A Computationally Efficient P_1 Radiation Model for Modern Combustion Systems Utilizing Pre-Conditioned Conjugate Gradient Methods

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ABSTRACT

The iterative convergence of the P_1 radiation model can be slow in optically thin scenarios when employing classical iterative methods. In order to remedy this shortcoming, an in-house P_1 radiation model was interfaced with high performance, scalable, linear solver libraries. Next, the accuracies of P_1 radiation model calculations was assessed by comparing its predictions against discrete ordinates (DO) model calculations for prototypical problems representative of modern combustion systems. Corresponding benchmark results were also included for comparison.

Utilizing Pre-Conditioners (PC) to the Conjugate Gradients (CG) method, the convergence time of the P_1 radiation model reduced by a factor of 30 for modest problem sizes and a factor of 70 for larger sized problems when compared against classical Gauss Seidel sweeps. Further, PC provided 50% computational savings compared to employing CG in a standalone mode. The P_1 model calculation times were about 25-30% of the DO model calculation time. The time to solution also scaled linearly with an increase in problem size. The weighted sum of gray gases model employed in this study in conjunction with the P_1 model provided good agreement against benchmark data with L_2 error norms (defined relative to corresponding DO calculations) improving when isotropic intensities were prevalent.

Keywords: Radiative transfer; Iterative Methods; WSGGM; Oxy-Combustion; P-1 model.

NOMENCLATURE

A	surface area of the face of the volume element normal to the x-axis
B	surface area of the face of the volume element normal to the y-axis
C	surface area of the face of the volume element normal to the z-axis
d	distance between adjacent lines
G	incident radiation, W/m^2
I	radiative intensity, $\text{W/m}^2\text{-Sr}$
k	absorption coefficient, m^{-1}
L	path length, m
L	Lower triangular matrix
M	pre-conditioning matrix
n_n	number of computational nodes along each dimension
P	Pressure, atm
P	square coefficient matrix
q	radiative heat flux vector, W/m^2
Q	right hand side vector of the linear matrix system
r	residual
$\hat{\mathbf{r}}$	location vector
R	condition number of matrix
$\hat{\mathbf{s}}$	unit vector in the direction of radiation intensity
T	temperature, K
T_b	blackbody emission temperature, K
U	Upper triangular matrix
V	volume of a grid element, m^3

w	angular weights
x, y, z	co-ordinate directions
Y	mole fractions of the gaseous species

Greek symbols

ε	emissivity
ζ	direction cosine in the z-direction
η	direction cosine in the y-direction
μ	direction cosine in the x-direction
σ	Stefan-Boltzmann constant
ρ	reflectivity
σ_s	scattering coefficient, m^{-1}
Ω	solid angle

Subscripts

b	blackbody
i	gray gas component
i, j, k	surface element indices
m	discrete angular direction of intensity
p	node at which the directional intensity or incident radiation is being solved
S	index that runs over all neighboring surface nodes
t	iteration number
w	wall

1. Introduction

The high computational cost associated with modeling radiative heat transfer is currently a significant bottleneck in computational fluid dynamics (CFD) simulations of combustion phenomena. For instance, in finely resolved (spatially and temporally) Large Eddy Simulations (LES) of combustion, 50 – 75% of the total solve time is associated with the radiation model [1 - 3] primarily due to the large number of transport equations being solved to adequately resolve the directional and wavelength dependencies of radiative transfer. While this cost cannot be significantly alleviated in LES simulations where the radiative fluxes are a primary variable of interest (assessing radiation hazards from fires for instance [4]), LES investigations where the primary focus is on studying ignition [5] and extinction behavior [6], flame stability and recirculation characteristics [3], may benefit from computationally efficient radiation modeling options where the fidelity of the coupling between the radiation model and the temperature field through the radiative source term may be deemed as “adequate.” The P_1 radiation model is one such option where a single nonhomogeneous, Helmholtz equation with Robin boundary conditions is solved for the incident radiation (G) instead of solving several separate transport equations for the radiative intensity (I) as undertaken in the popular discrete ordinates (DO) and Finite Volume (FV) radiation methods [7]. Despite this advantage, the P_1 method is known to yield poor predictions of wall radiative fluxes when the intensity distributions are anisotropic [4, 8] or suffer from poor convergence particularly in optically thin media where the governing equations are rendered stiff [9 - 11]. In fact, a recent study comparing the speeds and accuracies of the P_1 and DO models showed that while the cost per iteration was lower with the P_1 radiation model, the time to achieve a converged solution for the P_1 model may be higher if the iterative solver has not been optimized [9]. This shortcoming of employing classical iterative methods for solving the Helmholtz equation has been well recognized [12] and have resulted in the development of iterative methods and preconditioning strategies to improve the convergence rate when solving the Helmholtz equation [13, 14]. Therefore, *the first objective of this manuscript is*

