evaluated in the node advancement procedure already for the entire domain (nodes and intra-nodes). One major advancement in the stirring event was that eddy events needed to be executed on stretched grids. In order not to violate mass conservation and since the eddy event in the current formulation is defined on a
uniform grid only, the selected information range for an eddy event (according to eddy size and location) is interpolated onto a homogeneous grid first, then the eddy rejection tests are being executed followed by executing the triplet map if the eddy is accepted. This eddy is then interpolated back onto the stretched grid. The eddy rejection tests include testing the negative radicand of the eddy rate distribution function, an acceptance probability less than the random number sampled, or an eddy which elapsed time is less than the characteristic eddy turnover time scaled by the maturity constant. The stirring time step is adjusted according to the new acceptance probability if necessary. Finally, the one-dimensional solution is converted back to the three-dimensional solution (the inversion of this step took place at the beginning of the stirring event) and the node average is computed as already discussed above. With this, the stirring event is concluded and the next ODT event is executed based on the ODT selection process.

The newly introduced array structure resembles the "waver structure" idea as also discussed in Gonzalez-Juez, Schmidt and Kerstein [29] and allows for easier indexing in the usual euclidian orthogonal system, while at the same time saving computational cost. The waver structure is meant for finite-volume formulations where the indexing applied here is meant for finite-difference formulations. The array structure is built up of LES-size resolution with a ODT size resolution along the direction of interest. These arrays are overlapped in all three directions. This definition allows for easier boundary condition handling through utilization of ghost points and enables easy grid stretching and computing generic finite difference as the array elements are stored in a way which is a direct map to the independent coordinate arrays.

The actual geometrical and boundary conditions set up for the shear layer is very easy with an inlet, outlet in the streamwise direction, periodic in the spanwise direction and slip walls (zero gradient walls) in the transverse direction. The length of the domain is chosen, such that at least two vortex pairs can interact, the height is chosen such that the effect of the slip walls are negligible and the depth is chosen to accommodate the Oseen vortex pairs. At the inlet, streamwise and transverse velocity components are forced with a perturbation, respectively forcing velocity, which excites subharmonic modes. A randomly-walked phase is superimposed on the subharmonic modes. Forcing the inlet velocities enables formation of streamwise vortices and the randomly-walked phases ac-
6.1. Conclusions

Celerates the formation as well as add enough perturbation to the flow to trigger small- and large-scale turbulence structures to occur randomly as they do in nature. The fundamental mode corresponds to the Kelvin-Helmholtz mode and further subsequent pairing is achieved by forcing additional subharmonic modes. The modes obtained by solving the Rayleigh equation and is discussed by linear inviscid stability theory. For the spanwise velocity component as well as the transverse velocity component, four counter rotating Oseen vortex pairs are initialized, defined by location, size and strength. Through observation, it is found that the statistical solution is very sensitive to the definition of these initial rollers with streamwise vorticity. Inlet and initial condition for scalar resemble a Gaussian distribution for the temperature and a hyperbolic tangent function for mass fractions, identical to the streamwise velocity. The boundary condition for streamwise and transverse eddies is non-periodic meaning, if an eddy reaches across the boundary it is not allowed and a new eddy is sampled again. Spanwise eddies however are periodic and are allowed to reach to the other side if the eddy is larger than the physical grid boundary. The inlet is forced by fundamental and subharmonic modes and therefore no eddy events are needed, thus stirring at the inlet is suppressed.

Statistical data is sampled after two initial flushes over a total of eight convective flushes which when using a non-dimensional domain length of $L_x = 120$, a $U_m$ of 1.0 and a time step of $\Delta t = 0.05$, corresponds to a non-dimensional time of 960, or 19200 iterations, or 24000 iterations for the total of ten convective flushes, which in real-time is about 30 days for DNS and 7 days for LES-ODT. The simulations are carried out on one node at the NCSU Computer Science Department’s ARC cluster, with 16 cores at 1.8GHz and 32GB RAM. The DNS code is auto-parallelized with the compiler, while the LES-ODT code is accelerated with OpenMP and a speed-up factor of about 1.6 is achieved.

