ABSTRACT

BEN REJEB, SAMI. Thermal Radiation Modeling using LES-ODT Framework for Turbulent Combustion Flows. (Under the direction of Dr. Tarek Echekki).

The simulation of radiation effects in a turbulent combustion flow is performed using the Monte-Carlo Ray Tracing (MCRT) technique in the Large Eddy Simulation – One Dimensional Turbulence (LES-ODT) framework. The LES-ODT is a numerical tool used in turbulent combustion modeling. It consists of a hybrid simulation of the large scales within LES and another computational domain embedded in the LES that simulates the small scales contribution referred as ODT. In the LES-ODT framework, transport equations for mass, momentum and scalar are spatially filtered, while the effects of smaller scales are modeled [1, 80]. The large turbulence scales are flow specific and strongly dependent on the flow geometry and Reynolds number. The small scales tend to be more homogeneous and less affected by the boundary conditions [81]. LES-ODT is a promising model that situates itself between the two most common other models used in CFD: the Direct Numerical Simulation (DNS) and the Reynolds Averaged Navier-Stokes (RANS) providing a relatively close enough description of the process comparing to DNS with a significant saving in terms of CPU time and allocated memory.

Radiation is solved within the ODT domain at the subgrid scale where a combination of stochastic and deterministic solutions allows the treatment of different processes governing the transport and chemistry for scalars and momentum. The solutions are implemented in parallel on the ODT domains that are embedded in the LES computational domain.

The MCRT implementation is validated within a Direct Numerical Simulation (DNS) using a variation of the Spherical Harmonics (SH) method in a non-homogeneous auto-ignition isotropic turbulence simulation. This configuration exhibits different modes of combustion

(from ignition kernels to premixed and non-premixed flames) and a complex coupling between turbulent transport and molecular processes, diffusion, reaction and radiation, under highly transient conditions.

The implementation of MCRT in the LES-ODT framework is performed for different cases of optical thickness and absorption coefficient dependency. Results of the simulations were compared to filtered density contours for the same conditions. The comparison of the different statistics shows a satisfactory agreement.

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Thermal Radiation Modeling using LES-ODT Framework
for Turbulent Combustion Flows

by
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DEDICATION

To my parents, sister and friends.

BIOGRAPHY

The author was born in Tunis, Tunisia in 1982. He successfully finished the preparatory cycle for engineering studies at the Faculté des Sciences de Tunis in 2004. He obtained his Bachelor and Master of Science degrees in Energy Engineering from the National Engineering School of Monastir in 2007 and 2008. He performed his master research work at The Petroleum Institute, Abu Dhabi in the United Arab Emirates. After his graduation, he worked as a Process and Safety Engineer for an Oil and Gas engineering company contracting with SONATRACH, Algeria. He started his graduate work at North Carolina State University towards a Doctor of Philosophy degree in Mechanical Engineering in 2010.

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Chapter 1 Introduction

1.1. Background

Turbulent combustion is one of the most challenging processes to model since it generally involves the simultaneous computation of three-dimensional fluid dynamics process, turbulent mixing, chemical kinetics, and convective and radiative heat transfer. The latter distinguishes itself from other processes by its fourth power dependence on temperature as well as the complexity of numerically solving the radiative heat transfer equation (RTE). Previous studies have shown that it is necessary to study the effect of radiative heat transfer to improve combustion simulation results [2, 54]. As an illustration, the fraction of the total heat transfer due to radiation grows with combustor size and attains prominence for gaseous firing at characteristic lengths of about 1 m. Similarly, in furnaces for drawing optical fibers involving temperatures near the softening point of 1900 K, cooling by thermal radiation is important and needed in the modeling of the overall process [95]. Experimental and computational research work has been performed toward understanding and estimating the radiation effect. A large part of the experimental research focuses on the most common fuels and the radiation characteristics of their generated flame like coal [59], methane [61], air aerosols [62], or on the NO_x generation linked to the radiation contribution [60]. Numerical approaches integrate radiation contribution within turbulent combustion models. Those models consist of the solution of a set of conservation equations for momentum and scalars, plus additional auxiliary equations. Various turbulent combustion radiation models are encountered in a very broad

range of applications [1] like industrial burners, furnaces, and internal combustion engines simulations.

1.2. CFD Models for Turbulent Combustion

Turbulent combustion modeling is by itself a challenging process. It can be seen as an interaction between chemistry and turbulence [1]. Turbulence is affected by combustion because of the strong flow accelerations through the flame front induced by heat release and because of the large changes in fluid properties associated with temperature changes [64]. In addition, the previously mentioned complexity of solving for radiation heat transfer makes the model choice as well as the assumptions crucial in the turbulent combustion simulation. In this context, there are three main CFD approaches to simulate turbulent flows: Reynolds averaged Navier-Stokes (RANS), Direct Numerical Simulation (DNS), and Large-Eddy Simulation (LES).

Table 1.1 shows different characteristics, used models, and applications of the three CFD approaches to simulate turbulent combustion [64]. The three approaches are presented in the following sections.

Table 1.1 Different approaches for modeling turbulent flows [64]

Approach	DNS	LES	RANS
Resolved Scales	All scales	Large Scales	Mean flow field
Mesh	Very fine	Fine	Coarse
Domain size	Smallest	Intermediate	Largest
Relative Computational Cost	Very expensive	Medium	Low
Physics Modeling	Instantaneous equations	Filtered equations	Averaged equations
Turbulence Models Used	None	For subgrid scales	For all scales
Applications	Research	Expanding industrial usage	Widely used in industry

1.2.1. Direct Numerical Simulation (DNS)

The foundations of DNS were laid at the National Center for Atmospheric Research [90]. It started by performing a 32^2 computation of isotropic turbulence at a Reynolds number of 35 based on Taylor microscale [91]. DNS does not actually adopt a turbulence model. It numerically solves Navier-Stokes equations including the whole range of spatial and temporal scale [65]. DNS time step should be sufficiently small to satisfy accuracy and stability requirements. CPU time for DNS simulations can reach millions of CPU hours where 99% of the computational cost goes to the calculation of small scale energy that contains only 20% of the total energy. The computational cost for DNS increases proportionally with Reynolds Number Re^3 [66] which also means that the more the flow is turbulent the larger CPU time will be required. Another drawback of DNS is that it is mainly restricted to canonical systems (e.g. combustion in a small cubic box) or to some laboratory flames. The use of DNS is not widespread in industry. It is considered as a research tool, and not a brute-force solution to the Navier-Stokes equations for engineering problems [90]. It is more considered to be a valuable tool to develop simpler RANS or LES models [67–69] or for validation purposes.

1.2.2. Reynolds-Averaged Navier-Stokes (RANS)

In the RANS model, instead of solving for the instantaneous flow-field like in DNS, the statistical evolution of the flow is sought. The RANS model is based on averaging the Navier-Stokes equations using the ensemble, time or spatial averaging technique and only solving for the mean flow field. This will make RANS save most of the time used in DNS to solve for the small scales. However, ignoring the small scale contribution will affect the accuracy of the

model. The time averaging in RANS of Navier-Stokes equations is done in order to compute the Reynolds stresses. The most recognized ways to do this are the Linear Eddy Viscosity models [94], Nonlinear Eddy Viscosity models [93], and the Reynolds Stress model (RSM). In the Linear Viscosity category, we can find Algebraic or Zero-equation models, which do not require the solution of additional equations, One-Equation models (solve one turbulent transport equation), usually the turbulent kinetic energy like the Spalart-Allmaras model [94], and finally, Two-Equation models: the k-epsilon [70, 72] and k-omega models [73] that became industry standard models and are commonly used for most types of engineering problems. The k-epsilon model as a two equations model will solve for two transport variables: the turbulent kinetic energy and its rate of dissipation allowing the accountability of the history of the flow (convection and diffusion of turbulent energy) [92]. This model is efficient for free-shear layer flows with relatively small pressure gradients. However, it is not performing so well with large adverse pressure gradients making the k-epsilon model not appropriate for inlets and compressors. A variation of the k-epsilon model is the Re-Normalization Group (RNG) methods that renormalize the Navier-Stokes equations to account for the effect of smaller scales of motion. RANS model is more widely used in industry due to the fact that it is not restricted to any geometry and that it requires fewer meshing in comparison to the other methods. Many other variations of RANS exist in literature like the Unsteady RANS [74-75], Time-dependent RANS [76-78], and Hybrid RANS [71] or attached eddy simulation (DES) [79].

1.2.3. Large-Eddy Simulation (LES)

The Large-Eddy Simulation (LES) approach is based on the idea that the large eddies depend on the geometry while the smaller ones are universal in their character and statistics. In LES, the governing equations are generated through a low-pass spatial filtering process. Below the filter scales, the unresolved contributions are modeled and closure terms have to be represented. These terms concern primarily non-linear contributions in the original unfiltered equations [48]. While RANS provides only averaged results, Large Eddy Simulation (LES) is able to predict instantaneous flow characteristics [56, 57]. Among the non-linear contributions to the transport equations of scalars and momentum, two closure issues are most prominent. The first is related to subgrid scale (SGS) transport of momentum, the so-called SGS stress, or scalars (SGS fluxes). The traditional approach to LES closure of SGS scalars or fluxes is based on gradient diffusion type approximations such as the Smagorinsky model [99] and the dynamic model [100]. Those gradient diffusion types of models rely on deriving the closure information for unresolved physics using resolved scales. Some of the limitations encountered for turbulent mixing and combustion are the fact that non-unity Lewis, Prandtl, and Schmidt number effects may not be adequately modeled with gradient diffusion and counter-gradient diffusion that has been observed in computational and experimental studies [101-103] when heat release is present. Another important challenge in the LES of turbulent combustion is the modeling of source terms of chemistry or radiation. These terms are generally non-linear and display a myriad of time scales associated with different rates of a complex mechanism, which can involve thousands of reactions and hundreds of species for practical fuels. Even more critical in the modeling of these source terms is their tight coupling with molecular transport

mechanisms, such as diffusion. From this coupling, thin structures such as flames that characterize the combustion process can impose even stringer requirements on the spatial resolution to resolve these structures. This coupling is also modulated by the temporally evolving flow field. Large scale mixing increases the number of interfaces separating reactants and products (in premixed flames) or the fuel and the oxidizer (in non-premixed flames) and affects scalar gradients in the flow field, thus directly affects the rates of molecular transport processes and their coupling with chemistry. While large scale mixing is expected to be coupled with small scale mixing and chemistry for a wide range of practical combustion problems, reasonable assumptions can be made to attempt to decouple, at least partially, these processes. The validity of the assumption will depend on the conditions in a particular regime in which combustion occurs. The Eddy-Dissipation Concept (EDC) or the Eddy Break-Up (EBU) model is among the earlier approaches based on the comparison of rates of mixing versus rates of chemistry. In addition, we can find approaches adapted from RANS like the Flamelet model, the Conditional Moment Closure (CMC) model, and the transported Filtered Density Function (FDF) model [48].

LES was shown to be efficient in applications related to gas turbine engines [58] and laboratory flames [59]. In terms of CPU time, LES is more costly than RANS and less costly than DNS. However, it solves the large-scale motion of the turbulence that contains most of the turbulence kinetic energy [1] and can be easily implemented in a multiscale framework like LES-ODT (One-Dimensional Turbulence) [82] or LEM-LES (Linear Eddy Model) [83] to account for the small scales. These models are design to overcome inherent assumptions about the combustion mode or regime. More importantly, they address the coupling between turbulent transport,

chemistry and molecular transport with reasonable fidelity. In LEM and ODT, the coupling of mixing and chemistry is predicted at all scales by resolving the turbulent advection, molecular transport, and chemistry in one-dimension in physical space.

Some other LES models are: the Smagorinsky-Lilly Model, the Dynamic Subgrid-scale Model, the RNG-LES model, Wall-adapting local eddy-viscosity WALE model, the Kinetic Energy Subgrid-scale model, and the Near-wall Treatment for LES models.

1.2.4. The Linear Eddy Model (LEM)

The Linear Eddy Model (LEM) was first developed by Kerstein [98]. It is a one-dimensional model for representing the flame structure in turbulent flows. The scalar distribution can be seen as a one-dimensional reference field between Kolmogorov scale and grid scales. In the LEM model, a series of re-arranging stochastic events take place. These events represent the effects of a certain turbulent structure of size l , smaller than the grid size at a location η_0 within the one-dimensional domain. This vortex distorts the η field obtained by the one-dimensional equation, creating new maxima and minima in the interval $[\eta_0, \eta_0 + \eta]$. The vortex size l is chosen randomly based on the inertial scale range while η_0 is obtained from a uniform distribution in η . The number of events is chosen to match the turbulent diffusivity of the flow. For flows whose turbulence properties known empirically, this approach has been proven useful; however, for general flows, we need a more advanced model [48].

1.2.5. The One-Dimensional Turbulence Model

The One-Dimensional Turbulence (ODT) model was also developed by Kerstein [104] as a refinement of the LEM method. ODT has full spatial and temporal resolution. It simulates turbulent transport and dynamic fluctuations in velocity and fluid properties that one might measure along a one-dimensional (1D) line of sight through an actual 3D turbulent flow [105]. Both ODT and LEM treat the turbulent advection and molecular diffusion similarly. ODT distinguishes itself from the LEM by the mixing model. In fact, it is a self-contained turbulence model that not only solves for scalars but also velocity vectors at subgrid scales, which provide information about the shear field, thereby a mechanism for driving the turbulence. Therefore, ODT is a more advanced model compared to LEM since it fully resolves simulations of pure mixing, chemical reaction, and related scalar processes in turbulence. Another advantage of ODT over LEM is that the distribution function in ODT is not predetermined, rather it advances in time and is computed based on the turbulent kinetic energy. Furthermore, ODT has an advantage of allowing affordable simulation of high Reynolds number turbulent flows over a full range of dynamically relevant length scales. Thus, ODT is a more robust and advanced model than LEM and provides a sound representation of turbulent advection, molecular diffusion, and chemical reaction. ODT can be either a stand-alone model or a subgrid closure model for LES [48].

The simulation by Echehki [106] of turbulent hydrogen-air flames is the first implementation of ODT for reacting flows. The results obtained using ODT show good agreement with experimental statistics of thermo-chemical scalars. Moreover, ODT predictions and

measurements of differential-diffusion effects show that those effects are important in the near-field and decrease as moving to downstream.

1.3. Motivation

As described earlier, some promising new methods like LES-ODT are overcoming the complexity of solving turbulent combustion problems by providing a better balance of accuracy and CPU/memory effort. Such methods like LES-ODT or LEM-LES are based on coupling large scales models with subgrid treatment of small scales. ODT model came as a refinement of the Linear Eddy Model (LEM) as the latter has some limitations such as not fully considering the local turbulent properties like turbulent intensity as well as its limitation to only flows whose turbulence properties are known empirically. The major difference between LEM and ODT lies in the probability distribution function (PDF). It is from the PDF that the maps representing turbulent eddies are sampled. While LEM is sampled as a fixed function form, the PDF in ODT is relevant with eddy time scale and local flow state [1]. Other advantages of the ODT model are:

- ODT has the ability to provide closure for both scalars and momentum; thus, one has the flexibility to choose the closure for scalars or momentum or both.
- In ODT, both momentum and scalars are coupled within ODT fine space and time resolutions which are comparable with DNS resolution; and this fine resolution coupling is very crucial near physical boundaries where the boundary conditions for both scalars and momentum are implemented.

- In the LEM-LES model, splicing method is used for large scale transport between different LEM segments. The LES-ODT formulation of Cao and Echehki [49] proposed an alternative representation for large scale transport based on ODT domains extending beyond a single LES cell, so the large scale transport along ODT domain direction can be resolved within ODT itself without interacting with other ODT domains or LES.

As stated earlier, not accounting for radiation will significantly alter the turbulent combustion model. Solution methods for radiative heat transfer were proposed [2, 3, 84]. Some of them overcome the complexity of the Radiative Transfer Equation (RTE), an integro-differential equation in five independent variables, by decomposing it to a set of relatively easier equations such as the Spherical Harmonics (SH) method [85], the Discrete Ordinates Method (DOM) [12, 86] which employs a discrete direction to complete numerical quadrature [13], and the Discrete Transfer Method (DTM) [87]. However, the advantage of relative simplicity provided by those models can be balanced by some limitations. The simplified SH at first order is for example not suitable for quantitative radiation modeling in jet flame configurations [88]. Another kind of methods to simulate radiative heat transfer is the Monte-Carlo Ray Tracing method (MCRT) [3]. The MCRT is a statistical method that can be applied to problems of arbitrary difficulty with relative ease. It also facilitates the treatment of turbulence-radiation interactions without any approximation [88]. On the other side, this method is computationally expensive, in terms of CPU time as well as memory.

1.4. Radiation Models

1.4.1. The Spherical Harmonics Method

The Spherical Harmonics (SH) method, was first introduced by Pierre Simon Laplace in 1782. It consists of the angular portion of a set of solutions to Laplace's equation represented in spherical coordinates and forming an orthogonal system [11]. The SH method provides an approximate solution of the Radiative Transfer Equation (RTE) by transforming it into a set of simultaneous, easier to solve, partial differential equations (PDEs) [3]. The approach was first proposed in 1917 by Jeans [27] in his work on radiative heat transfer in stars. A more detailed description of the method can be found in the monographs of Kourganoff [28], Davidson [29], and Murray's [30]. Cheng [14, 15] gave a P-N derivation of the general multidimensional case in Cartesian coordinates. Khan and Thomas [16] derived the P-N approximation to the radiative transport equation for a medium with a spatially varying refractive index. Modest and Yang [17, 18] developed the elliptic PDE formulation of the high-order P-N method for three-dimensional geometries. Bhuvaneswari and Wu [19] applied the low-order P-N approximation to transient radiative transfer in graded index media with pulse irradiation.

One of the challenges of the SH method is that low-order approximations are usually only accurate in media with near-isotropic radiative intensity. Increasing the order will slowly improve accuracy while rapidly increasing the mathematical complexity of the formulation. Some of these challenges are addressed by researchers in the neutron transport community including Gelbard [31], who introduced the simplified P_N -approximation, or SP_N . What makes SP_N more appealing is the fact that it can be accurate even at low orders, especially for optically thin media [3].