to utilize different iterative solvers and preconditioners to assess the convergence behavior of an in-house P_1 radiation model in practical combustion scenarios of current interest and lead to the identification of optimum solver and preconditioner combination. This is undertaken by interfacing the model with the open-source, scalable linear solver and pre-conditioner library, Portable Extensible Toolkit for Scientific Computation (PETSc) [15]. Next, the accuracies of the P_1 radiation model are assessed by comparisons against benchmark solutions of radiative transfer in emission dominated (i.e., isotropic intensities), optically thick, combustion scenarios of current interest. Fortunately, oxy fuel combustion which is one of the leading technologies being actively investigated for carbon-capture [16, 17] could result in media conditions that favor the use of the P_1 radiation model. Optically thick oxy-combustion scenarios may result from: the high concentrations of radiatively participating gases (H_2O and CO_2) within the combustor resulting from flue gas recycle, the added opacity due to the presence of particles [18, 19], or when the combustor is operated at high pressures [20, 21]. In fact, recent studies indicate that in optically thick media the use of high fidelity gas radiative property models may be more important than accurately accounting for the angular variations in radiative transfer [22 - 24]. Cai et al. [22] evaluated different formulations of the spherical harmonics methodology in an artificially enhanced turbulent diffusion flame and determined that a high fidelity radiative property model with a spherical harmonics formulation can result in reasonably good accuracies when compared against similar solutions obtained with the photon Monte Carlo method. Poitou et al. [23] concluded that the impact of angular discretization strategies in the DOM was minimal and that using a global spectral model in conjunction with mesh coarsening in the radiation calculations could result in significant computational savings in LES simulations. Similar conclusions were reached by Krishnamoorthy [4, 24] where the radiative source term predictions by the P_1 radiation model within a pool fire of moderate opacity were comparable to those obtained using the discrete ordinates method and FV model calculations performed using 512 angular directions.

In order to optimize speed and accuracies, computationally tractable radiative property models for gas mixtures representative of oxy-combustion scenarios have been proposed by several researchers in recent years and their performances assessed against benchmark solutions available for prototypical radiation problems [25 - 30]. Most of the proposed models fall under the category of weighted-sum-of-gray-gases (WSGG) models where the emissivities (ε) of gas mixtures are expressed in terms of temperature independent absorption coefficients and temperature dependent weighting fractions for emission. Here ε is computed as a weighted sum of gray gas emissivities as:

$$\varepsilon = \sum_{i=0}^n a_i(T) [1 - \exp(-k_i(P_c + P_w)L)] \quad (1)$$

In Eq. (1), a_i and k_i are the emission weighting factor and the absorption coefficient for the i th gray gas component respectively, P_c and P_w are the partial pressures of CO_2 and H_2O respectively, n is the number of gray gases and L is the path length. The coefficients a_i and k_i are obtained from a fit to total emissivity data with the constraint that the sum of coefficients a_i is equal to unity. The transparent regions of the spectrum are accounted for by the term $i=0$. The temperature dependence of a_i can be expressed in a polynomial form. Differences among the databases employed in the WSGG formulation in conjunction with the accuracies of the emissivity-curve-fits can result in 10-30% variations in the emissivity and radiative transfer predictions among the different WSGG models [31 - 34]. Consequently, various studies expounding on the accuracies of the spectroscopic databases and WSGG models at different media conditions (temperatures, pressures and gas compositions) [21, 31 – 33, 35, 36] have been undertaken.