6.1.2 Flow-Physical Findings

Two benchmark cases are used to adjust the model constants. These are a constant density, reacting case and a variable density non-reacting case. Both cases are chosen to isolate numerical effects, which is variable density coupling between ODT and LES for the first case and turbulence-chemistry interactions for the non-reacting shear layer.
Choosing constant density, but with chemical reaction activated, essentially decouples the heat release due to reaction from the fluid mechanics, as density is not changing with temperature. For both benchmark cases flow fields of temperature, product mass fraction, reaction rate and flame front show good agreement. The constant density case shows break-up into smaller three-dimensional structures downstream. The agreement between LES-ODT and DNS for the first and second-order scalar statistics as well as shear layer growth rates are perfect. The non-reacting shear layer case is an important demonstration of the LES-ODT model and prove of its capabilities to simulate passive scalar mixing. The reaction rate is set to zero for this run, temperature and species are defined at the inlet.

Having found the ODT parameters, the fully variable density, reacting shear layer was simulated under Lewis number parameter variations of 0.5, 1.0 and 2.0. As reported in literature, the growth rate of the variable density reacting shear layer is suppressed by a factor of 0.7. The turbulence intensities are also suppressed by a considerable amount of about 10% or less. This suppression of shear layer growth is due to increase of volumetric heat expansion and the production of baroclinic torque. This goes along with less production of turbulent kinetic energy due to increased temperature and reduced density. Increasing the Lewis number continues the observed trends between constant density and variable density reacting flows. Due to increase in thermal diffusivity, the growth rate is further suppressed, while turbulence intensity is further reduced and widened for temperature, and for mass fractions the inverse is true.

In all cases, the flow field exhibited a deflection toward the low-speed side. This asymmetric behavior is also reported in literature and is due to the entrainment of high-speed fluid, giving the rollers a greater "downward spin" around the $z$ axis ($-y$-direction), where the "upward spin" ($+y$-direction) is defined by the low-speed velocity, which means that the original $y$ elevation of a fluid element under consideration can not be reached again due to loss in kinetic energy, due to mixing and diffusion. This process is continued toward the exit of the domain and results in a deflected shape of the shear layer. Would the high-speed velocity be in the lower halve of the domain, the shear layer would be deflected toward the upward direction, opposite to the case at hand. The flame sheets are thin, due to fast chemistry ($Da \gg 1$), rib vortices with streamwise vorticity
are negligible and the flow is dominated by streamwise vortices that grow downstream due to vortex pairing caused by fluid entrainment. Three-dimensional effects are greatest for the constant density case, as the volumetric heat expansion is not present, enhanced by streamwise and spanwise vortices, leading to high mixing rates. 

For variable density cases the results for means and growth rates show good agreement, while turbulence intensities for velocities and scalars only show reasonable agreement between LES-ODT and DNS. These indicate that variable density coupling between ODT and LES through filtered ODT density still needs more work, which will be addressed in the following section, which states recommendations for future work.

6.2 Recommendations

A possible explanation for the disagreements in the first and second order statistics between LES-ODT and DNS for the variable density cases is that a constant filtered ODT density across the Runge-Kutta steps in the LES solution procedure may be a crude approximation. There may however not be a simple solution to the problem that could be solved by parameter settings. A thorough solution approach is to call the ODT subgrid solver at each Runge-Kutta substep. This can turn out to be very expensive and is certainly not doable with the current state of parallelization of the code. Thus, the effort to improve variable density coupling between ODT and LES, actually goes along with porting the code to an already parallelized platform, like OpenFoam and others. One other reason could be that maybe the reaction and heat release modeling in ODT needs to be revisited. Also, one should consider implementing a variable density pressure scrambling model, as discussed in McDermott [71].