1.4.2. The Discrete Ordinate Method (DOM)

The discrete Ordinate Method (DOM) was developed 50 years ago by Chandrasekhar for analyzing radiation heat transfer within a plane-parallel medium while considering absorption, multiple scattering, and collimated incidence. Since then, the numerical method has been utilized to study radiative heat transfer in one- and multi-dimensional rectangular, spherical and cylindrical geometries [12]. Chandrasekhar [96] discretized the equation of transfer by considering a set of discrete directions according to a Gauss-Legendre quadrature [97]. The resulting system of ordinary-differential equations was solved analytically to yield highly accurate results from low-order approximations.

1.4.3. The Monte-Carlo Ray Tracing (MCRT) method

One of the other methods proposed for estimating the radiative contribution in turbulent combustion flows is the Monte Carlo Ray Tracing (MCRT) [3]. This method is different from the more widely used finite difference and finite element techniques as it does not numerically solve the Radiative Transfer Equation (RTE). It is actually a statistical method based on tracing the history of a statistically meaningful number of random photons. The MCRT originated in the 1940's [4] where it was used in an attempt to model neutron diffusion in fission material for the development of the atomic bomb during World War II. The first time it was used in a thermal radiation perspective was in the early 1960's by Fleck [5], and Howell and Perlmutter [6].

In the standard MCRT methods, each photon is traced from its point of emission to its point of absorption (at the wall, or where it leaves the domain) as described in figure 1.1. This approach

is, however, not efficient when the medium is optically thin and/or the walls are highly reflective [21-25] since the photon may exit without any contribution to the statistics. Modest [24-25] overcame this problem by applying the concept of energy partitioning where the energy is gradually attenuated along the photon path rather than being absorbed at a single point.

In general, the advantages of the MCRT method compared to numerical methods are the avoidance of numerically solving the RTE, the relative ease to deal with complex geometries, and the ability to handle the variation of the radiative properties with direction [3].

Figure 1.1 Photon emitting energy along its path until it is fully absorbed

As far as thermal radiation is concerned, MCRT is particularly suited to solve the RTE since energy travels in discrete parcels (photons) over relatively long distances along a straight path before interacting with matter [3].

On the other side, in the presence of a participating medium, ray tracing becomes more challenging since the participating medium plays a key role in many high-temperature

applications, such as combustion problems. A major difficulty is the evaluation of the optical thickness that a ray passes through, since the temperature and concentration fields tend to be highly inhomogeneous and turbulent. Moreover, similarly to any other statistical method, the efficiency of MCRT is related to the sampling. In fact, the accuracy of its prediction will depend primarily on the sample size. If the number of photons is too low, not enough physics will be captured. If it is too large, the CPU time will significantly increase.

Furthermore, the implementation of a MCRT method in multidimensional homogeneous problems can be limited by its demand for large computer storage space and its CPU time consumption [1]. Figure 1.2 shows that although the MCRT method requires more CPU time for simple problems, it actually presents a great convenience for more complex configurations.

1.5. Objectives

The scope of this research work is to integrate the radiative heat transfer contribution using the Monte-Carlo Ray Tracing (MCRT) method in the turbulent combustion LES-ODT framework. First, the radiation model is validated by implementing the MCRT method and the Spherical Harmonics SH-SP₁ model in a DNS simulation. Then, the MCRT model is implemented within the LES-ODT framework. Comparison between DNS and LES-ODT models with accounting the radiation effect in an isotropic turbulence autoignition case is performed.

Figure 1.2 Comparison of Monte Carlo and conventional solution techniques [3]

1.6. Outline

This dissertation is organized as follows: Chapter 2 introduces the DNS and LES-ODT formulation. Chapter 3 presents the formulation of the two used radiation models: the main one Monte Carlo Ray Tracing (MCRT) and the one used for the validation based on Spherical Harmonics (SH). Chapter 4 shows the validation results in a DNS simulation. Chapter 5 describes the formulation and implementation of the MCRT method in the LES-ODT framework and the simulation results with their comparison with MCRT in similar DNS cases. The last chapter provides general conclusions and recommendations for future work.

Chapter 2 DNS and LES-ODT Formulations and Numerical Implementation

The general formulation of both DNS and LES-ODT models is developed respectively by Mason [53] and Cao & Echehki [48]. In this chapter, the formulation will not account for the radiative heat contribution in the governing equations and will only present the general formulation. The radiative contribution is added in the implementation sections for DNS in section 4.2 and LES-ODT in section 5.3.

2.1. DNS Formulation

2.1.1. Objective

The objective of this paragraph is to establish the formulation of the DNS model. It consists of the numerical solution of non-dimensional transport equations for total mass, momentum, energy, and reactants mass fraction. Combustion is simulated by a single-step, second-order reaction with an Arrhenius reaction rate. The numerical formulation is characterized by third-order Runge-Kutta time integration, eleventh-order finite difference spatial derivatives schemes, and a fully consistent fractional-step method for the solution of the momentum equation. The DNS model is established under the ideal gas behavior and constant transport coefficients. The transport equations are solved using a low Mach number approximation where the effects of heat release are accounted for through variable density. The low Mach

number approximation is a solution to the presence of high-frequency acoustic waves that place severe restrictions on the size of the time step used to numerically integrate these equations [53]. When $Ma \ll 1$, such changes in density due to heat release are supported, but acoustic waves are not. The result is a system where density is only a function of temperature.

The governing equations for multicomponent reacting flows are, in general, very complex and numerical simulations of such flows typically require many simplifications. Governing equations in DNS for continuity, conservation of momentum, conservation of energy, conservation of species, and the equation of state are simplified under the following assumptions:

- Viscous stresses are given by Newton's law, i.e. the fluid is Newtonian.
- Bulk viscosity is zero (Stokes' hypothesis).
- Body forces are negligible.
- Specific heats C_p are constant and equal for all species.
- Molecular heat conduction is given by Fourier's law.
- Thermal conductivity is constant.
- Soret and Dufour effects are negligible. The Soret effect is mass diffusion due to temperature gradients and the Dufour effect is energy diffusion due to species gradients.
- All species behave as ideal gases.
- Thermal radiation is negligible.
- Mass diffusion velocities are given by Fick's law.
- Mass diffusivities D are the same for all species.

2.1.2. DNS Governing Equations

The non-dimensionalized governing equations under the low-Mach number assumption are expressed as:

Continuity equation:

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_i}{\partial x_i} = 0 \quad (2.1)$$

Momentum conservation equation:

$$\frac{\partial u_i}{\partial t} + u_j \frac{\partial u_i}{\partial x_j} = -\frac{1}{\rho} \frac{\partial P}{\partial x_i} + \frac{1}{\rho Re} \frac{\partial^2 u_i}{\partial x_i \partial x_j} + \frac{1}{3\rho Re} \frac{\partial}{\partial x_i} \left(\frac{\partial u_j}{\partial x_j} \right) \quad (2.2)$$

Energy conservation equation:

$$\frac{\partial T}{\partial t} + u_i \frac{\partial T}{\partial x_i} = \frac{1}{\rho Pr Re} \frac{\partial^2 T}{\partial x_i \partial x_i} + \omega \quad (2.3)$$

Mass conservation equation:

$$\frac{\partial Y_k}{\partial t} + u_i \frac{\partial Y_k}{\partial x_i} = \frac{1}{\rho Le Pr Re} \frac{\partial^2 Y_k}{\partial x_i \partial x_i} - \omega \quad (2.4)$$

where ω is the reaction rate and is expressed as:

$$\omega = Da \rho Y_F Y_O \exp \left[\frac{-\beta(1-T)}{1-\alpha(1-T)} \right] \quad (2.5)$$

where Y_F and Y_O are the fuel and oxidizer mass fractions.

Equation of State:

$$\rho \left[T \left(\frac{\alpha}{1-\alpha} \right) + 1 \right] = P_0 \quad (2.6)$$

These governing equations were developed using the following scaling:

$$x_i = \frac{(x_i)_d}{L_{ref}} \quad u_i = \frac{(u_i)_d}{U_{ref}} \quad \rho = \frac{\rho_d}{\rho_{ref}} \quad (2.7)$$

$$t = \frac{t_d U_{ref}}{L_{ref}} \quad p = \frac{p_d}{P_{ref} \frac{R_u}{W} T_{ref}} \quad T = \frac{T_d - T_{ref}}{T_{ad} - T_{ref}}$$

where the subscript “ d ” denotes the dimensional quantity and subscript “ ref ” indicates a reference or characteristic value.

In Eqs. (2.7), Ma is the Mach number, Pr is the Prandtl number, Le is the Lewis number, Re is the Reynolds number, Da is the Damkohler number, α is the non-dimensional temperature rise, and β is the non-dimensional activation energy. They are respectively defined as:

$$\begin{aligned} Ma &= \frac{U_{ref}}{(\gamma \frac{R_u}{W} T_{ref})^{1/2}} & Re &= \frac{\rho_{ref} L_{ref} U_{ref}}{\mu} & Pr &= \frac{c_p \mu}{\lambda} \\ Le &= \frac{\lambda}{\rho_{ref} C_p D} & \alpha &= \frac{T_{ad} - T_{ref}}{T_{ad}} & \beta &= \frac{E_a \alpha}{R_u T_{ad}} \end{aligned} \quad (2.8)$$

With the low-Mach number approximation, density changes due to heat release are allowed but acoustic waves are not. Pressure is non-dimensionalized using a thermodynamic scaling as opposed to a hydrodynamic scaling. This choice of scaling is important for the low Mach number approximation.

2.1.3. DNS Implementation

In the DNS model, non-staggered uniform grids are used in the formulation. This model allows all the dependent variables to be located at the same position. Therefore, momentum cells are collocated with the continuity cells eliminating the need for cell boundary interpolation. The pressure in the momentum equation is solved using the Poisson’s equation. Linearly implicit variation of third-order Runge-Kutta scheme is used to integrate the energy and the species

equations. Finally, spatial derivatives are computed using the fifth-order explicit finite-difference schemes.

Figure 2.1 DNS computational grid

The numerical implementation is done by computing the reaction rate term by using the most recent values of the temperature, density, and species mass fraction. Then, energy and species

equations are integrated. After the reaction rate term is integrated using the linearly implicit scheme, the density is obtained from the equation of state. Finally, the momentum equation is integrated in three steps: integrate the convection and diffusion terms to obtain the intermediate velocity field; solve the Poisson's equation for pressure; and update the velocity field. The flow chart of the numerical solution procedure adapted from Cao thesis [48] is presented below:

Figure 2.2 Flow chart of the numerical solution procedure

2.2. LES-ODT Formulation

2.2.1. Objectives

The objective of this paragraph is to establish the formulation of the LES-ODT model. It is mainly based on Cao and Echekki paper [49] and Cao thesis [48]. We can actually think about LES-ODT as a hybrid simulation of the large scales within LES and another computational domain embedded in the LES one referred as ODT. A 2D representation of the computational domain is shown in figure 2.3.

Both LES and ODT have different sets of governing equations but simulations are carried out simultaneously. ODT contains three key features to simulate turbulent combustion:

- A representation of 3D turbulent stirring with a stochastic process involving instantaneous mappings along each ODT 1D domain
- A representation of the molecular diffusion and reaction processes with deterministic solutions of unsteady reaction-diffusion transport equations along each ODT 1D domain
- A representation of the convection events along each ODT 1D domain.

The radiation effect is added in parallel to the molecular diffusion and reaction process representation within the second step.

2.2.2. Governing Equation

The LES governing equations solve only for the large scales. Since most of the turbulent combustion occurs in a scale smaller than the LES one, the small scale and reaction information are passed from ODT to LES after solving the ODT governing equations.

Figure 2.3 LES-ODT 2D grid layout

2.2.2.1. LES governing equations

The LES governing equations are obtained by performing the Favre-filtering on the transport equations for scalars and momentum in order to obtain the Favre-filtered velocity components $\bar{u}_1$, $\bar{u}_2$, and $\bar{u}_3$.

Continuity Equation:

$$\frac{\partial \bar{\rho}}{\partial t} + \frac{\partial \bar{\rho} \tilde{u}_j}{\partial x_j} = 0 \quad (2.9)$$

The filtered density $\bar{\rho}$ in LES does not account for the effect of heat release; therefore, it is obtained from the ODT solution.

Momentum Equation:

$$\bar{\rho} \frac{\partial \tilde{u}_i}{\partial t} = \frac{\partial}{\partial x_j} [\bar{\rho} (\tilde{u}_i \tilde{u}_j - \tilde{u}_i \tilde{u}_j)] + \left\{ -\frac{\partial \bar{P}}{\partial x_i} - \bar{\rho} \tilde{u}_j \frac{\partial \tilde{u}_i}{\partial x_j} + \frac{\partial \bar{\tau}_{i1}}{\partial x_1} + \frac{\partial \bar{\tau}_{i2}}{\partial x_2} \right\} \quad (2.10)$$

In Eq. 2.10, the viscous stress τ_{ij} is expressed as:

$$\tau_{ij} = \mu \left[\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \right] - \frac{2}{3} \mu \delta_{ij} \frac{\partial u_k}{\partial x_k} \quad (2.11)$$

where “ $\bar{}$ ” stands for LES filtered quantity and “ $\tilde{}$ ” for Favre-averaging expressed as:

$$\begin{cases} \phi = \tilde{\phi} + \phi'' \\ \tilde{\phi} = \frac{\bar{\rho} \phi}{\bar{\rho}} \end{cases} \quad (2.12)$$

The term $\bar{\rho} (\tilde{u}_i \tilde{u}_j - \tilde{u}_i \tilde{u}_j)$ in the momentum equation accounts for the subgrid stress.

2.2.2.2. ODT governing equations

The ODT governing equations are useful in the sense that they provide information on the physics of turbulence. They are obtained by writing the instantaneous transport equations for scalars and momentum along ODT 1D elements with contributions from LES resolved terms

in the continuity and momentum equations Eqs. (2.9) and (2.10). Those equations can be used for both variable and constant density flows.

Conservation of Momentum:

$$\rho \frac{\partial u_i}{\partial t} = \left[\frac{\partial}{\partial \eta} \left(\mu \frac{\partial u_i}{\partial x_\eta} \right) + \Omega_{u_i} \right] + \left\{ -\frac{\partial \hat{p}}{\partial x_i} - \rho \hat{u}_j \frac{\partial u_i}{\partial x_j} + \frac{\partial \hat{\tau}_{i1}}{\partial x_1} + \frac{\partial \hat{\tau}_{i2}}{\partial x_2} \right\} \quad (2.13)$$

Conservation of Energy:

$$\rho \frac{\partial T}{\partial t} = \left[\frac{1}{c_p} \frac{\partial P}{\partial t} + \frac{1}{c_p} \frac{\partial \hat{q}_\eta''}{\partial \eta} - \frac{1}{c_p} \sum_{k=1}^N h_k \dot{\omega}_k + \Omega_T \right] + \frac{1}{c_p} \left\{ -\rho \hat{u}_j \frac{\partial T}{\partial x_i} + \frac{\partial \hat{q}_1''}{\partial x_1} + \frac{\partial \hat{q}_2''}{\partial x_2} \right\} \quad (2.14)$$

Conservation of Mass Fraction:

$$\rho \frac{\partial Y_k}{\partial t} = \left[\frac{\partial J_{k,\eta}}{\partial \eta} + \dot{\omega}_k + \Omega_{Y_k} \right] + \left\{ -\rho \hat{u}_i \frac{\partial Y_k}{\partial x_i} + \frac{\partial \hat{f}_{k,1}}{\partial x_1} + \frac{\partial \hat{f}_{k,2}}{\partial x_2} \right\} \quad (2.15)$$

where $\mathbf{J}_{k,\eta}$ is defined as:

$$J_{k,\eta} = \left[\rho \left(D_k \frac{\partial Y_k}{\partial \eta} \right) \right] \quad (2.16)$$

In Eqs. (2.13)-(2.16), η denotes the spatial coordinate along the ODT direction. Terms with “ $\hat{}$ ” represent information passed from LES. The terms inside “[]” represent contributions from the resolved diffusion terms, the source terms, and the stochastic process along ODT 1D elements. However, non like ODT that solves along one direction, the stochastic contributions represent 3D transport events, including stirring, pressure scrambling, and contributions from fluctuating terms in the different variables. The stochastic contributions are therefore implemented as instantaneous stirring events through triplet maps, which are described in section 2.2. The molecular diffusion and reaction terms are obtained by solving the reaction-

diffusion transport equations and will be addressed in details in section 2.2.3. Terms inside “{ }” are the terms passed from LES that are not captured by the ODT 1D directions. These terms are crucial for momentum and scalar transport between ODT elements.

In Eqs. (2.13)-(2.15), Ω_{u_i} , Ω_T , and Ω_{Y_k} denote stochastically implemented subgrid scale turbulent transport. These terms are modeled with ‘eddy event’ in ODT. Molecular Diffusion

and chemical reaction are represented by $\frac{\partial}{\partial \eta} \left(\mu \frac{\partial u_i}{\partial x_\eta} \right)$, $\frac{1}{c_p} \frac{\partial \dot{q}_\eta''}{\partial \eta} - \frac{1}{c_p} \sum_{k=1}^N h_k \dot{\omega}_k$, and $\frac{\partial J_{k,\eta}}{\partial \eta} + \dot{\omega}_k$.

Those terms are 1D diffusive and can be numerically solved. Finally, $-\rho \hat{u}_j \frac{\partial u_i}{\partial x_j}$, $-\rho \hat{u}_j \frac{\partial T}{\partial x_i}$, and

$-\rho \hat{u}_i \frac{\partial Y_k}{\partial x_i}$ stand for the convection effect. Solving these terms involve node-convection at each ODT-node along with intra-node relaxation within each ODT domain.

2.2.3. The Molecular Diffusion and Reaction Processes in ODT

The molecular diffusion and reaction processes are characterized by small scales and therefore treated within the ODT simulation. The effect of the diffusion terms on the momentum equations is represented by the deterministic solution of 1D momentum transfer equation. Regarding scalar transport, 1D diffusion equations with reaction terms are solved. The diffusion terms are multiplied by a factor of 3 to account for the additional diffusion from the two directions that are normal to the ODT element.

The equations along ODT 1D elements can be obtained through decomposing Eqs. (2.13)-(2.15). Eqs. (2.18) and (2.19) are the equations solved to account for molecular diffusion and

reaction processes in ODT. The reaction rate terms are computed based on the instantaneous and local thermodynamic state of mixture.