In the context of WSGG models, it is worth mentioning that the Spectral-Line Weighted-Sum-of-Gray-Gases Model (SLW) developed by researchers at the Brigham Young University [37, 38] and the Full-Spectrum Correlated K (FSCK) models developed by Prof. Modest and Co-workers [22, 39, 40] are currently the most accurate variants of the model where the WSGG model

coefficients are computed directly from high resolution spectroscopic databases. However, to achieve high fidelity with the SLW and FSK models requires the use of 10-20 gray gases (or equivalently quadrature points) to be employed in the radiation calculations. Further, there are database retrieval costs associated with these models [38, 40]. Since *the computational cost comparisons between the P_1 and DO radiation models is the focus of this study*, the use of SLW or FSK methods in this study was not pursued since the overhead associated with database retrieval/interpolations and extrapolations could skew the comparisons [9]. All calculations in this study were therefore performed with the WSGG model proposed by Krishnamoorthy [29]. For the discrete ordinates (DO) method calculations, an in-house radiation code employing the T_4 angular quadrature set (corresponding to 128 directions) [41] was employed in the calculations.

2. Methods

2.1 Interfacing PETSc with the P_1 radiation model

Obtaining solutions to the discretized transport equations consumes the maximum time in most radiation algorithms. Therefore, the speed and parallelizability of an algorithm is often determined by the speed and parallelizability of the iterative solver employed in the solution procedure. Hence, it is extremely beneficial to interface the radiation algorithm to libraries of robust, scalable, nonlinear and linear solvers like the Portable Extensible Toolkit for Scientific Computation (PETSc) [15]. This provides the developers and users with an easy access to a suite of direct and iterative solvers and preconditioners that can be suitably selected depending on the problem being solved. Employing the solvers and preconditioners in PETSc to solve the system of linear equations arising from a finite volume discretization of the discrete ordinates method has been described previously in Krishnamoorthy et al. [42, 43]. Further, scaling of the radiation solver to 1000 processors was demonstrated. The transport equation for the P_1 approximation determines the distribution of the incident radiation (G) throughout the domain. If k represents the absorption coefficient, σ_s the scattering coefficient, C the linear-anisotropic phase function and T

the temperature, then the differential equation governing the P₁ approximation can be written as [7]:

$$\nabla(\Gamma \nabla G) - kG + 4k\sigma T^4 = 0 \quad (2)$$

where

$$\Gamma = \frac{I}{(3(k + \sigma_s) - C\sigma_s)} \quad (3)$$

If ε_w and T_w are the emissivities and temperature of the boundaries then the boundary condition associated with the above equation is

$$q_w = -\frac{\varepsilon_w}{2(2 - \varepsilon_w)}(4\sigma T_w^4 - G) \quad (4)$$

If the absorption coefficient and temperature within the domain are specified or can be obtained along with the boundary properties then Eq. (2) can be iteratively solved for the irradiation (G) throughout the domain. The radiative flux vector (q) and its divergence at a position vector r inside the domain can be calculated as [7]:

$$q(r) = -\Gamma \nabla G(r) \quad (5)$$

$$\nabla \bullet q(r) = k(r)(4\sigma T(r)^4 - G(r)) \quad (6)$$

Multiplying both sides of Eq. (2) by $dV = dxdydz$, and integrating over the volume elements results in the following equation for the face centered fluxes and the cell centered incident radiation

$$\begin{aligned} & \left[\left(\Gamma \frac{\partial G}{\partial x} \right)_e - \left(\Gamma \frac{\partial G}{\partial x} \right)_w \right] dydz + \left[\left(\Gamma \frac{\partial G}{\partial y} \right)_n - \left(\Gamma \frac{\partial G}{\partial y} \right)_s \right] dxdz + \left[\left(\Gamma \frac{\partial G}{\partial z} \right)_t - \left(\Gamma \frac{\partial G}{\partial z} \right)_b \right] dxdy \\ & - k_p G_p dV + 4k_p \sigma T_p^4 dV = 0 \end{aligned} \quad (7)$$