In the course of porting the LES-ODT concept to a higher programming language environments, parallelization efforts with graphics processing units (GPUs) in conjunction with the message passing interface (MPI) should also be explored, which are made easier by modern object oriented languages, like C++ or Java. A high-level programming language like OpenFoam is written in a form that allows easy implementation of governing equations, while providing the fundamental CFD capabilities of finite-volume discretization and parallelization. That way the developer can focus on physical aspects
of the model instead of programming challenges and finding bugs. The advantage of using finite-volume discretization is the capability to apply the model to complex geometries as they occur in engineering problems, like internal combustion engines, gas turbines, and other turbo machinery like jet engines and rocket engines.

Improvement of accuracy of the model can include extension the ODT stencils to higher orders in the finite-difference as well as the finite-volume concept, the improvement of filtering and interpolation operations. Downscaling (interpolation) can be improved by utilizing wavelet-assimilation based approaches, and upscaling (filtering) can be improved by utilizing Kalman filtering which combines LES and ODT density information. Both concepts have been explored by Fu [23], but both concepts require more work. Including the (1/3)-term that was omitted in the ODT momentum diffusion equation would improve the model accuracy. Utilization of different eddy-size and eddy-location pdf’s, which will allow more control over the distribution function could be beneficial for flows like a shear layer where most of the eddies are needed in the middle of the shear layer.

Automatization of the ODT parameter determination process is a crucial part in the generalization process of the ODT model. For example, eddy-sampling related parameters, like eddy rate constant, viscous penalty, stirring time step, target probability and maximum count for intensified sampling \((C, Z, P_{\text{targ}}, N_{\text{max}})\), can be found by analyzing the turbulent energy spectrum over the homogeneous direction from the large, LES resolved scales down to the dissipative Kolmogorov scales. For example in the case of the turbulent reacting shear layer, the homogeneous direction is the spanwise \((z)\)-direction. The turbulent energy spectrum between LES and ODT need to be evaluated and examined at several downstream locations. There should be no overlap but also not gaps between the two spectra. If there are, the constants need to be adjusted until the turbulent spectra match. Another margin to find the correct energy spectrum is to match the \((-5/3)\)-slope of the spectral curve while meeting the Nyquist limitations. For that purpose, locally defined parameters could be necessary, as the flow evolves through the domain. Having that information available, it will be easier to implement improved methods of upscaling and downscaling. In the course of doing that, one would further reduce the number of input parameters needed and the ODT model would become self-determined, and truly autonomous.
Understanding the turbulent energy spectrum goes along with increasing the understanding of the turbulent energy budgets at the subgrid level and their interactions with chemistry. This includes convection, production, dissipation, molecular diffusion and turbulent transport as well as turbulent work. As pressure does not exist at the subgrid level, pressure terms of transport, work and dilatation are omitted in the list, but may need to be reconsidered when trying to fully understand the inner effects of the ODT model as proposed. This deeper understanding will further and improve all future model advancements. For example, it is thinkable to omit the need for the Smagorinsky model as a LES closure method and replace it with fully consistent ODT subgrid information for velocities as has been proposed by McDermott [70].

Another step to strive for higher model complexity and practicability for engineering problems, is to introduce complex chemistry reaction mechanisms that are dependent of the flow velocities at equilibrium or in non-equilibrium. Introduction of complex reaction mechanisms with hundreds of different species always goes along with increased computational effort, which is another argument to port the code to higher-language software environments, but also the opportunity to couple LES-ODT with principal component analysis (PCA) and artificial neural networks (ANN), as proposed by Mirgolbabaei [78] and Mirgolbabaei and Echekki [79] for example to achieve a cost-efficient solution to complex chemical reactions. Coupling the model with other multi-physical aspects like radiation (Ben Rejeb [5]) and improvement of those need to be categorized as long-term efforts. These include multiphase-flows like soot formation and condensation, extinction and re-ignition, multistage ignition, high-speed flows as well as adaptive mesh refinement (AMR) and moving grids.
References