Diffusion for the Velocity Components:

$$\rho \frac{\partial u_i}{\partial t} = 3 \frac{\partial}{\partial \eta} \left(\mu \frac{\partial u_i}{\partial x_\eta} \right) \quad (2.17)$$

Reaction-Diffusion for the Temperature:

$$\rho \frac{\partial T}{\partial t} = \frac{1}{c_p} \frac{\partial P}{\partial t} + \frac{3}{c_p} \frac{\partial q''_\eta}{\partial \eta} - \frac{1}{c_p} \sum_{k=1}^N h_k \dot{\omega}_k \quad (2.18)$$

Reaction-Diffusion for Mass Fractions:

$$\rho \frac{\partial Y_k}{\partial t} = 3 \frac{\partial J_{k,\eta}}{\partial \eta} + \dot{\omega}_k \quad (2.19)$$

2.2.4. Turbulent Transport in ODT

In order to capture turbulence in a 3D configuration and knowing that ODT solves only along one direction, each individual eddy turnover, an ‘eddy event’, is emulated through a stochastic process by applying a random, instantaneous mapping to an interval of the domain corresponding to the range of the stirring motion being represented. Many ways for mapping can be found in literature like the triplet map introduced by Kerstein [50] which was originally implemented for LEM [50, 51].

2.2.4.1. The triplet mapping

One of the characteristics of the triplet mapping is that it satisfies the physical requirements of mass, momentum and energy conservation. Therefore, all integral properties remain the same before and after applying the triplet mapping.

$$f(y) \equiv y_0 + \begin{cases} 3(y - y_0) & \text{if } y_0 \leq y \leq y_0 + \frac{1}{3}l \\ 2l - 3(y - y_0) & \text{if } y_0 + \frac{1}{3}l \leq y \leq y_0 + \frac{2}{3}l \\ 3(y - y_0) - 2l & \text{if } y_0 + \frac{2}{3}l \leq y \leq y_0 + l \\ y - y_0 & \text{otherwise} \end{cases} \quad (2.20)$$

where $f(y)$ is the mapping function, y_0 is the starting location of the eddy, and l is the length scale of the eddy.

The mapping is done in three steps:

- Step 1: the domain interval $[y_0, y_0 + l]$ over which mapping needs to be done, is compressed to a third of its length.
- Step 2: three copies of the compressed domain will replace the original domain interval. Thus, the local gradients are increased geometrically and the turbulence cascade is enhanced.
- Step 3: the middle copy is reversed to get a continuous profile of the properties.

This operation is carried out on all transported quantities in ODT and mimics the rotational folding effect inherent in turbulent flows. Figure 2.4 shows the schematic of the triplet mapping process on a linear profile.

For the numerical implementation of the triplet map, the number of discrete points spanning the eddy should be a multiple of 3. A schematic of a triplet map event of a vector $v(y)$ over a

segment that is discretized with 9 discrete points is shown in figure 2.5. The end points of the eddy stay at the same location during triplet mapping. Because triplet mapping with eddy size equal to 3 does not change the field, the next available eddy size that is a multiple of 3 is 6.

Figure 2.4 The triplet map procedure

In figure 2.5, the points before mapping are denoted as diamonds. The points after mapping are represented by circles. The dashed line represents the original line segment and the dotted line the one after triplet mapping.

In practice, the smallest turbulence scales should span a range that is larger than this minimum set of grid points (i.e. larger than 6 grid points).

Figure 2.5 The discrete triplet map [48]

2.2.4.2. Pressure scrambling model

In order to ensure the energy conservation, Wunsch & Kerstein introduced the kernel function $K(y)$ since applying a triplet map to the density field will change the total potential energy while leaving the total kinetic energy unchanged. $K(y)$ is added to the velocity field within every eddy event and is defined as:

$$K(y) \equiv y - f(y) \quad (2.21)$$

2.2.5. Large-Scale Convection in ODT

The most sensitive step in the LES-ODT simulation is how to model a 3D phenomenon while solving along one direction. Diffusion, convection, stirring, or radiation can be adequately integrated with ODT temporal and spatial resolutions along that same ODT direction. But information needs to be passed from other directions as well.

At the ODT nodes, if those nodes match with the LES ones, information from other directions is passed from LES. Gradients from the 3 ODT directions are summed and averaged. This step is called node convection. For the ODT elements that are not on the nodes, the intra-node relaxation equations are used.

The transport equations for the ODT node convection case are expressed as:

Convection for velocity:

$$\frac{\partial u_i}{\partial t} = -\hat{u}_j \frac{\partial u_i}{\partial x_j} \quad (2.22)$$

Convection for temperature:

$$\frac{\partial T}{\partial t} = -\hat{u}_j \frac{\partial T}{\partial x_j} \quad (2.23)$$

Convection for mass fraction:

$$\frac{\partial Y_k}{\partial t} = -\hat{u}_j \frac{\partial Y_k}{\partial x_j} \quad (2.24)$$

where $\hat{u}_j$ is the velocity solved by LES.

In the intra-node relaxation configuration, the governing equations are expressed as:

Convection for velocity:

$$\frac{\partial u}{\partial t} = -\kappa \hat{u} \frac{\partial u}{\partial \eta} \quad (2.25)$$

Convection for temperature:

$$\frac{\partial T}{\partial t} = -\kappa \hat{u} \frac{\partial T}{\partial \eta} \quad (2.26)$$

Convection for mass fractions:

$$\frac{\partial Y_k}{\partial t} = -\kappa \hat{u} \frac{\partial Y_k}{\partial \eta} \quad (2.27)$$

where η is the special coordinate along ODT direction and κ is set to 3 to simulate the effect from each of the three directions.

2.2.6. LES-ODT implementation

First, the ODT domain is initialized by filtering a fine grid initial solution like a DNS initial field. Next, the LES is initialized by filtering the ODT initialization. The ODT stirring, diffusion and reaction, and convection are solved in the ODT configuration in parallel to the LES solution with different time steps. Meanwhile, interpolation of LES velocity field to the ODT one is performed. The iteration is done as soon as the ODT time step reaches the LES one. The implementation algorithm is shown in figure 2.6 (adapted from Cao thesis [48]).

Figure 2.6 Flowchart for LES-ODT time step

Chapter 3 Radiation Models Formulation

3.1. Objective

The objective of this chapter is to introduce and formulate the two radiation models used in the simulations: the Monte Carlo Ray Tracing and the Spherical Harmonics methods. For both methods, we first overview the general concept and then we show which models were chosen and how they were adapted and formulated for the simulations. In the first section, spherical harmonics and the general P_N -approximation methods are introduced and followed by the mathematical formulation of the chosen variation of the SH methods to be used, i.e., the P_1 -approximation. In the following section, the most common models used in the MCRT for radiation introduced by Wang and Modest [20] are presented then followed by a justification of the MCRT model chosen in our simulation. The choice of the photon number is also justified in the same section.

3.2. The Spherical Harmonics Method

The classical radiative heat transfer equation RTE for the spectral radiative intensity I_η is given below. As mentioned earlier, it has 5 variables: three space coordinates and two direction coordinates:

$$\frac{dI_\eta}{ds} = \hat{\mathbf{s}} \cdot \nabla I_\eta = \kappa_\eta I_{b\eta} - \beta_\eta I_\eta + \frac{\sigma_{s\eta}}{4\pi} \int_{4\pi} I_\eta(\hat{\mathbf{s}}_i) \Phi_\eta(\hat{\mathbf{s}}_i, \hat{\mathbf{s}}) d\Omega_i \quad (3.1)$$

where, $\hat{\mathbf{s}}$ and $\hat{\mathbf{s}}_i$ are unit direction vectors, η is the wave number, I_η is the radiative intensity for a wavenumber η (the local value of I_η depends on non local quantities, direction $\hat{\mathbf{s}}$, and wavenumber η), κ_η is the spectral absorption coefficient or linear absorption coefficient, $I_{b\eta}$ is the Planck function, $\sigma_{s\eta}$ is the spectral scattering coefficient or linear scattering coefficient, β_η is the spectral extinction coefficient, Ω is the solid angle, $\Phi_\eta(\hat{\mathbf{s}}_i, \hat{\mathbf{s}})$ is the scattering phase function. This function corresponds to the probability that a ray from incident direction $\hat{\mathbf{s}}_i$ is scattered into direction $\hat{\mathbf{s}}$.

Figure 3.1 Enclosure for derivation of radiative heat transfer

In order to estimate the radiative heat transfer, we need to solve for the radiative intensity I_η . In the general P_N -approximation, this intensity is expressed as a two-dimensional generalized Fourier series as described in the next paragraph.

3.2.1. General Formulation of the P_N-approximation

In a gray media, we can express the RTE as follow:

$$\hat{s} \cdot \vec{\nabla}_{\tau} I + I = (1 - \omega)I_b + \frac{\omega}{4\pi} \int_{4\pi} I(\hat{s}') \Phi(\hat{s}_l, \hat{s}) d\Omega' \quad (3.2)$$

Eq. (3.2) is non-dimensionalized using the extinction coefficient, i.e. $d\tau = \beta ds$ [3].

In the P_N-approximation, the radiative intensity field at location $\mathbf{r}$ may be considered as the value of a scalar function on the surface of a sphere of unit radius, surrounding the point $\mathbf{r}$.

Figure 3.2 Schematic representation of Y_l^m on the unit sphere and its nodal lines [89]

Therefore, we can express the radiative intensity as a two-dimensional generalized Fourier series [3] as follow:

$$I(\mathbf{r}, \hat{s}) = \sum_{l=0}^{\infty} \sum_{m=-l}^l I_m^l(\mathbf{r}) Y_l^m(\hat{s}) \quad (3.3)$$

where $I_m^l(r)$ are position-dependent coefficients, and $Y_l^m(\hat{s})$ are spherical harmonics defined as:

$$Y_l^m(\theta, \psi) = \begin{cases} \cos(m\psi)P_n^m(\cos\theta), & \text{for } m \geq 0, \\ \sin(m\psi)P_n^m(\cos\theta), & \text{for } m < 0, \end{cases} \quad (3.4)$$

where θ is the polar angle describing unit direction vector $\hat{s}$, ψ is the azimuthal angle describing unit direction vector $\hat{s}$, and P_n^m are the associated Legendre polynomials.

Figure 3.3 Coordinates for the one-dimensional plane-parallel medium

The P_N -approximation is made by replacing $I(r, \hat{s})$ in Eq. (3.2), which depends on space and direction, by $1 + 3 + \dots + (2N + 1) = (N + 1)^2$ unknown I_l^m that are functions of space only. Therefore, Eq. (3.3) which depends on space and direction will be replaced by $(N + 1)^2$ equations that depend only on space.

N is the order of the method. The most often employed order is the P_l method which is also used in this research work and addressed in the next section.

3.2.2. The P_1 -approximation

In Eq. (3.3), if we set $l = 1$, then we get the lowest order of the SP_N , i.e. SP_1 . Therefore, we can express the radiative intensity as:

$$I(r, \hat{s}) = I_0^0 Y_0^0 + I_1^{-1} Y_1^{-1} + I_1^0 Y_1^0 + I_1^1 Y_1^1 \quad (3.5)$$

The corresponding Legendre polynomials can be found in literature [32]: $P_0^0 = 1$, $P_1^{-1} = -\sin\theta$, $P_1^0 = \cos\theta$, and $P_1^1 = P_1^{-1} = -\sin\theta$. Therefore, Eq. (3.5) can be written as:

$$I(r, \theta, \psi) = I_0^0 + I_1^0 \cos\theta + I_1^{-1} \sin\theta \sin\psi + I_1^1 \sin\theta \cos\psi \quad (3.6)$$

Knowing that the unit direction vector $\hat{\mathbf{s}}$ is expressed in spherical coordinates as:

$$\hat{\mathbf{s}} \begin{bmatrix} \sin\theta \cos\psi \\ \sin\theta \sin\psi \\ \cos\theta \end{bmatrix} \quad (3.7)$$

We note that $\hat{\mathbf{s}}$ components correspond to three of the $I(r, \theta, \psi)$ coefficients (figure 3.2) and therefore we can express the radiative intensity as a function a vector proportional to $\hat{\mathbf{s}}$ plus a scalar corresponding to I_0^0 :

$$I(r, \hat{s}) = a(r) + \mathbf{b}(r) \cdot \hat{\mathbf{s}} \quad (3.8)$$

where $a(r)$ is a scalar depending on position $\mathbf{r}$, and $\mathbf{b}(r)$ is a vector depending on position $\mathbf{r}$. Eq. (3.8) has four unknowns: the scalar a and the three components of $\mathbf{b}$. These unknowns can actually be related to physical quantities. One of the ways to solve for a and $\mathbf{b}$, is to substitute Eq. (3.8) into the two following equations: the incident radiation and the radiative heat flux.

Figure 3.4 Representation of $I(r, \theta, \psi)$ at location $\mathbf{r}$

Knowing that:

$$\int_{4\pi} \hat{\mathbf{s}} d\Omega = \int_0^{2\pi} \int_0^\pi \begin{pmatrix} \sin\theta \cos\psi \\ \sin\theta \sin\psi \\ \cos\theta \end{pmatrix} \sin\theta d\theta d\psi = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix} = \mathbf{0} \quad (3.9)$$

we have:

$$G(r) = \int_{4\pi} I(r, \hat{\mathbf{s}}) d\Omega = a(r) \int_{4\pi} d\Omega + \mathbf{b}(r) \cdot \int_{4\pi} \hat{\mathbf{s}} d\Omega = 4\pi a(r) \quad (3.10)$$

where $G(r)$ is the incident radiation at location $\mathbf{r}$.

Similarly, substituting Eq. (3.8) into the definition of radiative heat flux gives:

$$\mathbf{Q}_{rad}(r) = \int_{4\pi} I(r, \hat{\mathbf{s}}) \hat{\mathbf{s}} d\Omega = a(r) \int_{4\pi} \hat{\mathbf{s}} d\Omega + b(r) \cdot \int_{4\pi} \hat{\mathbf{s}} \hat{\mathbf{s}} d\Omega = \frac{4\pi}{3} \mathbf{b}(r) \quad (3.11)$$

since,

$$\int_{4\pi} \hat{\mathbf{s}} \hat{\mathbf{s}} d\Omega = \frac{4\pi}{3} \boldsymbol{\delta} \quad (3.12)$$

where $\boldsymbol{\delta}$ is the unit tensor.

After expressing a and $\mathbf{b}$ in terms of physical values, we can rewrite Eq. (3.8) as:

$$I(r, \hat{s}) = \frac{1}{4\pi} [G(r) + 3\mathbf{Q}_{rad}(r) \cdot \hat{s}] \quad (3.13)$$

If we assume linear-anisotropic scattering:

$$\Phi(\hat{s}_i, \hat{s}) = 1 + A_1 \hat{s} \cdot \hat{s}' \quad (3.14)$$

we can express the scattering term as follows:

$$\begin{aligned} \int_{4\pi} I(\hat{s}') \Phi(\hat{s}_i, \hat{s}) d\Omega' &= \frac{1}{4\pi} \int_{4\pi} (G + 3\mathbf{Q}_{rad} \cdot \hat{s}') (1 + A_1 \hat{s} \cdot \hat{s}') d\Omega' \\ &= G + A_1 \mathbf{Q}_{rad} \cdot \hat{s} = G + A_1 \mathbf{Q}_{rad} \cdot \hat{s} \end{aligned} \quad (3.15)$$

Now, we can substitute the expression of the radiative intensity derived from the P₁-approximation in Eq. (3.13) into the RTE Eq. (3.2):

$$\frac{1}{4\pi} \nabla_{\tau} \cdot [\hat{s} (G + 3\mathbf{Q}_{rad} \cdot \hat{s})] + \frac{1}{4\pi} (G + 3\mathbf{Q}_{rad} \cdot \hat{s}) \approx (1 - \omega) I_b + \frac{\omega}{4\pi} (G + A_1 \mathbf{Q}_{rad} \cdot \hat{s}) \quad (3.16)$$

If we multiply Eq. (3.16) by Y_0^0 and integrate over all solid angles, we have:

$$\nabla_{\tau} \cdot \mathbf{Q}_{rad} = (1 - \omega)(4\pi I_b - G) \quad (3.17)$$

Similarly, we can also multiply Eq. (3.16) by $\hat{s}$ and integrate over all directions to have:

$$\nabla_{\tau} G = -(3 - A_1 \omega) \mathbf{Q}_{rad} \quad (3.18)$$

Another representation of the set of P₁ equations can be found by combining Eqs (3.17) and (3.18) to eliminate the heat flux. Therefore, we need to apply divergence on Eq. (3.18) and divide it by $-(3 - A_1 \omega)$ to get an expression of $\mathbf{Q}_{rad}$. Then we substitute it in into Eq. (3.17) to find:

$$\vec{\nabla}_{\tau}^2 G - (1 - \omega)(3 - A_1 \omega)G + (1 - \omega)(3 - A_1 \omega)4\pi I_b = 0 \quad (3.19)$$

This equation has a form of Helmholtz equation. It is elliptical and has the same behavior as a Laplacian equation. Thus, the solution at any point influences and depends upon the solution at every other point.

Previous mathematical development showed that solving the radiative intensity under P₁-approximation reduces to solving for G in a Helmholtz type equation. As mentioned in the overview in section 1.4.1, the purpose of the SH approximations is to make the RTE easier to solve by simplifying it to equations that were treated in the literature or within the coding community.

After solving for G , we can find the radiative source term by using Eq. (3.17).

Furthermore, if we neglect scattering, Eq. (3.19) can be simplified to:

$$\vec{\nabla}_\tau^2 G - 3G = -12\pi I_b \quad (3.20)$$

and

$$\nabla_\tau \cdot \mathbf{Q}_{rad} = 4\pi I_b - G \quad (3.21)$$

3.3. Monte-Carlo Ray Tracing (MCRT) Schemes

MCRT is a popular method in combustion modeling where the participating medium is represented by discrete point masses, such as the flow field and scalar fields in PDF Monte Carlo methods. Each point mass is assigned an optical thickness. This optical thickness determines the energy exchanged between the photon/ray and the particle. In fact, it expresses the quantity of light removed from a beam by scattering or absorption during its path through a medium. The optical thickness τ is expressed as [26]:

$$\frac{I}{I_0} = e^{-\tau} \quad (3.22)$$

where I_0 is the intensity of radiation at the source, and I is the observed intensity after a given path.