In this equation, the lower case subscripts represent face centered values and the upper case subscripts represent cell centered values. The subscript p corresponds to the node at which Eq. (2) is being approximated. The subscripts correspond to the interfaces of the control volume

under consideration with its neighboring cell to the east (e), west (w), north (n), south (s), top (t) and bottom (b) respectively. A central differencing scheme was employed to evaluate the fluxes (the derivatives). The medium properties (Γ , k and T) are all cell-centered variables. Γ at a control volume face is determined as a harmonic mean of the Γ of the cells adjoining that face. Eq. (7) can then be represented in the form [44]:

$$P_p G_p + \sum_S P_s G_s = Q_p \quad (8)$$

where the subscript p corresponds to the node at which Eq. (2) is being approximated, the index “ S ” runs over all the neighboring surface nodes in Eq. (7), P_s corresponds to the product of the geometric properties and medium properties and Q_p contains all the terms that are known. Therefore, Eq. (8) can be written in matrix form as:

$$\mathbf{P}\mathbf{G} = \mathbf{Q} \quad (9)$$

where $\mathbf{P}$ corresponds to a square coefficient matrix which is sparse, septa-diagonal (in 3D) and symmetric. If the control volume under consideration is adjacent to a boundary cell(s), then the corresponding flux(s) in Eq. (7) must be replaced by the boundary condition, Eq. (4).

The WSGGM is employed here as a non-gray gas model with the P_1 approximation. Eq. (2) in a non-scattering medium (all the test cases considered in this study) for the “ i^{th} ” gray gas may be written as:

$$\nabla \left(\frac{1}{3k_i} \nabla G_i \right) - k_i G_i + 4a_i(T) k_i \sigma T^4 = 0 \quad (10)$$

with the boundary conditions:

$$q_{w,i} = -\frac{\varepsilon_w}{2(2 - \varepsilon_w)} (4a_i(T) \sigma T_w^4 - G_i) \quad (11)$$

The heat fluxes and the source terms for the WSGGM were then evaluated as:

$$q_i(r) = \sum_i -\frac{1}{3k_i(r)} \nabla G_i(r) \quad (12)$$

$$\nabla \bullet q_i(r) = k_i(r)(4a_i(T)\sigma T(r)^4 - G_i(r)) \quad (13)$$

In this study, various preconditioning strategies were employed to speed the convergence of Eq. (9) in PETSc. A preconditioned, iterative method results in the splitting of the matrix “**P**” in Eq. (9) of the form:

$$\mathbf{P} = \mathbf{M} - \mathbf{N} \quad (14)$$

where **M** is the preconditioning matrix (usually containing the diagonal or a triangular part of **P**) and **N** contains the negative of the remaining elements of **P**. The matrix equations to be solved then reduce to the form:

$$\mathbf{M} G_t = (\mathbf{M} - \mathbf{P}) G_t + \mathbf{Q} \quad (15)$$

where t is the iteration number. It is best that the preconditioner **M** be convenient, sparse, invertible, and be as close an approximation to **P** as possible. Convergence is determined by the condition number or the ratio of the largest to smallest eigen-values of the matrix given by [45]:

$$\mathbf{R} = \mathbf{M}^{-1}(\mathbf{M} - \mathbf{P}) \quad (16)$$

The criterion for convergence is the L_2 -norm of the preconditioned residual [15]. The preconditioned residual is defined as

$$r_m = \mathbf{M}^{-1}\mathbf{Q} = \mathbf{M}^{-1}\mathbf{P}\mathbf{G} \quad (17)$$

Convergence is detected at iteration t if

$$\|r_t\|_2 < \max(\text{rtol} \times \|r_0\|_2, \text{atol}) \quad (18)$$

where *rtol* gives the relative decrease in the residual norm and the absolute size of the residual norm is given by “*atol*”. The value of “*rtol*” for all the cases run in this chapter was set at 10^{-6} , further decreasing the value of “*rtol*” did not increase the precision of the P_1 radiation model calculations reported in this study.