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A.1 Time Integration

The DNS scalar conservation equations for temperature and species can be written in short form as

\[ \frac{\delta \varphi_i}{\delta t} = -C_j + D_j \pm \dot{s}, \]  

(A.1)

where \( C \) represents the convective term and \( D \) represents the diffusive term, given as

\[ C_j = u_j \frac{\partial \varphi_i}{\partial x_j}, \]  

(A.2)

\[ D_j = \kappa_i \frac{\partial^2 \varphi_i}{\partial x_j^2}, \]  

(A.3)

with

\[ \kappa_i = \begin{cases} \frac{1}{\rho \text{RePr}}; & \text{for } i = 4 \\ \frac{1}{\rho \text{RePrLe}}; & \text{for } i = 5, 6 \end{cases} \]  

(A.4)

where \( \varphi_4 = T \) and \( \varphi_{5,6} = Y_F, Y_O \) and \( \varphi_{1,2,3} \) was already reserved for \( u_{1,2,3} = u, v, w \). The sign in front of the reaction rate term \( \dot{s} \) is positive for the energy equation and negative for the species equations.

The time integration for the convective and the diffusive terms of the species integration is accomplished using a linearly implicit variation of the third-order Runge-Kutta
A.2 Temperature- Species Coupling

The three-stage Runge-Kutta scheme in conjunction with the fractional-step method, is also used to integrate the DNS momentum equation, where the procedure is essentially equivalent to the time integration of the LES momentum equation (except for the turbulence closure terms in LES), as demonstrated in Section 3.1.

The reaction rate term is treated differently for stability reasons however, and integrated with a Crank-Nicolson scheme, which can be written as

\[
\frac{\varphi^k - \varphi^{k-1}}{\Delta t} = -\xi_k \left( -C^k + D^k \right) - \zeta_k \left( -C^{k-2} + D^{k-2} \right) \pm \chi_k \dot{s}_k \pm \psi_k \dot{s}^{k-1}.
\] (A.5)

The Runge-Kutta coefficients \( \xi_k \) and \( \zeta_k \) are given in Eq. (3.7) and the Crank-Nicolson coefficients \( \chi_k \) and \( \psi_k \) are (Le and Moin [62])

\[
\chi_1 = \psi_1 = 4/15 \quad \chi_2 = \psi_2 = 1/15 \quad \chi_3 = \psi_3 = 1/6
\] (A.6)

with

\[
\sum_{k=1}^{3} (\chi_k + \psi_k) = 1.
\] (A.7)

A.2 Temperature- Species Coupling

The unknown value \( s^k \) in Eq. (A.5) is related to \( s^{k-1} \) by first-order terms of the Taylor series expansion of \( s^k \) about \( s^{k-1} \). The first-order term is given as

\[
\dot{s}^k = \dot{s}^{k-1} + \frac{\partial \dot{s}^{k-1}}{\partial T} \Delta T_k + \frac{\partial \dot{s}^{k-1}}{\partial Y_F} \Delta Y_{F,k} + \frac{\partial \dot{s}^{k-1}}{\partial Y_O} \Delta Y_{O,k} + \frac{\partial \dot{s}^{k-1}}{\partial \rho} \Delta \rho_k
\] (A.8)

and \( \Delta t_k \) is the time-step of the Runge-Kutta scheme from \( (k - 1) \) to \( k \). The partial time derivatives \( T, Y_F, Y_O \) at \( (k - 1) \) are combined with the Runge-Kutta time step to yield

\[
\dot{s}^k = \dot{s}^{k-1} + \frac{\partial \dot{s}^{k-1}}{\partial T} \Delta T + \frac{\partial \dot{s}^{k-1}}{\partial Y_F} \Delta Y_F + \frac{\partial \dot{s}^{k-1}}{\partial Y_O} \Delta Y_O + \frac{\partial \dot{s}^{k-1}}{\partial \rho} \Delta \rho_k
\] (A.9)
where

$$\Delta T = T^k - T^{k-1} \quad \Delta Y_F = Y_F^k - Y_F^{k-1} \quad \Delta Y_O = Y_O^k - Y_O^{k-1}. \quad (A.10)$$