Two approaches are described in Wang and Modest paper [20]: the Point Particle Model (PPM), in which the shape of particle is not specified and the Spherical Particle Model (SPM) in which particles are assumed to be spheres with specified radiation properties across their volumes. Also, in order to determine the region of influence of the ray (the discrete points involved in the energy exchange) two ways of modeling are proposed: the Line Ray Model (LRM) and the Cone Ray Model (CRM).

Based on those models, three different interaction schemes between rays and particles are considered, i.e., line-SPM (Sphere-Particle Model), cone-PPM (Point-Particle Model) and cone-SPM.

3.3.1. Ray Models

3.3.1.1. Line Ray Model (LRM)

The LRM is the standard model for ray tracing in continuous media. The ray is considered to be a volume-less line where energy propagates one-dimensionally. Using the Line Ray Model requires that the particles are volumetric and are not considered as points. As shown in figure 3.5, particles are assigned nominal volumes (gray boxes) to allow the energy exchange with the ray.

3.3.1.2. Cone Ray Model (CRM)

The CRM represents the physical aspect of a photon bundle consisting of millions of individual photons occupying a small solid angle. Energy is assumed to propagate axi-symmetrically along the cone, with its strength decaying in the radial direction normal to the cone axis.

Figure 3.5 Illustration of the (a) CRM and (b) LRM methods

3.3.2. Particle Models

In the case of a medium represented by discrete particles, the total energy is divided into a number of rays considered as photon bundles released into random directions and the emitted energy comes from every point in the volume [20]. However, if the particle optical thickness is high, some of the emitting energy cannot escape from the particle due to self-absorption.

Therefore, in case of optically thin particle, the self-absorption is negligible and the energy emitted from a particle is expressed as:

$$Q_{emi,i} = 4\kappa_{\rho,i}m_i\sigma T_i^4 \quad (3.23)$$

where $\kappa_{\rho,i}$ is the density-based Planck-mean absorption coefficient at particle temperature T_i , σ is the Stephan-Boltzmann constant, and m_i is the particle mass.

3.3.2.1. The Point-Particle Model (PPM)

In the PPM scheme, particles are treated as shapeless point masses with a nominal volume, which may be calculated from their thermo-physical properties such as pressure and temperature. Under the ideal gas assumption, the nominal volume can be calculated as:

$$V_{o,i} = \frac{m_i R T_i}{p_i} \quad (3.24)$$

where m_i is the mass carried by particle i , T_i is its temperature, p_i is its total pressure, and R is the gas constant.

To enforce consistency in the discrete particle representation of the medium, the overall nominal volume of all particles should be the same as the actual geometric expanse of the medium. As a consequence, one may regard the nominal volume of a particle as its real volume. The advantage of this scheme is that the particle only contains its original information and no assumptions are used to estimate properties around it like in the Sphere-Particle Model. However, the disadvantage is that it is difficult to determine the interaction of a photon ray with a volume without shape.

Figure 3.6 2D representation of the PPM scheme

3.3.2.2. The Sphere-Particle Model

In the SPM scheme, each point-mass has a sphere influence region Ω_i surrounding it. The mass m_i is distributed in the sphere according to a density profile defined as:

$$\hat{\rho}_i(x) = \begin{cases} \rho_{o,i} W_{3D} \left(\frac{|x-x_i|}{R_i} \right), & |x - x_i| < R_i \\ 0, & |x - x_i| \geq R_i \end{cases} \quad (3.25)$$

where $\mathbf{x}_i$ is the spatial location vector of the point-mass i , R_i is the point-mass sphere influence radius, $\rho_{o,i}$ is the nominal density expressed as $\rho_{o,i} = \frac{m_i}{V_{o,i}} = \frac{p_i}{RT_i}$, and W_{3D} is a spherically symmetric weight function which decays from the center along radial direction and satisfies the condition $\int_{\Omega_i} W_{3D} \left(\frac{|x-x_i|}{R_i} \right) dx = V_{o,i}$ so that the total mass in the influence region is equal to the point mass.

In the SPM scheme, larger sphere influence regions (larger R_i) lead to more particle overlap and spatial gradient may be smoothed out. While smaller R_i will decrease the particle volume and therefore affect the interaction with the rays.

One special case of the SPM scheme is when it is associated with the Constant Density Sphere (CDS) assumption, where the density is assumed to be constant inside the region of influence,

i.e. $W_{3D} = \frac{R_i}{|x-x_i|}$, and the particle volume is equal to its nominal volume. Therefore, the influence radius will be expressed as follow:

$$R_i = \left(\frac{3V_{o,i}}{4\pi} \right)^{1/3} \quad (3.26)$$

3.3.3. Ray-Particle Models

3.3.3.1. Line-SPM scheme absorption model

Under the CDS assumption, the contribution of particle i to the optical thickness that ray j passes through is expressed as:

$$\Delta\tau_{ij} = 2\rho_{o,i}\kappa_{\rho,i}\sqrt{R_i^2 - r_{ij}^2} \quad (3.27)$$

where $\rho_{o,i}$ is the nominal density, $\kappa_{\rho,i}$ is the density-based Planck-mean absorption coefficient at particle temperature T_i , R_i is the particle influence radius, and r_{ij}^2 is the distance from the center of particle i to ray j .

The total optical thickness that ray j passes through is the summation of the contributions from the individual particles it interacts with:

$$\tau_j = \sum_{i \in I_j} \Delta\tau_{ij} \quad (3.28)$$

where I_j denotes all particles intersected by ray j .

Figure 3.7 Line-SPM representation of a 2D grid

3.3.3.2. Cone-PPM scheme absorption model

In the Cone-PPM scheme, it is possible to let the particle interact as a point and therefore avoid assumptions like CDS. The total optical thickness that the ray passes through along its path S is expressed as:

$$\tau = \sum_{i \in I} \frac{\kappa_{\rho,i} W_i m_i}{\pi R_{c,i}^2} \quad (3.29)$$

where $\kappa_{\rho,i}$ is the density-based Planck-mean absorption coefficient at particle i with temperature T_i , $R_{c,i}$ is the local cone radius, I denotes all the particles enclosed by the cone, m_i

is the mass carried by particle i , and W_i is the particle weight expressed as $W_i = W_{2D} \left(\frac{r_i}{R_{c,i}} \right) = W_{2D}(r'_i)$ and W_{2D} is a normalized two-dimensional center-symmetric profile. A proposed Gaussian-like weight function is expressed as:

$$W_{2D}(r') = \frac{60}{7} \begin{cases} \frac{1}{3} - 4r'^2 + 4r'^3, & 0 \leq r' < \frac{1}{2} \\ \frac{4}{3}(1 - r')^3, & \frac{1}{2} \leq r' < 1 \\ 0, & r' \geq 1 \end{cases} \quad (3.30)$$

Figure 3.8 Cone-ppm scheme [20]

3.3.3.3. Cone-SPM scheme absorption model

In this case, the cone intersects the spheres centered on the particles. The amount of sphere volume inside the cone will affect the energy exchange. The total optical thickness passed through by a ray under CDS is estimated as:

$$\tau = \sum_{i \in I} \kappa_i R_{c,i} f_i \quad (3.31)$$

where $R_{c,i}$ is the local cone radius at location i , and f_i is a function defined as:

$$f_i = \frac{1}{\pi} \int_{r'_{min}}^{r'_{max}} W_{2D}(r') A'_i(r') dr' \quad (3.32)$$

where r'_{min} is the normalized closest distance, r'_{max} is the farthest normalized distance, and $A'_i(r')$ is a cylindrical shell around the cone axis with radius r' .

Figure 3.9 Cone-SPM scheme [20]

3.3.4. Photon Distribution and Generation

Photons having the same wave length can be grouped in sets of N energy bundles of equal energy. Each bundle consists of many photons of single wavelength carrying the same amount of energy E/N . The probability that any particular bundle has a wavelength between λ and $\lambda + d\lambda$ is given by the probability density function $P(\lambda)$. The fraction of energy emitted over all wavelengths between 0 and λ is then:

$$R(\lambda) = \int_0^\lambda P(\lambda) d\lambda = \frac{\int_0^\lambda E_\lambda d\lambda}{\int_0^\infty E_\lambda d\lambda} \quad (3.33)$$

$R(\lambda)$ also stands for the probability that any given energy bundle has a wavelength between 0 and λ . This is known as the Cumulative Distribution Function (CDF). Eq. (3.33) implies that if we want to simulate emission from a surface with N energy bundles of equal energy, then the fraction $R(\lambda)$ of those bundles must have wavelengths smaller than λ .

Now, if we consider a pool of random numbers equally distributed between the values 0 and 1. A fraction R of these random numbers has values less than R itself. So if we consider one single random number R_0 and proceed with the same logic, inverting Eq. (3.33), we can associate a wave length $\lambda(R_0)$ to R_0 , i.e., the wavelength corresponding to a cumulative distribution function of value R_0 , and we assign this wavelength to an energy bundle. Repeating this action many times, the fraction R_0 of all energy bundles will have wavelengths below $\lambda(R_0)$, since the fraction R_0 of all the random numbers will be below this value. Thus, in order to model correctly the spectral variation of surface emission using N bundles of equal energy, their wavelengths may be determined by picking N random numbers between 0 and 1 and inverting Eq. (3.33) [3].

3.3.5. Formulation

3.3.5.1. Heat Transfer Relations for Radiative Exchange between Surfaces

Assuming the absence of participating medium and neglecting refraction, the radiative heat flux leaving or going into a certain surface, using MCRT technique, is the difference between

the emission from the surface and the fraction of energy originally emitted from the surface at $\mathbf{r}'$, which eventually gets absorbed at location $\mathbf{r}$:

$$q(r) = \epsilon(r)\sigma T^4(r) - \int_A \epsilon(r')T^4(r') \frac{dF_{dA' \rightarrow dA}}{dA} dA' \quad (3.34)$$

where $q(r)$ is the local surface heat flux at location $\mathbf{r}$, $T(r)$ is the surface temperature at location $\mathbf{r}$, $\epsilon(r)$ is the total hemispherical emittance of the surface at $\mathbf{r}$, A is the surface area of the enclosure, and $dF_{dA' \rightarrow dA}$ is the generalized radiation exchange factor between surface elements dA' and dA .

$dF_{dA' \rightarrow dA}$ can actually be defined as the fraction of the total energy emitted by dA' that is absorbed by dA , either directly or after any number and type of reflections.

If the enclosure is not closed, i.e., had opening into space, some artificial closing surfaces must be introduced. Keeping the surface artificially closed is necessary to maintain the conservation of energy. The enclosure surface is then divided into J subsurfaces, and Eq. (3.34) reduces to:

$$Q_i = \int_{A_i} q_i dA_i = \epsilon_i \sigma T_i^4 A_i - \sum_{j=1}^J \epsilon_j \sigma T_j^4 A_j F_{j \rightarrow i} - q_{ext} A_s F_{s \rightarrow i}, \quad 1 \leq i \leq J, \quad (3.35)$$

where q_{ext} is the external energy entering through any opening in the enclosure, A_s is the area of the opening irradiated from external sources, and ϵ_j and T_j are suitable average values for each subsurface, i.e.,

$$\epsilon_j \sigma T_j^4 = \frac{1}{A_j} \int_{A_j} \epsilon \sigma T^4 dA \quad (3.35)$$

where ϵ_j is the total hemispherical emittance at j .

Figure 3.10 Path of the fraction of energy emitted by dA' (in red) and absorbed by dA

Unlike the heat flow rates Q_i that depend on all surface temperatures in the enclosure, the exchange factors $F_{i \rightarrow j}$'s either do not (gray surfaces) or depend only on the temperature of the emitting surface (non gray surfaces). It is accurate to assume that surface reflectances (and absorptances) are independent of temperature and therefore, based on the Second Law of Thermodynamics, the net exchange between two equal temperature surfaces must be zero. The summation rule and reciprocity also hold for exchange factors i.e.,

$$\sum_{j=1}^J F_{i \rightarrow j} = 1 \quad (3.36)$$

where $F_{i \rightarrow j}$ is the exchange factor from i to j .

$$\epsilon_i A_i F_{i \rightarrow j} = \epsilon_j A_j F_{j \rightarrow i} \quad (3.37)$$

A large statistical sample of energy bundles N_i is emitted from surface A_i , each of them carrying the amount of radiative energy:

$$\Delta E_i = \frac{\epsilon_i \sigma T^4 A_i}{N_i} \quad (3.38)$$

If N_{ij} of these bundles become absorbed by surface A_j either after direct travel or after any number of reflections [3], the exchange factor may be calculated from:

$$F_{i \rightarrow j} = \lim_{N_i \rightarrow \infty} \left(\frac{N_{ij}}{N_i} \right) \approx \left(\frac{N_{ij}}{N_i} \right)_{N_i \gg 1} \quad (3.39)$$

3.3.5.2. Random Number Relations for Surface Exchange

For each of the emitted bundles, the point of emission, direction of emission, and wavelength of emission need to be determined. However, if all surfaces of the enclosure are gray, then the wavelength of the bundle does not enter the calculations and its determination may be omitted [3].

- Points of Emission: the purpose of this paragraph is to express the emission points as a function of random numbers and geometry parameters. The total emitted energy from a surface A_j is written as follow:

$$E_j = \int_{A_j} \epsilon \sigma T^4 dA \quad (3.40)$$

rewriting the same expression with double integral:

$$E_j = \int_{x=0}^X \int_{y=0}^Y \epsilon \sigma T^4 dy dx = \int_0^X E'_j dx \quad (3.41)$$

where

$$E'_j(x) = \int_0^Y \epsilon \sigma T^4 dy. \quad (3.42)$$

Thus, if we apply Eq. (3.33), we find:

$$R_x = \frac{1}{E_j} \int_0^x E'_j dx \quad (3.43)$$

where R_x is the x -direction cumulative distribution function.

To find the x location of the emission point as a function of the random number R_x , this expression can be inverted:

$$x = x(R_x) \quad (3.44)$$

Once the x location is determined, we similarly apply Eq. (3.33), leading to an expression for the y -location of emission:

$$R_y = \frac{1}{E_j'} \int_0^y \epsilon \sigma T^4 dy \quad (3.45)$$

where R_y is the y -direction cumulative distribution function and

$$y = y(R_y, x) \quad (3.46)$$

As we can see in Eq. (3.46), the y location of the emission point not only depends on the random number R_y but also on the x location. In order to make the y location independent from the x one, the emissive power may be separated in x and y , i.e., if

$$E = \epsilon \sigma T^4 = E_x(x) E_y(y) \quad (3.47)$$

Eqs. (3.43) and (3.45) become:

$$R_x = \frac{\int_0^x E_x(x) dx}{\int_0^X E_x(x) dx} \quad (3.48)$$

and

$$R_y = \frac{\int_0^y E_y(y) dy}{\int_0^Y E_y(y) dy} \quad (3.49)$$

In the case of isothermal surface with constant emittance, we can write x and y as follow:

$$x = X R_x \text{ and } y = Y R_y \quad (3.50)$$

- Directions of Emission: the spectral emissive power for a given position and wavelength is:

$$E_\lambda = \int_{2\pi} \epsilon'_\lambda I_{b\lambda} \cos \theta \, d\Omega = \frac{1}{\pi} E_{b\lambda} \int_0^{2\pi} \int_0^{\pi/2} \epsilon'_\lambda \cos \theta \sin \theta \, d\theta \, d\psi \quad (3.51)$$

Similarly to the choice of the emission point coordinates in 2D, we write:

$$R_\psi = \frac{E_{b\lambda}}{\pi E_\lambda} \int_0^\psi \int_0^{\pi/2} \epsilon'_\lambda \cos \theta \sin \theta \, d\theta \, d\psi = \frac{1}{\pi} \int_0^\psi \int_0^{\pi/2} \frac{\epsilon'_\lambda}{\epsilon_\lambda} \cos \theta \sin \theta \, d\theta \, d\psi \quad (3.52)$$

or

$$\psi = \psi(R_\psi, x, y, \lambda) \quad (3.53)$$

where R_ψ is the azimuthal cumulative distribution function.

We note from Eq. (3.52) that unless the emittance changes across the surface, ψ does not depend on the emission location. However, ψ depends on the chosen wavelength unless spectral and directional dependence of the emittance are separable. Once the azimuthal angle ψ is found, the polar angle θ is determined from:

$$R_\theta = \frac{\int_0^\theta \epsilon'_\lambda \cos \theta \sin \theta \, d\theta}{\int_0^{\pi/2} \epsilon'_\lambda \cos \theta \sin \theta \, d\theta} \quad (3.54)$$

or

$$\theta = \theta(R_\theta, x, y, \lambda, \psi) \quad (3.55)$$

where R_θ is the polar cumulative distribution function.

Most surfaces tend to be isotropic so that the directional emittance does not depend on azimuthal angle ψ . Then:

$$R_\psi = \frac{\psi}{2\pi} \text{ or } \psi = 2\pi R_\psi \quad (3.56)$$

Also the choice of the polar angle becomes independent from the azimuthal angle and thus, for a diffuse emitter, Eq. (3.54) becomes:

$$R_\theta = \sin^2 \theta \text{ or } \theta = \sin^{-1} \sqrt{R_\theta} \quad (3.57)$$

Chapter 4 Radiation Simulation in DNS: Comparison of SH and MCRT

4.1. Objective

The objective of this chapter is to validate the two considered radiation models: the Monte-Carlo Ray Tracing and the Spherical Harmonics. The validation is made by comparing temperature profiles in a non-homogeneous autoignition with preheated oxidizer in isotropic turbulence using 3D Direct Numerical Simulation (DNS). The simulation is carried out using a constant density assumption resulting in the implementation of periodic boundary conditions in this statistically homogeneous mixture. We also assume a simple one-step reaction rate model with an Arrhenius form.