2.2 The discrete ordinates radiation model

An in-house radiation code was employed to solve the discrete ordinates transport equation in this study. If μ_m , η_m and ζ_m , represent the direction cosines associated with each

ordinate direction, k represent the absorption coefficient and I_b represent the black body emissive power, then the differential equation governing the discrete ordinates method in the absence of scattering can be written for each direction “ m ” as [7]:

$$\mu_m \frac{\partial I_m}{\partial x} + \eta_m \frac{\partial I_m}{\partial y} + \zeta_m \frac{\partial I_m}{\partial z} = -kI_m + kI_b \quad (19)$$

The radiative heat fluxes within the domain or at a surface and the radiative flux divergence were determined by integrating the intensities over all solid angles using weighting factors (w_m) as [7]:

$$q(r) = \int_{4\pi} I(r, \hat{s}) \hat{s} d\Omega \approx \sum_m w_m I_m(r, \hat{s}) \hat{s}_m \quad (20)$$

$$\nabla \bullet q(r) = k(r)(4\pi I_b(r) - G(r)) \quad (21)$$

G , the incident radiation was calculated as:

$$G(r) = \int_{4\pi} I(r, \hat{s}) d\Omega \approx \sum_m w_m I_m(r, \hat{s}) \quad (22)$$

Multiplying both sides of Eq. (19) by $dV = dx dy dz$, and integrating over the volume elements, the intensity I_m at the center of each control volume in a uniform, structured grid is related to the face centered values of the intensities as

$$\mu_m A [I_{m,i+l} - I_{m,i}] + \eta_m B [I_{m,j+l} - I_{m,j}] + \zeta_m C [I_{m,k+l} - I_{m,k}] = -kI_m V + kI_b V \quad (23)$$

where A , B and C represent the surface areas of the faces of the volume element that are normal to the x-, y- and z- axis respectively, and i , j and k represent the surface element indices along the x-, y- and z- axis, respectively. An upwind differencing scheme was employed to relate the face centered values to the cell centered values. For directions with positive direction cosines, this results in:

$$I_{m,i+l} = I_{m,j+l} = I_{m,k+l} = I_m \quad (24)$$

A similar analysis can be carried out for other combinations of direction cosines as well.

Substituting Eq. (24) in Eq. (23) we get:

$$[\mu_m A + \eta_m B + \zeta_m B + kV]I_m = \mu_m AI_{m,i} + \eta_m BI_{m,j} + \zeta_m BI_{m,k} + kI_b V \quad (25)$$

Thus, Eq. (25) also corresponds to a discretized set of linear algebraic equations of the form:

$$P_p I_{m,p} + \sum_S P_S I_{m,S} = Q_p \quad (26)$$

where the subscript p corresponds to the node at which Eq. (19) is being approximated, the index “ S ” runs over all the neighboring surface nodes in Eq. (25), P_S corresponds to the product of the direction cosines with the geometric properties (surface areas) and Q_p contains all the terms that are known. Eq. (26) can be written in matrix form as

$$\mathbf{P}\mathbf{I}_m = \mathbf{Q} \quad (27)$$

where “ $\mathbf{P}$ ” corresponds to a square coefficient matrix. If $I_{m,i}$, $I_{m,j}$ or $I_{m,k}$ correspond to intensity from a boundary, they must be suitably replaced by the boundary conditions. Eq. (27) corresponds to a linear system of equations for each direction in which the RTE is being solved. For the problems considered in this paper, the square coefficient matrix ($\mathbf{P}$) is a sparse non-symmetric matrix with three other bands running parallel to the diagonal. The number of bands on the upper or lower triangular part of the matrix depend on the direction in which the RTE is being solved. Gauss-Seidel sweeps were employed to solve the matrix equations corresponding to the discrete ordinates method in this paper.

The different cases investigated in this study are summarized in Table 1. Considering the wide range of variability in the magnitudes of the radiative source and flux predictions among the different cases, a root-mean-square (RMS) error norm also known as L_2 Error Norm was evaluated as defined by Burns and Christon [46] in order to express the overall solution accuracy of the numerical method in a compact form. First, the relative error at each node is calculated as:

$$e_{\varphi,P} = 100 \frac{(\varphi_{P_1} - \varphi_{DO})_P}{\|\varphi_{DO}\|_{max}} \quad (28)$$

where e is the relative error, φ refers to the radiative flux or flux divergence calculated at each nodal location (p), DO and P_1 refer to discrete ordinates solution values and P_1 values,

respectively. $\|\varphi_{DO}\|_{\max}$ refers to the maximum DO value along the line. The percentage RMS error norm can then be calculated as:

$$\|e\|_{RMS} = 100 \times \left\{ \frac{\sum_{i=1}^{n_n} e_{\varphi,i}^2}{n_n} \right\}^{\frac{1}{2}} \quad (29)$$

where n_n is the number of computational nodes along each dimension.