Substituting Eq. (A.10) in Eq. (A.5) and coupling with Eq. (A.9), a system of three coupled equations for $\Delta T$, $\Delta Y_F$, $\Delta Y_O$ is obtained, and can be written in matrix form as

$$
\begin{bmatrix}
1 - \Delta t \chi_k \frac{\partial s^{k-1}}{\partial T} & -\Delta t \chi_k \frac{\partial s^{k-1}}{\partial Y_F} & -\Delta t \chi_k \frac{\partial s^{k-1}}{\partial Y_O} \\
\Delta t \chi_k \frac{\partial s^{k-1}}{\partial T} & 1 + \Delta t \chi_k \frac{\partial s^{k-1}}{\partial Y_F} & -\Delta t \chi_k \frac{\partial s^{k-1}}{\partial Y_O} \\
-\Delta t \chi_k \frac{\partial s^{k-1}}{\partial T} & -\Delta t \chi_k \frac{\partial s^{k-1}}{\partial Y_F} & 1 + \Delta t \chi_k \frac{\partial s^{k-1}}{\partial Y_O}
\end{bmatrix}
\begin{bmatrix}
\Delta T \\
\Delta Y_F \\
\Delta Y_O
\end{bmatrix} =
$$

$$
\begin{bmatrix}
\Delta t(\chi_k + \psi_k) s^{k-1} + \Delta t \chi_k \frac{\partial s^{k-1}}{\partial \rho} \frac{\partial \rho^{k-1}}{\partial t} \Delta t_k - \xi_k \left(-C_T^{k-1} + D_T^{k-1}\right) + \zeta_k \left(-C_T^{k-2} + D_T^{k-2}\right) \\
-\Delta t(\chi_k + \psi_k) s^{k-1} + \Delta t \chi_k \frac{\partial s^{k-1}}{\partial \rho} \frac{\partial \rho^{k-1}}{\partial t} \Delta t_k - \xi_k \left(-C_{Y_F}^{k-1} + D_{Y_F}^{k-1}\right) + \zeta_k \left(-C_{Y_F}^{k-2} + D_{Y_F}^{k-2}\right) \\
-\Delta t(\chi_k + \psi_k) s^{k-1} + \Delta t \chi_k \frac{\partial s^{k-1}}{\partial \rho} \frac{\partial \rho^{k-1}}{\partial t} \Delta t_k - \xi_k \left(-C_{Y_O}^{k-1} + D_{Y_O}^{k-1}\right) + \zeta_k \left(-C_{Y_O}^{k-2} + D_{Y_O}^{k-2}\right)
\end{bmatrix}
$$

(A.11)

Partial derivatives for the reaction rate can be obtained from Eq. (5.4) and the time-derivative for the density is calculated from Eqs. (3.14a)-(3.14c). Mason [69] solves the system of equations directly by multiplying the right-hand side with the inverse of the 3x3 matrix on the left-hand side.
A.3 Solution Procedure

Within each time step and at each Runge-Kutta sub-step, the order in which the governing equations are solved is outlined in Fig. A.1.

After the reaction-rate term is evaluated, the energy and species transport equations are integrated, while applying the boundary conditions.

Figure A.1: Solution of the DNS governing equations.
The integration of the reaction-rate term, as shown in the previous two sections (A.1 and A.2), follows, and the density is updated with the new temperature value based on the equation of state. The integration of the DNS momentum equation with application of the boundary condition follows, with an update of the pressure through the Poisson equation and an update of the velocity through the velocity-correction step, as explained in Section 3.1.3 and in Eq.(3.19).

The continuity equation is used to check the solution for divergence. If the continuity of the velocity is not met, the solver stops the solution algorithm.