4.2. MCRT Implementation in the DNS Code

4.2.1. Formulation

The energy equation treatment in DNS was described in section 2.2. In order to account for the radiation effect, the radiation source term is added to the right hand side of Eq. (2.3) as follows:

$$\frac{\partial T}{\partial t} + u_i \frac{\partial T}{\partial x_i} = \frac{1}{\rho Pr Re} \frac{\partial^2 T}{\partial x_i \partial x_i} + \omega - \frac{1}{\rho C_p} \frac{\partial Q_{rad}}{\partial x_i} \quad (4.2)$$

where $\mathbf{Q}_{rad}$ is the radiation heat flux in the i^{th} direction. In dimensionless form, the reaction rate is expressed as:

$$\omega = Da \rho Y_F Y_O \exp \left[\frac{-\beta(1-T)}{1-\alpha(1-T)} \right] \quad (4.3)$$

where Da is the Damkohler number, β is the non-dimensional activation energy (the Zel'dovich number), and α is heat release parameter, which is a measure of the temperature rise during combustion. In order to estimate $\mathbf{Q}_{rad}$ in the DNS domain, a set of N_p photons is emitted at each time iteration (the photons are considered to have the same wavelength). The emission point and the direction are set as established in section 3.3.4. Each DNS particle will be considered to emit energy according to Plank's Law as follow:

$$Q_{emit,i} = 4K_{p,i}m_i\sigma T_i^{*4} \quad (4.4)$$

where $Q_{emit,i}$ is the energy emitted by the DNS grid i , m_i is the particle mass, $K_{p,i}$ is the absorption coefficient, T_i^* is the non-dimensionalized temperature at grid i , and $K_{p,i}$ is the non-dimensionalized absorption coefficient.

The total emitted energy is expressed as:

$$Q_E = \sum_i^{DNS \text{ grids}} Q_{emit,i} \quad (4.5)$$

where Q_E is the total emitted energy.

Each photon will initially carry an energy Q_{photon} . It is that initial energy that will be absorbed in the medium. In DNS, Q_{photon} is determined by the energy emitted by the closest particle to the photon as shown in the figure 4.1.

Figure 4.1 The Photon initial energy is equal to the emitted energy of the closest DNS particle

At each step, the photon exchanges energy with the DNS grids as shown in figure 4.2, according to a specific absorption model like those described in section 3.3.

After estimating the energy emitted and absorbed by each DNS grid, we can evaluate the radiation source term at grid i as:

$$\frac{\partial Q_{rad}}{\partial x_i} = Q_{emit,i} - Q_{abs,i} \quad (4.6)$$

where Q_{rad} is the radiation source term at the DNS grid i , $Q_{emit,i}$ is the emitted energy at the DNS grid i , and $Q_{abs,i}$ is the absorbed energy at the DNS grid i .

Figure 4.2 Photon exchanging energy with DNS grids along its path in 2D configuration

4.2.1.1. Temperature Non-Dimensionalization

Temperature is treated in the code as a dimensionless variable T^* as expressed below:

$$T^* = \frac{T_d - T_{ref}}{T_{ad} - T_{ref}} \quad (4.7)$$

where T_d is the dimensionalized temperature.

To get the dimensionalized temperature expression, we can reverse Eq. (4.7):

$$T_d = [T_{ref} + (T_{ad} - T_{ref})T^*] \quad (4.8)$$

T_{ad} and T_{ref} correspond respectively to T burned, T_b and T unburned, T_u . They are related by the non-dimensional temperature rise:

$$\alpha = \frac{T_b - T_u}{T_b} \quad (4.9)$$

So we can write T_b as:

$$T_b = \frac{T_u}{(1-\alpha)} \quad (4.10)$$

We need to determine the dimensionalized temperature in order to estimate the absorption coefficient as shown in the next section.

4.2.1.2. Absorption Coefficient

Some models found in the literature provide an estimation of the absorption coefficient where a fictitious nonscattering gray gas was studied [8]. The Planck-mean absorption coefficient can be expressed as:

$$\kappa_{p,d} = C_k(Y_p + \epsilon_y) \left[c_0 + c_1 \left(\frac{A}{T} \right)^1 + c_2 \left(\frac{A}{T} \right)^2 + c_3 \left(\frac{A}{T} \right)^3 + c_4 \left(\frac{A}{T} \right)^4 + c_5 \left(\frac{A}{T} \right)^5 \right] \quad (4.11)$$

where $\kappa_{p,d}$ is the (dimensionalized) absorption coefficient, coefficients; A and $(c_0 - c_5)$ are the water vapor values from [8] and presented in table 4.1, Y_p is the product mass fraction, ϵ_y is an arbitrary, small, positive threshold to ensure that κ_p is nonzero everywhere, and C_k is a non-dimensionalization term.

The water vapor parameters were taken to estimate the absorption coefficients shown in Table 4.1.

Table 4.1 Water vapor parameters to determine the absorption coefficient

Coefficient	A	c ₀	c ₁	c ₂	c ₃	c ₄	c ₅
Value	1000	-0.23093	-1.12390	9.41530	-2.99880	0.51382	-1.8684×10^{-5}

4.2.1.3. Boundary Conditions Treatment

The treatment of boundary conditions with radiation problems remains a formidable challenge even for the most trivial conditions. For example, in periodic boundary conditions any flux of physics, including rays of radiation, must be reinserted into the computational domain along the periodic plane. However, under optically-thin radiative conditions, the rays may track a long path and multiple insertions before they are absorbed.

Non-periodic boundary conditions may also be problematic. In general, we can only account for radiation coming from the computational volume; but, we cannot account for radiation emitted from outside of this control volume. For example, one obvious remedy for an isothermal boundary conditions is to allow the boundary to re-emit any amount that it absorbs such that there is no net radiative term contributes to an increase or a decrease in temperature. In the present formulation, we have adopted the following boundary conditions treatments in our computational code. In the case of periodic boundary conditions, the photon is reemitted from the other side of the boundary in accordance with the periodicity. In the non-periodic isothermal case, the photon is re-mitted from the same point it reached the boundary, to the opposite direction, with a different path from its original one. The non-periodic case

implementation is done considering that the temperature needs to remain fixed. In this case, it is as if another photon is emitted from the outer environment at the same location at the boundary to compensate the energy loss.

Figure 4.3 Photon path in case of periodic (left) and non-periodic (right) boundary condition

4.2.2. Algorithm

A schematic of the algorithm is shown in figure 4.4, which displays the main steps involved in MCRT for DNS.

Figure 4.4 Procedure graph for MCRT in DNS

First, a pseudo-random sequence is initialized at the beginning of the radiation subroutine in order to establish the random numbers used to determine the emission point and direction. For a Monte-Carlo simulation, usually a high number of photons is needed. This number can be fairly high for establishing an externally determined set of random numbers that will need to be stored and would require a prohibitive amount of computer storage. Another option is to rely on the computer itself to generate random numbers. The question will be then how random those numbers are since they are generated by a logic functioning device. Substantial research has been carried out on how to generate sets of sufficiently random numbers using pseudorandom number generators [3]. The randomness of those numbers depends on the quality of the generator as well as the choice of the starting point and should be tested by different “randomness tests” [4]. In this research work, to generate random numbers we first initialize the pseudo-random number sequence calling the FORTRAN intrinsic function `RANDOM_SEED` that initializes a sequence by restarting or querying the state of the pseudorandom number generator used by `RANDOM_NUMBER`. For each random variable, we call `RANDOM_NUMBER` that returns a single pseudorandom number or an array of pseudorandom numbers from the uniform distribution over the range $[0,1[$.

The runtime-library implements George Marsaglia's KISS (Keep It Simple Stupid) random number generator (RNG). This RNG combines:

1. The congruential generator with a period of 2^{32} ,
2. A 3-shift shift-register generator with a period of $2^{32}-1$,
3. Two 16-bit multiply-with-carry generators with a period of $597273182964842497 > 2^{59}$.

The overall period will then exceed 2^{123} [7].

The next step is to estimate the energy emitted by each particle, $Q_{emit,i}$'s, the dimensionalized temperature at each grid, $T_{d,i}$'s, and the absorption coefficients, $K_{p,i}$'s. The dimensionalized temperatures in all DNS grids are calculated as described in section 4.2.1.1. After calculating the dimensionalized temperatures, we can use the correlations found in the literature of the absorption coefficient $K_{p,i}$ at each grid. Both $T_{d,i}$ and $K_{p,i}$ values will establish the emitted energy, $Q_{emit,i}$, at each DNS grid. After setting all the emission parameters, a loop for the N_p photons is started in order to estimate the absorbed energy. This loop will emit each photon one by one. First, the starting point is determined according to Eq. (3.50) (The z -coordinate was established similarly to x and y). It is noted here that X , Y and Z will be equal to the number of DNS grids along directions x , y , and z . Also, since the random number generator selects numbers between $[0,1[$ where zero is included, a check was added in order to only keep coordinates between $]1, N_x[$, $]1, N_y[$, and $]1, N_z[$, where N_x , N_y , and N_z are the number of DNS grids along each direction. This implies that a photon can never be emitted from the boundaries. Similarly, the direction vector is set according to Eqs. (3.55) and (3.57). The conversion to Cartesian coordinates is done as follows:

$$\begin{cases} xdir = \sin(\theta) \cos(\psi) \\ ydir = \sin(\theta) \sin(\psi) \\ zdir = \cos(\theta) \end{cases} \quad (4.12)$$

Part of tracking the photon is to determine the two points where its path will meet the boundaries. A scalar product of the vector formed by those two points and the direction vector will determine which boundary the photon will reach as shown in figure 4.5.

If a photon reaches a boundary, in the case of periodic boundary conditions, the photon exits the boundary and is re-emitted from the opposite one. In the case of non-periodic boundary conditions, the photon is re-emitted from the same boundary with a different opposite direction. The emitted photon exchanges energy according to the selected absorption model like one of the models described in section 3.3. As soon as the photon energy dips below a certain value E_{p0} , the photon is eliminated. Finally, after all photons have emitted all their energy, the photons loop is closed and the radiation source term is calculated according to Eq. (4.6). The energy conservation equation is then updated.

Figure 4.5 The two points where the photon would meet the boundaries

4.3. P₁-approximation Implementation in the DNS code

4.3.1. Overview of the MUDPACK software

In literature and within the CFD community, many codes and packages solving elliptic partial differential equations are available. One of them is MUDPACK which is a FORTRAN multigrid software developed by John C. Adams [33] for elliptic partial differential equations. It consists of a package of portable subprograms which use multigrid iteration for solving real or complex elliptic partial differential equations. The solution regions are rectangles in two dimensions and boxes in three dimensions. The equations are automatically discretized using second-order finite differencing.

MUDPACK was downloaded from the Computational Information Systems Laboratory (CISL), University Corporation for Atmospheric Research website [34].

The choice of MUDPACK was motivated by the fact that it deals with parameterized PDEs, in a similar solution region to our configuration in 3D. Moreover, other advantages of MUDPACK are that multigrid iteration [38-43], combines classical iterative techniques, such as Gauss-Seidel line or point relaxation, with subgrid refinement procedures to yield a method superior to iterative techniques alone. By iterating and transferring approximations and corrections at subgrid levels, a good initial guess and rapid convergence at the fine grid level can be achieved. Multigrid iteration requires less storage and computation than direct methods for nonseparable elliptic PDEs [44] and is competitive with direct methods such as cyclic reduction [37, 45-47] for separable equations. In particular, three-dimensional problems can often be handled at reasonable computational cost.

The software is written in much the same format as the separable elliptic PDE package FISHPACK [35]. It extends the domain of solvable problems to include both separable and nonseparable PDEs.

4.3.2. Algorithm

The purpose of the SP_N approximation is to make the RTE easier to solve. The implementation of the SP_1 will basically consist of adapting the MUDPACK subroutines to the code. A special attention should be made to the fact that MUDPACK subroutines are written mainly in FORTRAN77 if the code is in a more updated version of FORTRAN.

The right hand side of Eq. (3.20) consists of the Planck function multiplied by a scalar coefficient. First, we need to dimensionalize temperature to estimate the Planck function. This is done the same way as in section 4.2.2. Then the MUDPACK subroutines are called in order to solve for the incident radiation. MUDPACK offers the possibility to set all the coefficients of the elliptic PDE that needs to be solved under the subroutine '*cof*'. The RHS is determined in the first step of the algorithm while the coefficients are determined according to Eq. (3.20). After getting the solution of the incident radiation in all the domain, we can find the radiation source term as in Eq. (3.21).

Figure 4.6 Procedure graph for implementing the SP-1 approximation

4.4. Initialization

4.4.1. Initialization of the Vector Field

The initialization of the turbulent velocity field for an isotropic state is performed in the associated Fourier space based on the random distribution of the turbulent kinetic energy. The analytical relation between the distribution of the turbulent kinetic energy and the wave number is described by the von Karman-Pao correction for near-dissipation scales and it is given in Eq. (4.14)

$$E(k) = A \frac{(u_{turb}^2)^5}{\varepsilon_d} \frac{(k/k_e)^4}{[1+(k/k_e)^2]^{17/6}} \cdot \exp\left(-\frac{3}{2}\alpha(k/k_d)^{4/3}\right) \quad (4.14)$$

where $A=1.5$, $\alpha=1.5$, u_{turb} is the root mean square velocity, ε_d is the dissipation number, k_e is the wave number of the most energetic scale and it represents the peak of the turbulent kinetic energy distribution, k_d is the wave number corresponding to the Kolmogorov dissipation scale and it represents the maximum level of dissipation [48].

4.4.2. Initialization of the Scalar Field

The initial scalar field is generated by initializing the mixture fraction field in the associated Fourier space with von Karman-Pao spectrum. The initial spatial distribution of the mixture fraction varies from pure fuel to pure oxidizer over a characteristic length scale, which is defined as:

$$L_c = \frac{\int_0^\infty Q_z(r) dr}{Q_z(0)} \quad (4.15)$$

where Z denotes mixture fraction and $Q_z(r)$ is defined as:

$$Q_z(r) = \langle Z''(x)Z''(x+r) \rangle \quad (4.16)$$

In this equation, $Q_z(r)$ is the two-point correlation function for the local mixture fraction fluctuation at a distance r . The length scale, L_c , measures the characteristic scale over which the mixture evolves from the fuel to the oxidizer, and vice versa. The resulting initial scalar field is characterized by fuel-centered and oxidizer-centered ‘blobs’ of fluid between which the mixture fraction changes.

A mean value of the mixture fraction is imposed to the fluctuating mixture field to yield an average value of 0.5, which is the stoichiometric mixture fraction. Moreover, the values of the mixture fraction are adjusted with a coefficient and a $\tanh$ profile is used to maintain the mixture field to be from 0 to 1. Figure 3.1 shows the initial mixture fraction field. In the present study, the mixture fraction range is from 0.15 to 0.85.

Figure 4.7 Initial mixture field

To initialize the temperature field, we use the energy balance equation assuming constant specific heats for both the fuel and the oxidizer:

$$Y_F h_F + Y_O h_O = Y_F h_{mix} + Y_O h_{mix} = (Y_F + Y_O) h_{mix} = h_{mix} \quad (4.17)$$

where Y_F is the fuel mass fraction defined by $Y_F = Z$, Y_O is the oxidizer mass fraction defined as $Y_O = 1 - Z$, h_F is the enthalpy of the fuel stream, h_O is the enthalpy of the oxidizer steam, and h_{mix} is the enthalpy of the mixture.

If we assume constant specific heat for both the fuel and the oxidizer, we have:

$$Y_F T_F + Y_O T_O = T_{mix} \quad (4.18)$$

where T_F is the temperature of the fuel steam, T_O is the temperature of the oxidizer stream, and T_{mix} is the temperature of the mixture.

Substituting the expressions of Y_F and Y_O , we get:

$$T = T_F + (1 - Z)(T_O - T_F) \quad (4.19)$$

In the stoichiometric condition, we have:

$$T_{st} = T_F + (1 - Z_{st})(T_O - T_F) \quad (4.20)$$

where T_{st} is the stoichiometric mixture fraction, which is equal to 0.5, and Z_{st} is the corresponding temperature at the stoichiometric mixture fraction prior to the combustion onset.

Because the oxidizer is preheated relatively to the fuel to provide a mechanism for the autoignition of the mixture, the stoichiometric temperature is set to zero. Therefore, Eq. (4.20) is reduced to [48]:

$$T_F = -T_O \quad (4.21)$$

Figure 4.8 Initial temperature field

4.5. Absorption Model

Radiation absorption models are presented in detail in section 3.3. Two parameters are taken in consideration in order to determine the most appropriate absorption model to be used : the CPU time and the model performance. The Cone schemes have not been explored due to the required high CPU time. A trial was made for this method, and one DNS iteration lasted only several hours and therefore was not considered in this research work. Wang and Modest [20] presented and discussed the three absorption models and showed similar results for radiative heat transfer modeling.

In this research work, one approach is proposed to model the line-SPM scheme. The idea consists of moving a sphere along the ray path (or the cone axis in case the cone scheme is adopted). As shown in figures 4.9 and 4.10.

Figure 4.9 Constant radius moving sphere configuration

If the desired absorption model is line-SPM, then the sphere will have a constant radius equal to the particles' nominal volume one (assuming the Constant Density Sphere condition where all sphere surrounding particles will have the same radius as described in section 3.3.3). If a particle is inside the sphere, then the distance between it and the ray, shown as d in figure 4.9, is equal to or less than the particle sphere radius R_i and, therefore, that particle is involved in the energy exchange. If the desired absorption model is cone based, as shown in figure 4.10, then the sphere will have variable radius starting from zero at the emission point and increasing according to the user preference to set the cone opening. The increasing moving sphere will constitute a cone along its path.

Figure 4.10 Increasing radius moving sphere configuration

In the sphere approach, attention should be made to overlapping. A particle involved in one exchange should be removed from any further exchange to avoid being included one more time in the progressing sphere.

4.6. Determination of the Number of Photons

As introduced in section 1.4.3, the photon number is crucial in MCRT simulations. Too few photons are not enough to detect the problem physics and contribute to increase the statistical errors. Too many photons will dramatically increase the CPU time.

Radiation source terms are studied for simulations with different photon numbers. The contours' ranges are set to be from the maximum and minimum values for each case in order to show the considerable difference of the radiation source terms ranges depending on photon numbers.

Figure 4.11 Radiation source term 3D contour for (a) 10^5 , (b) 10^4 , and (c) 10^3 photons

Figure 4.12 Radiation source term contour at the center x slice for (a) 10^5 , (b) 10^4 , and (c) 10^3 photons

Figure 4.13 Radiation source term contour at the center x slice for (a) 10^5 , (b) 10^4 , and (c) 10^3 photons

We also know intuitively that the radiation source term shows the same patens as temperature since it can be considered as a distribution of energy. Therefore, the temperature contour for

the no-radiation case at the same time step is shown in figure 4.14 in order to compare the behavior of the radiation source term in accordance with temperature for different photon numbers.