3. Results and Discussion

3.1. Comparisons of Iterative Solver Performance

First, the convergence characteristics of the P_1 method when employing a classical Gauss Seidel iterative method to solve Eq. (9) is demonstrated for Case 2. Convergence was determined when the relative percentage variation in G between iterations was less than 10^{-6} . In the WSGGM employed in this study [29], four gray gases and a transparent gas were employed. The absorption coefficient (and consequently the opacity of the medium) in the WSGGM increases from the first to the fourth gray gas while the fifth gray gas is transparent. Table 2 summarizes the time as well as the number of iterations to achieve convergence across each gray gas during the solution to case 2. The “degrees of freedom” correspond to the number of unknowns being solved in the matrix equation Eq. 9 in the mesh $(80 \times 41 \times 41)$ and a refined mesh $(80 \times 82 \times 82)$ respectively. It is clear that the maximum time is spent in the transparent gray gas iteration. Further, the time and number of iterations to achieve convergence reduce significantly as we move from gray gas 1 to gray gas 4 as the k_i (absorption coefficient of the i^{th} gray gas) in the WSGGM increases. Table 3 summarizes the scaled timing results to achieve convergence when employing the different solvers and preconditioners to solve the P_1 radiation model equation during the simulation of Case 2. For brevity, the timing results are calculated and scaled relative to the fastest calculation reported in the table i.e., the Conjugate Gradient (CG) [49] solver calculation employing Successive Over Relaxation (SOR) preconditioning strategy at 134K degrees of freedom.

Utilizing Pre-Conditioners (PC) to the Conjugate Gradients (CG) method, the convergence time of the P_1 radiation model is seen to reduce by a factor of 30 for modest problem sizes and a factor of 70 for larger sized problems when compared against classical Gauss Seidel sweeps. Further, PC provided 25-50% computational savings compared to employing CG in a standalone mode with the increased savings associated with larger sized problems. We also notice that when PC is employed, the time to solution scales nearly linearly with an increase in problem size offering no significant bottlenecks i.e., the solve time with CG with incomplete LU factorization (ILU) for instance increases by a factor of 11 as the problem size increases 8 times (from 134K to 1076K). This scaling behavior offers the possibility of tackling really large LES calculations in a computationally efficient manner in a parallel computing environment. Finally, we notice that the optimized calculation times with the P_1 model are about 25-30% of the corresponding DO model solve times which were undertaken employing classical Gauss Seidel sweeps.

Very briefly, ILU preconditioning is a variant of Gaussian Elimination, or LU factorization and results in the factoring of the $\mathbf{P}$ matrix in Eq. 14, of the form:

$$\mathbf{P} = \mathbf{LU} + \mathbf{N} \quad (29)$$

where $\mathbf{L}$ is upper triangular, $\mathbf{U}$ is lower triangular and $\mathbf{N}$ is a non-zero residual matrix. Comparing Eq. (29) with Eq. (14), it is easy to recognize that preconditioning matrix in this case is just:

$$\mathbf{M} = \mathbf{LU} \quad (30)$$

Additional calculations were performed by interfacing the DO model with PETSc to explore the identification of optimum solvers and pre-conditioners. In this context, it is important to first note that unlike the discretized P_1 radiation model which results in a sparse, symmetric, septa-diagonal matrix in 3D, the discretized DO model for the problems investigated in this study, results in a sparse non-symmetric matrix system with three diagonals (that run parallel to the main diagonal) distributed on the upper and lower triangular portion of the matrix. The number of diagonals on either side of the main diagonal depends on the direction of the DO sweep [42, 43]. Due to this difference in matrix type (non-symmetry), the GMRES solver (as opposed to CG for the P_1

radiation model) has previously been determined to be the optimum solver choice for the DO model [42, 43]. However, Table 3 shows that for the problems investigated in this study, the GMRES solver with the best pre-conditioning options (SOR/ILU) was at least 4 times slower than classical Gauss-Siedel (GS) sweeps for the same problem. Further, the differences between GS and GMRES solve times are even more pronounced as the problem size (i.e., matrix size) increased. Therefore, all subsequent DO calculations in this study were carried out using GS sweeps. In spite of these results, it is important to recognize that iterative solutions to the DO model equations using scalable GMRES solvers could still have their place and might prove beneficial in parallel computing environments and/or when scattering and reflective walls are present.