Figure 4.14 No radiation temperature contour (a) 3D, (b) x center face, and (c) y center face

Isosurfaces contours at 25% of the maximum emitted energy are shown in figure 4.15 to display the volume filling for different photon number cases.

Figure 4.15 Isosurfaces for (a) 10^5 , (b) 10^4 , and (c) 10^3 photons

It is only for the 10^5 photons case where we can see the same trends for temperature and radiation source term. In figures 4.11-4.13, the case of 10^4 photons shows contours that are not similar to the temperature ones in figure 4.14 and, therefore, can-not be considered although its fast CPU time. We can also see from figure 4.15 that the 10^5 photons simulation has a better reaching of the boundaries that constituted a major convergence criteria while running simulations. While it is hardly the case for the 10^4 configuration and almost never the case for the 10^3 one.

The same number of photon also showed a consistent validation with the Spherical Harmonics method presented in the following section. Therefore, it can be concluded that 10^5 is a good compromise between reasonable CPU time and good representation of the physics.

4.7. Simulation results

The numerical simulation is made by adopting the following models:

- The 3D non-dimensional transport equations are solved using a low-Mach number DNS code.
- 3rd order Runge-Kutta method is used for temporal integration and 9th-order explicit scheme is used for spatial differentiation.
- A single- step, 2nd order, irreversible reaction mechanism is used for chemistry.
- The scalar and velocity fields are initialized using Von Karman-Pao spectrum and the oxidizer is preheated.
- Periodic boundary conditions are imposed in all directions.
- The radiation absorption model is the line-SPM.

Moreover, the simulation parameters are shown on table 4.2.

Tracking the maximum temperature T_{max} can show the radiation influence on the solution region. Intuitively, radiation will contribute to the energy exchange by favoring heat transfer from hot regions to cold regions and therefore by reducing the maximum and minimum temperatures.

Table 4.2 DNS simulation parameters

Parameter	Value
Domain size	3.6 x 3.6 x 3.6
Grid points	129 x 129 x 129
Time step	0.001
Re	6000
Pr	0.7
Density	Constant

The T_{max} profile as a function of time is shown in figure 4.16 for different cases: no radiation, radiation using SH method (right), and radiation using MCRT method (left).

As we can see from figure 4.16, two main phases occur in the radiation case:

During phase 1 in figure 4.16, we observe a first ignition peak where reaction occurs but quickly gets attenuated. This can be explained by the fact that at early time steps, mixing is not well established yet. Thus, radiation prevails right after chemistry starts and tries to equilibrate temperature. The temperature contours at the center slice of the cube are shown in figure 4.17 at iteration 50 for the no radiation case, SH, and MCRT.

We can notice the similarity of the temperature contours in all 3 cases but with different values of temperature. The no radiation case has greater maximum and minimum values than the radiation models and show more contrast in the temperature. While both radiation models show a more homogenized temperature profile. This is explained by the fact that radiation favorites energy transfer and therefore tends to equilibrate the energy distribution.

Figure 4.16 $T_{\max}$ profile as a function of time for (a) no radiation, (b) MCRT, and (c) SH

Figure 4.17 Temperature contour at the center slice $x = 1.8$ for (up) no radiation, (Right) MCRT, and (Left) SH at iteration 50

The temperature contours at the center of the cube are shown in figure 4.18 at the end of phase one where the reaction will start to take over after more mixing is established.

During phase 2, shown in figure 4.16, after some time steps, mixing increases as turbulence grows which allows more reaction. This corresponds to the second temperature increase in phase two. After some time, when reactants are more and more consumed, radiation prevails again and stabilizes temperature. The temperature contour profile is shown in figure 4.19 at the center of the cube at iteration 1000, in which temperature is stabilized.

Figure 4.18 Temperature contour at the center slice $x=1.8$ for (up) no radiation, (Right) MCRT, and (Left) SH at iteration 100

We can also notice, like in phase 1, that the temperature profile is homogenized in both radiation models as compared to the no radiation case.

4.8. Conclusion

Both methods, the statistical (MCRT) and analytical one (SH), showed the same behavior: qualitatively by displaying the same radiation effect on the domain and its competition with chemistry and quantitatively by reaching almost the same values at similar time steps.

One main difference can be seen in the T_{max} profile in figure 4.16 at the transition period in the second temperature increase. This can be explained by the fact that the SP_1 consists of many PDEs where each can have a dominant behavior at different times.

Figure 4.19 Temperature contour at the center slice $x = 1.8$ for (up) no radiation, (Right) MCRT, and (Left) SH at iteration 1000

Chapter 5 MCRT simulation in LES-ODT

5.1. Objective

The objective of this chapter is to apply the established MCRT radiation model in the LES-ODT framework and validate the results with DNS. Absorption and emission models, photon number, and other parameters have been set up for DNS in Chapter 4. They will be adapted to LES-ODT. In this chapter LES-ODT and DNS simulations of non-homogeneous autoignition in isotropic turbulence are conducted using the MCRT method to simulate radiation. The main simulation parameters are shown in table 5.1.

Table 5.1 Main simulation parameters for both LES-ODT and DNS

Parameter	Value
Domain size	3.6 x 3.6 x 3.6
Grid points	129 x 129 x 129
Time step	0.01
Re	6000
Pr	0.7
Density	Constant
Absorption model	Line-SPM
Photon emission	Closest particle

5.2. MCRT for LES-ODT overview

The same concept of emitting a photon with certain energy until that energy is dissipated also is applied in the LES-ODT formulation. Temperature is integrated in the ODT subgrid scale along with reaction and diffusion. The radiation source term is added to the reaction-diffusion operator for the temperature transport equation in ODT in Eq. (2.19) as follow:

$$\rho \frac{\partial T}{\partial t} = \frac{1}{c_p} \frac{\partial \dot{q}_\eta''}{\partial \eta} - \frac{1}{c_p} \sum_{k=1}^N h_k \dot{\omega}_k - \frac{1}{\rho c_p} \nabla \cdot \mathbf{Q}_{rad} \quad , \quad (5.1)$$

where $\mathbf{Q}_{rad}$ is the radiation source term.

However, the ODT presents two main challenges from the DNS model. First, the DNS grid fills the entire volume while ODT has a lower number of grids and, therefore, fills less volume as shown below in figure 5.1.

Figure 5.1 DNS and LES-ODT distribution

Second, while DNS has no preferred direction, ODT can only treat scalars along one direction.

Many suggestions were discussed in order to overcome this issue:

- **Consider the ODT domains in one direction as a slab:** which allows us to average the ODT scalars in a thin 3D slab centered on an ODT direction.

Figure 5.2 Example of slabs in the three different directions

Each slab consists of a box having two sides equal to an LES grid in length and another thin side equal to an ODT grid in width. There are three different kind of slabs according to the three different spatial directions as shown in figure 5.2.

- **Build a DNS like grid:** previous work done by Shekhawat and Echehki [9] established a DNS-like grid generated from the ODT one as described in figure 5.3.

Figure 5.3 A 2D equivalent of DNS-like field generation from the ODT field

The scalar variable value at a point inside a LES grid is found by averaging the ODT variables embedded in the same LES grid. Applying this to each LES grid gives us a DNS-like scalar field. However, such an approach requires a DNS-like resolution, an attribute that is undesirable and runs counter to the potentially less-memory intensive LES-ODT approach.

In this research work, photons emit energy equal to the energy emitted by the closest particle and one of the absorption models described in section 3.3 will be considered. Both line-SPM and cone-PPM adaptation to LES-ODT is shown in figure 5.4.

Figure 5.4 Cone-SPM (right) and line-SPM (left) in LES-ODT framework

Figure 5.5 Temperature configuration in ODT and Cartesian coordinates

5.3. MCRT implementation in the LES-ODT code

Most of the steps in LES-ODT algorithm are similar to the DNS one as shown in figure 5.6. The main difference is the conversion of the ODT temperature, expressed according to a domain based reference, to Cartesian coordinates. In the code, the ODT temperature is established as a function of two variables: the ODT domain and the ODT grid number on the same domain as shown in the figure 5.5.

The temperature at the blue ODT grid shown in figure 5.5 is established as $\phi(3,5)$ where 5 stands for the ODT domain number and 3 stands for the grid number on that domain. A subroutine was developed in order to convert temperature to Cartesian reference. It is much more convenient to have temperature expressed in Cartesian coordinates as it will enable a more straightforward use of geometry and trigonometry.

5.4. Initialization

The initialization of the LES-ODT flow field consists of initializing velocity vectors, temperature, and the fuel and the oxidizer mass fractions in all three directions, x , y , and z in accordance with the DNS one. First, the initial flow field is generated using DNS employing the steps presented in section 4.4. Second, the flow field from DNS is interpolated to the ODT field via tri-linear interpolation. Finally, the initial LES flow field is obtained from filtering the ODT flow field using the box filter [48].

Figure 5.6 Procedure graph for MCRT in LES-ODT

5.5. Absorption model

The same absorption model used for DNS is used in the LES-ODT simulation in order to ensure consistency in the validation between both frameworks. The adopted Line-SPM scheme is detailed in section 3.3.3. The main difference between LES-ODT and DNS is that the particles' spheres nominal volume is different. In fact, in order to ensure the consistency of the model, the sum of all the particles' volumes should be equal to the total volume [20].

A sanity check was made toward verifying if the absorption model will show consistent results. A simulation was ran with constant initial temperature equal to 0.1 and no chemistry. In this simulation, no thermal energy is created by chemical reaction and radiation will constitute the only one energy transfer way. Radiation source term profile and range are shown in figure 5.7.

Figure 5.7 Radiation source term for uniform initial temperature and no chemistry simulation

For constant initial temperature and no chemistry, we note that the radiation source term has very small value. This result can be physically interpreted by the fact that there is almost no radiation transfer. Thus, this result shows that the energy emitted was absorbed in a consistent way within the volume and comfort the idea of using the line-SPM scheme for LES-ODT.

5.6. Determination of the Number of Photons

We may intuitively assume that the same number of photon can be used since we are working on the same configuration as in DNS. However, the sphere centered on the ODT particle is larger than the DNS one as shown in section 5.5, which may affect the absorption process and potentially requires less photons for the MCRT simulation. However, we want to keep the same photon number as in the DNS simulation since we want to compare LES-ODT and DNS results on the same basis. The following paragraph will show that consistent results are achieved by a 10^5 photons configuration.

5.7. Simulations

The purpose of this section is to qualitatively evaluate the radiation model. Three cases are treated: 1) a main case whose simulation parameters are shown in table 5.1, 2) a simulation with thinner optical thickness, and 3) a non-reacting case. Three different outputs are made for three different time steps. The first iteration that can constitute a reference to monitor the evolution of the radiation effect, the 50th iteration, which corresponds to the onset of autoignition, and finally the 200th iteration where the chemical reaction is fully established.

The temperature and radiation source terms contours at the first iteration are shown in figures 5.8-5.25.

Figure 5.8 Temperature 3D contours for (a) no-radiation, (b) LES-ODT, and (c) DNS at iteration 1

Figure 5.9 Temperature contours at the $x=1.8$ plane for (a) no-radiation, (b) LES-ODT, and (c) DNS at iteration 1

Figure 5.10 Temperature contours at the $y = 1.8$ plane for (a) no-radiation, (b) LES-ODT, and (c) DNS at iteration. 1

Figure 5.11 Radiation source term 3D contour for (a) LES-ODT and (b) DNS at iteration 1

Figure 5.12 Radiation source term contour at $x=1.8$ plane for (a) LES-ODT and (b) DNS at iteration 1

Figure 5.13 Radiation source term contour at $y=1.8$ plane for (a) LES-ODT and (b) DNS at iteration 1

Figure 5.14 Temperature 3D contours for (a) no-radiation, (b) LES-ODT, and (c) DNS at iteration 50

Figure 5.15 Temperature contours at the $x = 1.8$ plane for (a) no-radiation, (b) LES-ODT, and (c) DNS at iteration 50

Figure 5.16 Temperature contours at the $y = 1.8$ plane for (a) no-radiation, (b) LES-ODT, and (c) DNS at iteration 50

Figure 5.17 Radiation source term 3D contour for (a) LES-ODT and (b) DNS at iteration 50

Figure 5.18 Radiation source term contour at $x=1.8$ plane for (a) LES-ODT and (b) DNS at iteration 50

Figure 5.19 Radiation source term contour at $y=1.8$ plane for (a) LES-ODT and (b) DNS at iteration 50

Figure 5.20 Temperature 3D contours for (a) no-radiation, (b) LES-ODT, and (c) DNS at iteration 200

Figure 5.21 Temperature contours at the $x = 1.8$ plane for (a) no-radiation, (b) LES-ODT, and (c) DNS at iteration 200

Figure 5.22 Temperature contours at the $y = 1.8$ plane for (a) no-radiation, (b) LES-ODT, and (c) DNS at iteration 200

Figure 5.23 Radiation source term 3D contour for (a) LES-ODT and (b) DNS at iteration 200

Figure 5.24 Radiation source term contour at $x=1.8$ plane for (a) LES-ODT and (b) DNS at iteration 200

Figure 5.25 Radiation source term contour at $y=1.8$ plane for (a) LES-ODT and (b) DNS at iteration 200

Figures 5.8-5.25 show that for both temperature and radiation source term contours, the same trends are observed between the cases where there is no radiation and where radiation is simulated. For both LES-ODT or DNS, the hot and cold spots are located at the same zones. However, we note that maxima and minima are higher for the no-radiation case than the DNS and LES-ODT cases. In fact, radiation contributes to the energy transfer from the warmer sub-volumes to the cooler ones and, thus, contributes to the temperature homogeneity in the domain.

In addition, looking at the LES-ODT and DNS contours, we can see a qualitative similarity in the trends between both cases. However, quantitative values can-not be evaluated from the plots as errors caused by filtering may occur. The next section will be dedicated to the quantitative study of both cases by evaluating errors between the two methods and the turbulence-radiative interaction.

The next step is to consider an optically thinner medium. Optical thickness can be associated with a dimensionless parameter κL , where L is the turbulent length scale and κ is the absorption coefficient. In this simulation, we considered this parameters 10 times less than the one used in the previous one. Results are compared with the previous case by showing the plots at the same range in both cases. Temperature and radiation source term contours for the optically thinner medium are shown in figures 5.26-5.31 at the 50th iteration.

Figure 5.26 Temperature 3D contour at iteration 50 for (a) DNS (b) optically thicker DNS, (c) LES-ODT, and (d) LES-ODT optically thicker LES-ODT

Figure 5.27 Temperature contour at $x=1.8$ plane for (a) DNS (b) optically thicker DNS, (c) LES-ODT, and (d) LES-ODT optically thicker LES-ODT at iteration 50

Figure 5.28 Temperature contour at $y=1.8$ plane for (a) DNS (b) optically thicker DNS, (c) LES-ODT, and (d) LES-ODT optically thicker LES-ODT at iteration 50

Figure 5.29 Radiation source term contours at iteration 50 for (a) DNS (b) optically thinner DNS, (c) LES-ODT, and (d) LES-ODT optically thinner LES-ODT

Figure 5.30 Radiation source term contour at $x=1.8$ plane for (a) DNS (b) optically thinner DNS, (c) LES-ODT, and (d) LES-ODT optically thinner LES-ODT at iteration 50

Figure 5.31 Radiation source term contour at $y=1.8$ plane for (a) DNS (b) optically thinner DNS, (c) LES-ODT, and (d) LES-ODT optically thinner LES-ODT at iteration 50

We note from figures 5.26-5.31 that for the optically thinner configuration, the radiation effect is enhanced; and therefore more energy transfer occurs. That is why the temperature tends to be more homogeneous across the computational domain. Both LES-ODT and DNS models are showing consistent qualitative behavior with the change of optical thickness. They also show the same similarities as compared to each other by displaying the hot and cold zones at the same spots. Both 3D contours of temperature and radiation source term are shown in figure at the 200th iteration to confirm the effect of optical thickness and the similarity between LES-ODT and DNS.

Figure 5.32 Temperature 3D contour at iteration 200 for (a) DNS (b) optically thicker DNS, (c) LES-ODT, and (d) LES-ODT optically thicker LES-ODT

Figure 5.33 Radiation source term contours at iteration 50 for (a) DNS (b) optically thinner DNS, (c) LES-ODT, and (d) LES-ODT optically thinner LES-ODT

Next, a non-reacting simulation is performed in order to isolate the radiation effect from the heat release associated with chemical reaction. We first look at the temperature behavior that may be different from the previous cases. In fact, as there is no source of energy production due to the absence of chemistry, temperature will tend to homogenize relatively quickly as shown in figures 5.34-5.45.

Figure 5.34 Temperature 3D contours for (a) no-radiation, (b) LES-ODT, and (c) DNS at iteration 30

Figure 5.35 Temperature contours at the $x = 1.8$ plane for (a) no-radiation, (b) LES-ODT, and (c) DNS at iteration 30

Figure 5.36 Temperature contours at the $y = 1.8$ plane for (a) no-radiation, (b) LES-ODT, and (c) DNS at iteration 30

Figure 5.37 Radiation source term contours for (a) LES-ODT and (b) DNS at iteration 30

Figure 5.38 Radiation source term contour at $x=1.8$ plane for (a) LES-ODT and (b) DNS at iteration 30

Figure 5.39 Radiation source term contour at $y=1.8$ plane for (a) LES-ODT and (b) DNS at iteration 30

Figure 5.40 Temperature 3D contours for (a) no-radiation, (b) LES-ODT, and (c) DNS at iteration 90

Figure 5.41 Temperature contours at the $x = 1.8$ plane for (a) no-radiation, (b) LES-ODT, and (c) DNS at iteration 90

Figure 5.42 Temperature contours at the $y = 1.8$ plane for (a) no-radiation, (b) LES-ODT, and (c) DNS at iteration 90

Figure 5.43 Radiation source term contours for (a) LES-ODT and (b) DNS at iteration 90

Figure 5.44 Radiation source term contour at $x=1.8$ plane for (a) LES-ODT and (b) DNS at iteration 90

Figure 5.45 Radiation source term contour at $y=1.8$ plane for (a) LES-ODT and (b) DNS at iteration 90

The non-reacting case also shows consistency between the cases where there is no radiation, the LES-ODT, and the DNS one. However, similarities between LES-ODT and DNS, although present, are less obvious than the two other study cases. This can be explained more by the quantitative study in the following paragraph.

5.8. Quantitative study

After our qualitative comparison of the predictions of LES-ODT and DNS from the ignition phase till chemical reaction is established, we attempt, in this section, to quantitatively compare LES-ODT with DNS results. For this purpose, we attempt to compare the Root Mean Square (RMS) as compared to fluctuations for filtered quantities. We also use conditional statistics in order to compare averages, RMS, and Turbulence-Radiative Interaction (TRI) parameters. The conditioning is based on the mixture fraction, which is the primary variable adopted in the modeling of autoignition problems. The mixture fraction is evaluated at any time in terms of the mass fractions of the fuel and the oxidizer, based on the equal Lewis number condition for the fuel, the oxidizer, and the product as follow [48]:

$$Z = (1 + Y_f - Y_o)/2 \quad (5.2)$$

Different cases of optical thickness and absorption parameters were considered. For the optically thinner case, the optical thickness characterized by $L_{ref}\kappa$ is divided by a factor of 10. The absorption coefficient has a significant influence on the radiative heat transfer. It is present in both the emission and absorption terms. The expression for the absorption coefficient, detailed in section 4.2.1.2, is a function of temperature and product mass. In

autoignition problems, the product mass fraction is not significant prior to or at the ignition phase; and, therefore, a model based on products mass fraction may affect the absorption coefficient estimation. We aim to explore the effect of the absorption coefficient on the radiation transfer process by varying its dependency. Two cases are compared: an absorption coefficient depending on the product mass fraction and the case where it does not as shown respectively in Eqs. (5.3) and (5.4). In the second case, the absorption coefficient will depend only on temperature.

$$\kappa_{p,d} = C_k(Y_p + \epsilon_y) \left[c_0 + c_1 \left(\frac{A}{T} \right)^1 + c_2 \left(\frac{A}{T} \right)^2 + c_3 \left(\frac{A}{T} \right)^3 + c_4 \left(\frac{A}{T} \right)^4 + c_5 \left(\frac{A}{T} \right)^5 \right] \quad (5.3)$$

$$\kappa_{p,d} = C_k \left[c_0 + c_1 \left(\frac{A}{T} \right)^1 + c_2 \left(\frac{A}{T} \right)^2 + c_3 \left(\frac{A}{T} \right)^3 + c_4 \left(\frac{A}{T} \right)^4 + c_5 \left(\frac{A}{T} \right)^5 \right] \quad (5.4)$$

where A and $(c_0 - c_5)$ are the water vapor values from [8] and presented in the table 4.1; Y_p is the product mass fraction; ϵ_y is an arbitrary, small, positive threshold to ensure that κ_p is nonzero everywhere; C_k is a non-dimensionalization term.

5.8.1. RMS for filtered quantities

In this section, we compare the Root Mean Square (RMS) error between LES-ODT and DNS fields for both filtered temperature and radiation source term as expressed in Eq. (5.5). The RMS error may be normalized by the fluctuations in one of the two fields (DNS or LES-ODT) to provide a measure of the error that is independent of the scale of the variables evaluated or their dimensions/units as given by the following expression:

$$\frac{RMS}{fluctuations} = \frac{\sqrt{\langle X_{ODT}^2 - X_{DNS}^2 \rangle}}{\sqrt{\langle X^2 \rangle - \langle X \rangle^2}} \quad (5.5)$$

where X stands for either temperature or radiation source term.

The expressions in both numerator and denominator in the RHS are spatially averaged over the 3D LES grid. The fluctuations can be estimated either with the DNS or LES-ODT case. The DNS fluctuations were considered for the following results as it provides larger error than if LES-ODT was considered.

Errors are shown in figures 5.46 and 5.47 for the main case, the optically thinner, and the non-reacting case at different stages of the combustion. Both plots, the temperature and the radiation source term for LES-ODT and DNS show that the error is below 5% for both cases of different optical thicknesses. However, the error increases for the case where there is no chemistry. This is explained by the fact that with the chemistry effect turned off, the radiation source term is the only source term for energy transfer; and, therefore, the error is amplified. Also in the no-chemistry case, the temperature homogenized at around the 100th iteration as shown in figure 5.39 where the temperature range is around -0.035 and 0.04 . The physics that is left has no strong effect on the process.

We can also observe from figures 5.46 and 5.47 that the behavior of the temperature and radiation source term is similar between the two cases. For the main case, the error starts high and, then, decreases in time. For the optically thinner case, the error tends to be more relatively constant. This is explained by the fact that in the optically thinner medium, radiation transfer beyond the near field is favored; and, therefore, the interaction between rays and particles is enhanced and the error is reduced.

Figure 5.46 Filtered temperature RMS / fluctuations for the 3 studied cases

Figure 5.47 Filtered radiation source term RMS / temperature fluctuations for the 3 studied cases

5.8.2. Conditional statistics on averages

In this section, conditional statistics are used to compare temperature and radiation source term averages. Averages are calculated within intervals of mixture fractions for both ODT and DNS non filtered quantities according to Eq. (5.6) as shown in figures 5.48-5.51.

$$\langle X|Z \rangle = \frac{\sum_{i \in Z_{int}} X_i}{N_i} \quad (5.6)$$

where Z stands for mixture fraction as described in Eq. (5.2), $\langle X|Z \rangle$ is the conditional average of variable X that can stand for temperature or radiation source term, Z_{int} is the interval of mixture fraction, and N_i is the number of particles in the considered interval of mixture fraction Z_{int} .

Cases of different optical thicknesses and absorption coefficient are studied. For the optical thickness cases, the simulation is continued until most of the reactants are consumed. For the absorption coefficient configurations, more focus is given on the autoignition and chemical reaction stages.

DNS and ODT temperature and radiation source term conditional means are shown in Figures 5.48-5.51. The label and subscripts “*no_yp*” denotes absorption coefficient depending only on temperature while “*thn*” denotes the optically thinner medium. Radiation contribution is set to be stronger in the absorption coefficient dependency case by multiplying the radiation source term by a factor of 10.

Figure 5.48 Comparison of conditional averages of temperature between LES-ODT and DNS at different times for different optical thicknesses

Figure 5.49 Comparison of conditional averages of temperature between LES-ODT and DNS at different times for both absorption coefficient configurations

Figure 5.50 Comparison of conditional averages of radiation source term between LES-ODT and DNS at different times for different optical thicknesses

Figure 5.51 Comparison of conditional averages of radiation source term between LES-ODT and DNS at different times for both absorption coefficient configurations

Conditional averages either for temperature or source term show agreement between LES-ODT and DNS results for the four treated cases. Except some differences especially in the radiation source term cases, magnitudes and trends are consistent. The irregularities are mainly

located at the boundaries of the mixture fraction range. This result can be explained by the fact that, at the boundaries, there is not enough data points to establish sufficient statistics. In addition, the mixture fraction range shrinks with time because of the mixing. The shrinking of this range during the autoignition process is captured by LES-ODT accurately.

Note that maximum temperature increases from 860 K/0.44 (0.44 stands for the non-dimensional temperature) at iteration 50 to reach around 880 K/0.5 at iteration 500. This corresponds to the fact that kernels start ignition at lean mixture conditions and propagate from lean to rich conditions. At iteration 900 the temperature decreases below its value at iteration 50 and the mixture fraction range shrinks to almost converge around 0.5. The temperature decrease can be attributed to the radiation effect. In fact, after most of reactants are consumed, the radiation source term will have a dominant effect and will tend to homogenize temperature in the medium. We note here the excellent agreement between LES-ODT and DNS in counterbalancing chemistry.

Regarding differences between the two optical thicknesses simulations, conditional temperature averages show consistently lower values in the case of optically thicker medium that also correspond to higher radiation source term averages. As far as cases of different absorption coefficients, we observe a better agreement in magnitude in the case where the absorption coefficient is a function of the products' mass fraction. In the autoignition phase (the phase we want to focus on for the absorption coefficient dependency), both cases are in good agreement. Regarding the conditional radiation source term, the case where the product mass fraction is considered shows more variation in the slope compared to the case where it is not. At later time, around the 500th iteration, the radiation source term shows a higher slope.

The behavior of the slope though remains the same and the effect on temperature between LES-ODT and DNS of removing the product mass fraction dependencies does not affect similarity. It is important to note here that the difference of magnitude between cases of different absorption coefficient dependency is related to the fact that the product mass fraction has a contribution of the order of 10^{-1} .

5.8.3. Conditional RMS

Conditional RMS statistics are computed for both LES-ODT and DNS cases for temperature and radiation source term as expressed in Eq. (5.7):

$$\langle X_{rms}|Z \rangle = \sqrt{\frac{\sum_{i \in Z_{int}} \langle X|Z \rangle^2 - X_i}{N_i}} \quad (5.7)$$

The same cases of different optical thickness (figure 5.52 and 5.54) and absorption coefficient dependencies (figure 5.53 and 5.55) are considered for RMS statistics.

One would expect that since LES-ODT model has 46 times fewer particles than DNS, RMS profile would show obvious inconsistencies. It is actually not the case as we can observe in figures 5.52-5.55 similar RMS profiles not only in trends but also in magnitude. In addition, similarities of the radiation source term in figures 5.53 and 5.55 conditional RMS consolidates the choice of the adopted radiation model.

Figure 5.55 shows that in the case the absorption coefficient is depending on the product mass fraction (i.e. chemistry) a peak is observed to move from lower to higher mixture fraction until it reaches the value of 0.5. This peak, absent when there is no dependency on product mass fraction in figure 5.55, corresponds to the chemistry effect. We can also see the moving peak

in the temperature RMS profiles in figures 5.52 and 5.53. From this we can conclude that LES-ODT successfully predicts the physics that are represented by DNS. The physics include the onset of ignition, reaction progress, the locations and the magnitude of the peak values in the mixture fraction space, and the radiation effect.

Figure 5.52 Comparison of conditional temperature RMS between LES-ODT and DNS at different times for different optical thicknesses

Figure 5.5.53 Comparison of conditional temperature RMS between LES-ODT and DNS at different times for both absorption coefficient configurations

Figure 5.5.54 Comparison of conditional radiation source term RMS between LES-ODT and DNS at different times for different optical thicknesses

Figure 5.5.55 Comparison of conditional divergence source term RMS between LES-ODT and DNS at different times for both absorption coefficient configurations

5.8.4. Conditional TRI correlations

The radiative heat source term in Eq. (3.1) consists of the difference between the emitted and absorbed energy terms. The Turbulence Radiation Interaction (TRI) is observed when Eq. (3.1) is averaged as follows [64]:

$$\langle \nabla \cdot \mathbf{Q}_{rad} \rangle = 4\langle \kappa_p \sigma T^4 \rangle - \langle \kappa_p G \rangle \quad (5.6)$$

where G is the radiative intensity.

TRI correlations as described in Deshmukh and Modest study [64] are used to estimate the emission, absorption, and temperature TRI correlations.

5.8.4.1. Absorption TRI

Absorption TRI is expressed as follow:

$$TRI_a = \frac{\langle \kappa_p' G' | Z \rangle}{\langle \kappa_p | Z \rangle \langle G | Z \rangle} \quad (5.7)$$

where superscript “ ‘ ” stands for fluctuations.

Cases of conditional absorption TRI for different optical thicknesses and absorption coefficient dependencies are shown in this section.

From the optical thickness profiles in figure 5.56, we can observe a higher absorption in the case of optically thicker medium. A considerable difference is noted in the cases of absorption coefficient dependency in figure 5.57. In fact, the conditional absorption TRI has a positive higher peak in the case of product mass fraction dependency. It is negative and has a lower magnitude in the other case. This underlines the importance of the absorption coefficient model choice when simulating radiation.

Figure 5.5.56 Comparison of conditional absorption TRI between LES-ODT and DNS at different times for different optical thicknesses

Figure 5.5.57 Comparison of conditional absorption TRI between LES-ODT and DNS at different times for both absorption coefficient configurations

Figure 5.5.58 Comparison of conditional absorption TRI between LES-ODT and DNS at different times for both absorption coefficient configurations

The case without product mass fraction dependency shows a better agreement and track the peaks very well. This cannot be seen at figure 5.57 due to the same scale drawing. Conditional absorption TRI for the case of non-dependency on product mass fraction is shown in figure 5.58. We can observe that for product mass fraction dependency in figure 5.57, DNS and LES-ODT absorption TRI do not have matching peaks at early iterations (autoignition phase). However, starting from iteration 300, those peaks match. This is explained by the fact that at the autoignition phase, there is no considerable presence of products; and, therefore, the absorption coefficient (if based on product mass fraction) can be affected. In the case of non-dependency, the peaks match perfectly.

5.8.4.2. Emission TRI

The emission TRI is expressed as:

$$TRI_e = \frac{\langle \kappa_p' I_b' | Z \rangle}{\langle \kappa_p | Z \rangle \langle I_b | Z \rangle} \quad (5.8)$$

where I_b is the Plank function.

In the case of optical thickness simulations in figure 5.59, the emission TRI correlation is almost not affected by the change in optical thickness. This is not the case for absorption TRI in figure 5.56 where the difference in magnitude between both cases of optical thickness is noticeable. This is an expected observation though since the emitted energy is not much affected by the change in optical thickness; whereas, the absorption one does. Absorption TRI actually decreases with the decrease of optical thickness and is only considerable at high optical thickness ($\kappa L > 1$) as observed by Deshmukh [64]. We also observe from figures 5.57 and 5.60

that the peak magnitude is different for emission and absorption TRI. In fact, the emitted radiation is mostly absorbed locally or travels only small distance before being absorbed. The fluctuations in the incident radiation G , a nonlocal quantity, are highly correlated with those of the absorption coefficient, a local quantity. At any given location, the incident radiation G results from radiation from all solid angles and thus, it is an average value in a general sense for a wrinkled flame as compared to emission which is solely dependent on the local quantities [64]. Therefore, the peak value for absorption TRI is different than that for emission TRI.

Figure 5.5.59 Comparison of conditional emission TRI between LES-ODT and DNS at different times for different optical thicknesses

Figure 5.5.60 Comparison of conditional emission TRI between LES-ODT and DNS at different times for both absorption coefficient configurations

5.8.4.3. Temperature TRI

Next we compare the temperature TRI statistics. The temperature TRI is expressed as:

$$TRI_T = \frac{\langle T^4|Z \rangle}{\langle T|Z \rangle^4} \quad (5.9)$$

Comparison of conditional temperature TRI profiles are shown in figures 5.61 and 5.62.

The temperature TRI peak location changes along mixture fraction and time in figures 5.61 and 5.62 is similar to the same peak performance of temperature RMS observed in figures 5.53. In fact, around the peak, the presence of hot products is increasing, there is preheating of reactants, heat release by chemical reaction of reactants and also radiation from hot products. As such, the temperature is increasing rapidly and the local temperature fluctuations are also high, resulting in a high value for the correlation. Temperature TRI does not seem to be affected by optical thickness as we can see in Fig. 5.61. However, the effect of absorption coefficient dependency is noticeable. This can be explained by the difference in emission and absorption TRI magnitudes for both cases.

Figure 5.5.61 Comparison of conditional temperature TRI between LES-ODT and DNS at different times for different optical thicknesses

Figure 5.5.62 Comparison of conditional temperature TRI between LES-ODT and DNS at different times for both absorption coefficient configurations

5.9. Conclusion

In this chapter, we have attempted to validate, both qualitatively and quantitatively, the LES-ODT MCRT model using DNS simulations of the same problem of autoignition in a non-homogeneous mixture. The qualitative comparison show similar dependencies on optical thickness effects and identify the effects of chemistry and no-chemistry on various scalars' statistics.

Quantitative comparisons were also made using 1) estimates of the RMS error based on the filtered DNS and LES-ODT solutions at different times of the mixture evolution. The comparison showed that a model for the absorption coefficient that does not include the products' mass fraction performs much better than with the model involving the products' mass fraction. This is expected since the initial conditions and up until the onset of autoignition, the products are characterized by relatively low concentrations.

Conditional statistics were carried out on temperature, radiation terms and measures of turbulence-radiation interactions (TRI). The TRI are important to assess the contribution of unresolved fluctuations in averaged or filtered solutions. The predictions of TRI also is the main challenge of any radiation model. The results show that the LES-ODT model performs very well under different conditions involving variations of the optical thickness and absorption coefficient dependency.

Chapter 6 Conclusions and Recommendations for Future Work

Validation of the MCRT radiation model was first performed in comparison with the Spherical Harmonics method. Although one is statistical and the other one is analytical, both models showed the same effects compared to the no-radiation case by homogenizing the temperature distribution and favoring heat transfer in the medium. Successful validation of the radiation model led next to its implementation in the LES-ODT framework. Successful validation with the DNS results corresponding to the same configuration of autoignition in a heterogeneous mixture and decaying isotropic turbulence was observed qualitatively and quantitatively. The qualitative effect of radiation was seen on the similar scale for both models in different configurations (optically thinner medium and no-chemistry case). The quantitative analysis showed that error of filtered quantities between LES-ODT and DNS models was reasonable and was kept below 10%. Conditional statistics results of different variables including averages, RMS, and TRI correlations confirmed the qualitative behavior similarity between LES-ODT and DNS. The conditional analysis was performed for different cases of optical thickness and absorption coefficient dependencies. Validation of the LES-ODT model formulation by comparing the radiation parameters conditional statistics from LES-ODT with that from DNS is an important indicator of the LES-ODT model performance.

Some recommendations for future work are suggested. The spectral radiative properties of gases can be included. For the photon Monte Carlo method, the information of wavenumbers

can be added to the particle data structure of the photons without resulting in significant additional computational cost [64]. Similarly to Cao work [48] in studying effects of Re , Da and Le variations. One can explore those variations effect on TRI. The effect of turbulence on radiation can be studied by variation of turbulence intensity over a wide range. The variation of Da can show the effect of chemical time scales on TRI. The changes in Le can show the effect of mixing of species to the optical thickness of the medium. Finally, other absorption models like the Cone-PPM and Cone-SPM schemes can be modeled in LES-ODT in order to evaluate the most appropriate one to this framework.

REFERENCES

- [1] Echehki T., Mastorakos E., Turbulent Combustion Modeling Advances: New Trends and Perspectives, Springer, 2011.
- [2] Viskanta R., Menguc M.P., Radiation Heat Transfer in Combustion Systems, Prog. Energy Combust. Sci., 13, 97-160, 1987.
- [3] Modest M.F., Radiative Heat Transfer, Academic Press, Third Edition, 2013.
- [4] Hammersley J.M., Handscomb D.C., Monte Carlo Methods, John Wiley & Sons, New York, 1964.
- [5] Fleck J.A., The calculation of non-linear radiation transport by Monte Carlo method, Technical Report UCRL-7838, Lawrence Radiation Laboratory, 1961.
- [6] Howell J.R., Perlmutter M., Monte Carlo solution of thermal transfer through radiant media between gray walls, ASME Journal of Heat Transfer, 86, no.1, 116-122, 1964.
- [7] http://gcc.gnu.org/onlinedocs/gfortran/RANDOM_005fSEED.html
- [8] Combustion Research Facility Sandia National Laboratory, International Workshop on Measurement and Computation of Turbulent Nonpremixed Flames. (<http://www.ca.sandia.gov/TNF/radiation.html>), 2002.
- [9] Shekhawat Y., One-Dimensional Turbulence Based Multiscale Radiation Heat Transfer Model in Participating (Absorbing-Emitting) Gray Media, M.S. Thesis, Department of Mechanical and Aerospace Engineering, North Carolina State University, 2011.
- [10] Wang A. Investigations of Turbulent-Radiation Interactions in Turbulent Flames Using Hybrid Finite Volume/Monte Carlo Approach, PhD Dissertation, Penn State University, 2007.
- [11] Courant R., Hilbert D., Methods of Mathematical Physics, Volume I, Wiley-Interscience, 1962.
- [12] Thynell S.T., Discrete-ordinates method in radiative heat transfer, International Journal of Engineering Science, 36, Issues 12–14, 1651–1675, 1998.

- [13] Zhu K.Y., Huang Y., Wang J., Combination of spherical harmonics and spectral method for radiative heat transfer in one-dimensional anisotropic scattering medium with graded index, *International Journal of Heat and Mass Transfer* 62,200–204, 2013.
- [14] Cheng P., Two-dimensional radiating gas flow by a moment method, *AIAA J.*, 2(9), 1662–1664, 1964.
- [15] Cheng P., Dynamics of a radiating gas with application to flow over a wavy wall, *AIAA J.* 4(2),238–254,1966
- [16] Khan T., Thomas A., Comparison of PN or spherical harmonics approximation for scattering media with spatially varying and spatially constant refractive indices, *Opt. Commun.*, 255,(1–3),130–166, 2005.
- [17] Yang J., Modest M.F., Elliptic PDE formulation of general, three-dimensional high-order PN-approximations for radiative transfer, *J. Quant. Spectro. Radiat. Transfer*, 104,(2),217–227, 2007.
- [18] Modest M.F., Yang J., Elliptic PDE formulation and boundary conditions of the spherical harmonics method of arbitrary order for general three-dimensional geometries, *J. Quant. Spectro. Radiat. Transfer*,109(9),1641–1666,2008.
- [19] Bhuvaneswari M., Wu C.Y., Differential approximations for transient radiative transfer in refractive planar media with pulse irradiation, *J. Quant. Spectro. Radiat. Transfer*, 110(6–7),389–401, 2009.
- [20] Wang, A., Modest M., Photon Monte Carlo Simulation for Radiative Transfer in Gaseous Media Represented by Discrete Particle Fields, *Journal of Heat Transfer*, 128,1049, 2006.
- [21] Heinisch R.P., Sparrow, E.M., Shamsundar N., “Radiant Emission from Baffled Conical Cavities”, *J. Opt. Soc. Am.*, 63_2_, pp. 152–158, 1973.
- [22] Shamsundar N., Sparrow E.M., Heinisch R.P., “Monte Carlo Solutions—Effect of Energy Partitioning and Number of Rays”, *Int. J. Heat Mass Transfer*, 16, 690–694, 1973.
- [23] Modest M.F., Poon S.C., “Determination of Three-Dimensional Radiative Exchange Factors for the Space Shuttle by Monte Carlo”, *ASME paper No. 77-HT-49*, 1977.
- [24] Modest M.F., “Determination of Radiative Exchange Factors for Three Dimensional Geometries With Nonideal Surface Properties”, *Numer. Heat Transfer*, 1, pp.403–416, 1978.

- [25] Walters D.V., Buckius R.O., "Monte Carlo Methods for Radiative Heat Transfer in Scattering Media". Annual Review of Heat Transfer, Vol.5, Hemisphere, New York, pp. 131–176, 1992.
- [26] Kitchin, Christopher Robert, Stars, Nebulae and the Interstellar Medium: Observational Physics and Astrophysics. CRC Press, 1987.
- [27] Jeans J.H., "The equations of radiative transfer of energy", Monthly Notices Royal Astronomical Society, 78, 28–36, 1917.
- [28] Kourganoff V., Basic Methods in Transfer Problems, Dover Publications, New York, 1963.
- [29] Davison B., Neutron Transport Theory, Oxford University Press, London, 1958.
- [30] Murray R.L., Nuclear Reactor Physics, Prentice Hall, Englewood Cliffs, NJ, 1957.
- [31] Gelbard E.M., "Simplified spherical harmonics equations and their use in shielding problems", Technical Report WAPD-T-1182, Bettis Atomic Power Laboratory, 1961.
- [32] MacRobert T.M., Spherical Harmonics, 3rd ed., Pergamon Press, New York, 1967.
- [33] Adams J., "Multigrid Software for Elliptic Partial Differential Equations: MUDPACK", NCAR Technical Note-357+STR, 51 pages, Feb. 1991, The link for this document is <http://nldr.library.ucar.edu/repository/assets/technotes/asset-000-000-000-167.pdf>.
- [34] MUDPACK, National Center for Atmospheric Research (<https://www2.cisl.ucar.edu/resources/legacy/mudpack>)
- [35] Adams J., "MUDPACK: Multigrid Software for Linear Elliptic Partial Differential Equations", SCD User Doc, Version 2.0, NCAR, February 1990.
- [36] Andrienko D.A., Surzhikov S.T., Shang J.S., Spherical harmonics method applied to the multi-dimensional radiation transfer, Computer Physics Communications, 184, 2287–2298, 2013.
- [37] Adams J., Swarztrauber P., Sweet R., "Efficient Fortran Subprograms for the Solution of Elliptic Partial Differential Equations", Elliptic Problem Solvers, Academic Press, 333–390, 1982.
- [38] Brandt A., "Multi-level Adaptive Solutions to Boundary Value Problems", Math. Comp., 31, pp. 333–390, 1977.

- [39] Briggs W., "A Multigrid Tutorial", SIAM, Philadelphia, 1987.
- [40] Fulton S., Ciesielski R., Schubert W., Multigrid methods for elliptic problems: a review. Monthly Weather Review, 114:943-959, 1986.
- [41] Hackbush W., Trottenberg U., "Multigrid Methods", Springer-Verlag, Berlin, 1982.
- [42] Jespersen D., "Multigrid Methods for Partial Differential Equations", Studies in Numerical Analysis, Vol.24, MAA, 1984.
- [43] McCormick S., "Multigrid Methods", Vol 3 of SIAM Frontiers Series, SIAM, Philadelphia, 1987.
- [44] Adams J., "Comparison of direct and iterative methods for approximating nonseparable elliptic PDEs at NCAR", SCD Computing News, 10,12-14, 1989.
- [45] Buzbee B., Golub G., Nielson C., "On direct methods for solving Poisson's equations", SIAM J. Numer.Anal., 7,627-656, 1970.
- [46] Swarztrauber P., "Fast Poisson Solvers", Studies in Numerical Analysis, Math. Assoc, America, pp.319-369, 1985.
- [47] Sweet R., "A Parallel and Vector Variant of the Cyclic Reduction Algorithm", SIAM J. Sci. and Stat. Comp., 9,761-766, 1988.
- [48] Cao S., A novel hybrid scheme for Large Eddy Simulation of turbulent combustion based on the One-Dimensional Turbulence model, Ph.D. thesis, North Carolina State University, 2006.
- [49] Cao S., Echekki T., A low-dimensional stochastic closure model for combustion large-eddy simulation, Journal of Turbulence, 9(2):1–35, 2008.
- [50] Kerstein A.R., Ashurst W.T., Wunsch S., Nilsen V., One-dimensional turbulence: vector formulation and application to free shear flows, Journal of Fluid Mechanics, 447:85–109, Oct. 2001.
- [51] Kerstein A.R., Linear-eddy modeling of turbulent transport. Part V: Geometry of scalar interfaces. Physics of Fluids A: Fluid Dynamics, 3(5):1110, 1991.
- [52] Kerstein A.R., Linear-Eddy modeling of turbulent transport.Part 4.Structure of diffusion flames. Combustion Science and Technology, 81(1-3):75–96, Jan. 1992.

- [53] Mason S.D., Turbulence Transport in Spatially Developing Reacting Shear Layers, Ph.D. thesis, Department of Mechanical Engineering, University of Wisconsin-Madison, 2000.
- [54] Coelho P.J., “Approximate solutions of the filtered radiative transfer equation in large eddy simulations of turbulent reactive flows”, *Combustion and Flame*, 156(5),1099–1110, 2009.
- [55] Andersson K., Johnson F., Flame and radiation characteristics of gas-fired O₂/CO₂ combustion. *Fuel* Volume 86, Issues 5–6, Pages 656–668, MARCH-April 2007.
- [56] Sagaut P., Introduction à la simulation des grandes échelles pour les écoulements de fluide incompressible. *Mathématiques & Applications*, Vol. 30, 1998.
- [57] Poinso T., Veynante D., Theoretical and Numerical Combustion. Edwards, 2001.
- [58] Boileau M., Staffelbach G., Cuenot B., Poinso T., Bérat C., “LES of an ignition sequence in a gas turbine engine”. *Combustion and Flame*, 154(1-2), pp. 2–22, 2008.
- [59] Nottin C., Knikker R., Boger M., Veynante D., “Large eddy simulations of anoustically excited turbulent premixed flame”. *Symposium (International) on Combustion*, 28(1), pp. 67–73, 2000.
- [60] Lavoie G.A., Heywood J.B., Keck J.C., Experimental and theoretical study of Nitric Oxide formation in internal combustion engines. *Combustion Science and Technology*. Volume 1, Issue 4, 1970.
- [61] Khanna V., Goel R., Ellzey J.L., Measurements of Emissions and Radiation for Methane Combustion within a Porous Medium Burner. *Combustion Science and Technology*, Volume 99, Issue 1-3, 1994.
- [62] Shoshin Y., Dreizn E., Particle combustion rates in premixed flames of polydisperse metal—air aerosols. *Combustion and Flame*, Volume 133, Issue 3, Pages 275–287, May 2003.
- [63] Wang L., Yang J., Modest M.F., Haworth D.C., Application of the full-spectrum k-distribution method to photon Monte Carlo solvers. *Journal of Quantitative spectroscopy & Radiative Transfer*, 104,297–304, 2007.
- [64] Deshmukh K.V., Direct Numerical Simulation and Radiation Monte Carlo for Turbulence-Radiation Interactions in Combustion Systems. PhD Thesis at The Pennsylvania State University, 2009.
- [65] Veynante D. Poinso T., Theoretical and Numerical Combustion, R.T. Edwards, Inc.,Flourtown, PA 2nd edn. 2005.

- [66] Shi Y., Ge H.W., Reitz R.D., Computational Optimization of Internal Combustion Engines. Springer, Jun 22, 2011.
- [67] Givi P., Model-free simulation of turbulent reactive flows, *Progr. Energy Combust. Sci.*, 15: 1–107, 1989.
- [68] Poinso T., Candel S., Trounev A., Application of direct numerical simulation to premixed turbulent combustion, *Progr. Energy Combust. Sci.*, 21: 531–576, 1996.
- [69] Vervisch L., Poinso T., Direct Numerical Simulation of non-premixed turbulent flames, *Ann. Rev. Fluid Mech.*, 30: 655–692, 1998.
- [70] Shih T.H., Liou W.W., Shabbir A., Yang Z., Zhu J., A new $k-\epsilon$ eddy viscosity model for high reynolds number turbulent flows. *Computers & Fluids*, Volume 24, Issue 3, Pages 227–238, March 1995.
- [71] Davidson L., The PANS $k-\epsilon$ model in a zonal hybrid RANS–LES formulation. *International Journal of Heat and Fluid Flow*, Volume 46, Pages 112–126, April 2014.
- [72] Lam C.K.G., Bremhorst K., A Modified Form of the $k-\epsilon$ Model for Predicting Wall Turbulence, *J. Fluids Eng.* 103(3), 456–460, Sep 01, 1981.
- [73] Menter F.R., Influence of Freestream Values on $k-\epsilon$ Turbulence Model Predictions. *AIAA Journal*, Vol. 30, NO.6,
- [74] Sadiki A., Maltsev A., Wegner B., Flemming F., Kempf A., Janicka J., Unsteady methods (URANS and LES) for simulation of combustion systems. *International Journal of Thermal Sciences*, 45(8):760–773, Aug. 2006.
- [75] Wegner B., Maltsev A., Schneider C., Sadiki A., Dreizler A., Janicka J., Assessment of unsteady RANS in predicting swirl flow instability based on LES and experiments. *International Journal of Heat and Fluid Flow*, 25(3):528–536, June 2004.
- [76] Hanjalic K., Kenjeres S., ‘T-RANS’ Simulation of Deterministic Eddy Structure in Flows Driven by Thermal Buoyancy and Lorentz Force. *Flow, turbulence and combustion*, 66(4):427–451, 2001.
- [77] Kenjeres S., Hanjalic K., Transient analysis of Rayleigh Benard convection with a RANS model. *International journal of heat and uidow*, 20(3):329–340, June 1999.
- [78] Kenjeres S., Hanjalic K., LES, T-RANS and hybrid simulations of thermal convection at high Ra numbers, *International Journal of Heat and Fluid Flow*, 27(5):800–810, Oct. 2006.

- [79] Spalart P., Allmaras S., A one-equation turbulence model for aerodynamic flows. *Recherche Aerospatiale*, (1):5–21, 1994.
- [80] Pitsch H., Large-eddy simulation of turbulent combustion. *Ann. Rev. Fluid Mech.* 38, 453–482, 2006.
- [81] Pope S.B., *Turbulent Flows*, Cambridge University Press, Cambridge, U.K. 2000.
- [82] Schmidt R.C., Kerstein A.R., McDermott R., ODTLES: A multi-scale model for 3D turbulent flow based on one-dimensional turbulence modeling. *Computer Methods in Applied Mechanics and Engineering*, 199(13-16):865–880, Feb. 2010.
- [83] Chakravarthy V., Menon S., Subgrid modeling of turbulent premixed flames in the flamelet regime. *Flow, Turbulence and Combustion*, 65(2):133–161, 2000.
- [84] MENGUC M., WEBB B., Radiative Heat Transfer, in SMOOT, L., ed., *Fundamentals of Coal Combustion: for Clean and Efficient Use*, Elsevier, 375–432, 1993.
- [85] LI G., MODEST M.F., Application of composition PDF methods in the investigation of turbulence-radiation interactions, *J. Quant. Spectr. and Radiat. Trans.*, 73, 461–472, 2002.
- [86] COELHO P.J., TEERLING O.J., ROEKAERTS D., Spectral radiative effects and turbulence/radiation interaction in a nonluminous turbulent jet diffusion flame, *Combust. and Flame*, 133, 75–91, 2003.
- [87] CUMBER P.S., Improvements to the discrete transfer method of calculating radiative heat transfer. *International Journal of Heat and Mass Transfer*, Volume 38, Issue 12, Pages 2251–2258, August 1995.
- [88] WANG L., MODEST M.F., HAWORTH D.C., TURNS S.R., Modeling Nongray Soot and Gas-Phase Radiation in Luminous Turbulent Nonpremixed Jet Flames, *Combustion Theory and Modeling*, 9(3), 479–498.
- [89] Christophe Dang Ngoc Chan, Representation of a spherical harmonic by discrepancy to a sphere.
- [90] Moinand P., Mahesh K., Direct Numerical Simulation: A tool in Turbulence Research. *Annu. Rev. Fluid Mech.*, 30:539–78, 1998.
- [91] Fox D.G., Lilly D.K., Numerical simulation of turbulent flows. *Reviews of Geophysics*, Volume 10, Issue 1, pages 51–72, February 1972.

- [92] Yakhot V., Orszag S.A., Thangam S., Gatski T.B., Speziale C.G. (1992), "Development of turbulence models for shear flows by a double expansion technique", *Physics of Fluids A*, Vol. 4, No.7, pp1510-1520, 1992.
- [93] Craft T.J., Launder B.E., Suga K., Development and application of a cubic eddy-viscosity model of turbulence. *International Journal of Heat and Fluid Flow*, Volume 17, Issue 2, Pages 108–115, April 1996.
- [94] Spalart P.R., Allmaras S.R., "A One-Equation Turbulence Model for Aerodynamic Flows" AIAA, Paper 92-0439, 1992.
- [95] Yin Z., Jaluria Y., *HTD-* Vol. 323, 1, 207, 1996.
- [96] Chandrasekhar S., *Radiative Transfer*. Dover Publications, New York, 1960.
- [97] Abramowitz M., Stegun I.A., *Handbook of Mathematical Functions*, Dover, New York, 1972.
- [98] Kerstein A.R., *A linear-eddy model of turbulent scalar transport and mixing*. Combustion Science and Technology, Taylor & Francis, 1988.
- [99] Smagorinsky J., General circulation experiments with the primitive equations I. The basic experiment. *American Meteorological Society*. Volume 91, Issue 3, March 1963.
- [100] Germano M., Piomelli U., Moin P., Cabot W.H., A dynamic subgrid-scale eddy viscosity model. *Phys. Fluids A*, 3, 1760, 1991.
- [101] Angelberger C., Veynante D., Egolfopoulos F., Poinso T., Large eddy simulations of combustion instabilities in premixed flames. Center for Turbulence Research. Proceedings of the Summer Program, 1998.
- [102] Veynante D., Poinso T., Effects of pressure gradients on turbulent premixed flames. *Journal of Fluid Mechanics*, Cambridge University Press, Volume 353, pp 83-114, 1997.
- [103] Caldeira-Pires A., Heitor M.V., Characteristics of turbulent heat transport in nonpremixed jet flames. *Combustion and Flame*, Volume 124, Issues 1–2, Pages 213-224, January 2001.