3.2. Atmospheric Pressure Natural Gas Combustion: Air and Oxy-Fired

In Cases 1 and 2, the predictions of P_1 and DO models are first assessed at conditions representative of natural gas combustion in air as well as with dry flue gas recycle (FGR). The benchmark predictions of Liu [47] and Porter et al. [9] employing the EM2C Statistical Narrow Band Model (EM2C SNB) are also included for comparison. The purpose here is not to quantify the accuracies of the Perry (5 gg) model since the differences in the property databases as well as the model approximations used by Liu [47] and Porter et al. [9] to generate their data precludes such a comparison. Figures 1 (a, b) show the centerline radiative source (which is the negative of the radiative flux divergence in Eqs. 6 and 21) distributions and incident wall radiative flux distributions along (2 m, 1 m, z) predicted by the various models in case 1. Figures 2 (a, b) show the distributions of the radiative source along the centerline of the enclosure and incident wall radiative flux distributions along (2 m, 1 m, z) for case 2. From Figures 1 and 2, we notice that for the natural gas combustion scenarios, the P_1 and DO model predictions are close to each other. The L_2 error norms for the different cases are computed according to Eq. 29 and reported in Table 4. A slight improvement in the agreement between the P_1 and DO models is observed in Case 2 (dry FGR) possibly due to an increase in opacity resulting from higher concentrations of

radiatively participating gases. Previous comparisons of the P_1 radiation model predictions against those of Monte Carlo and Finite Volume radiation model predictions in turbulent diffusion flames and pool fires have shown that the P_1 radiation model accuracies improves in emission dominated, optically thick media that yield isotropic intensity distributions within the domain [22, 24]. The absence of wall reflections and particle scattering in Cases 1 and 2 favor such a scenario.

3.3. High Pressure Natural Gas Combustion with Dry FGR

The temperature and specie profiles in the high pressure natural gas combustion scenario of cases 3 and 4 were obtained from Kez et al. [21] which were in turn based on curve-fitting the CFD simulations of Ströhle et al. [48]. The predictions of the radiative source and radiative heat flux distributions in cases 3 and 4 employing the P_1 model are compared against those obtained from the DO model in Figures 3 and 4. In Figures 3 and 4, the benchmark predictions reported in Kez et al. [21] employing the EM2C SNB are also shown. In their study, Kez et al. [21] also evaluated the performances of three WSGGM [27, 30, 50] and determined the WSGGM proposed by Bordbar et al [30] to be the most accurate in the investigated scenarios. Therefore, the results from employing the Bordbar et al [30] WSGGM reported in Kez et al. [21] are also included here for comparison against our DO predictions since both calculations were performed on identical mesh sizes employing the T_4 quadrature scheme in the DO method. Unlike cases 1 and 2, cases 3 and 4 correspond to sharper temperature gradients within a smaller geometry. Further, the temperature profiles in case 3 exhibited greater gradients when compared against case 4. Consequently, the L_2 error norm values (especially of the radiative source term) in Table 4 are reflective of the magnitude of the temperature gradients within the domain. In order to ascertain this, Case 2 calculations were repeated for different temperature gradients and the L_2 error norms were assessed. In Case 2, the gas temperature was considered to be non-uniform but symmetrical about the centerline of the enclosure and specified in the functional form:

$$T = (T_c - T_e)f(r/R) + T_e \quad (31)$$

Here, T_c is the gas temperature along the centerline of the enclosure that increases linearly from 400 K at the inlet ($z = 0$) to a maximum value (T_{max}) at $z = 0.375$ m and then decreases linearly to 800 K at the exit ($z = 4$ m). T_e is the exit temperature at $z = 4$ m. In order to simulate different temperature gradients, T_{max} of 1800 K, 2400 K and 3000 K were considered representing oxy-methane flames at different oxidizer compositions based on previous simulations that we have carried out [34]. Inside the enclosure a circular region or a cylinder around the centerline can be imagined, where $R = 1.0$ m is the radius of the cylinder. The radial variation in gas temperature inside the circular region was specified as per the equation:

$$f(r/R) = 1 - 2(r/R)^2 + 3(r/R)^3 \quad (32)$$

where r is the distance from the centerline of the enclosure. The gas temperatures outside the circular region, i.e. between the cylinder with radius $R = 1.0$ m and the walls of rectangular enclosure were defined as uniform and equal to the exit temperature, T_e . The variation of the L_2 Error Norm (Eq. 29) with T_{max} when employing the P_1 radiation model to solve Case 2 is shown in Table 5. A clear relationship between the L_2 error norm and the temperature gradient is seen. Even when reflective walls or scattering particles are absent, steep temperature gradients in an emission dominated medium can result in anisotropic intensities (since there is a hot medium on one side and a cold medium on the other) and increase the errors associated with the P_1 radiation model.

3.4. Influence of Particles: Biomass Combustion with Air-Firing and Oxy-Firing

Oxy-combustion using biomass is currently being considered as an excellent carbon negative option for power generation [51]. The furnace dimensions, wall boundary conditions, gas and temperature profiles for Case 5 have been adopted from Bahador and Sunden [52] concerning thermal radiation in biomass combustors under air-fired conditions. Employing realistic ash particle size distributions in conjunction with Mie theory to estimate the absorption

and scattering coefficients, scattering phase function of the ash particles, they concluded that the scattering of the ash particle was not important. However, ash concentrations had a strong impact on the absorption coefficients and consequently the radiative source and wall heat flux predictions. Similar conclusions regarding the minimal role played by ash scattering in particle combustors have also been reached by Marakis et al. [18] and Adams [53]. More recently, simulations of co-firing biomass and coal under oxy-combustion conditions carried out by Krishnamoorthy and Caitlyn [54] also concluded that determining the particle size distributions within the combustor had a greater bearing on the wall radiative fluxes predictions than the accuracy of the scattering phase function. Therefore, particle scattering was neglected in Cases 5 and 6 and the particle contribution to radiation was accounted for by specifying a constant particle absorption coefficient of 0.05 m^{-1} throughout the combustor. Our previous studies on biomass combustion [54] along with the Planck mean absorption coefficients at different volume fractions reported in [52] deem 0.05 m^{-1} to be an acceptable value for the purposes of this analysis. Since biomass combustion in an oxygen-enriched scenario with FGR was not investigated by Bahador and Sunden [52], we report here a case 6 where only the gas composition corresponding to case 5 have been changed to correspond to oxy combustion with FGR. Note that this is identical to the composition in Case 2 and is a reasonable representation of dry FGR as determined from our previous simulations of these scenarios [54]. In order to provide a reference benchmark for comparison, calculations employing the multiplicative approach in the SLW model [55] employing 21 logarithmic spaced intervals were also performed with the DO method and are reported in this study. The absorption cross-section of H_2O was in the range $3.0\text{e-}05$ to $120.0 \text{ m}^2/\text{mole}$ and the absorption cross-section of CO_2 was in the range $1.0\text{e-}08$ to $200.0 \text{ m}^2/\text{mole}$. The reference temperature for the SLW calculations was determined by volume averaging the fourth power of temperature throughout domain. The engineering correlations for the full spectrum k-distributions of H_2O were obtained from Denison and Webb [37] whereas

those for CO_2 were obtained from Modest and Mehta [56] since they were based on the more updated CDS-1000 spectroscopic database.

Figures 5 (a, b) show the centerline radiative source distributions and incident wall radiative flux distributions along (2 m, 1 m, z) predicted by the various models in case 5. Figures 6 (a, b) show the distributions of the radiative source along the centerline of the enclosure and incident wall radiative flux distributions along (2 m, 1 m, z) for case 6. From Figures 5 and 6, we notice an excellent agreement between the P_1 and DO model predictions for the radiative source term and a reasonable agreement in the wall radiative heat fluxes. The L_2 error norms reported in Table 4, again show a slight improvement in the agreement between the P_1 and DO models is observed in Case 6 (dry FGR) in comparison to Case 5 possibly due to an increase in opacity resulting from higher concentrations of radiatively participating gases. Higher opacities in an emission dominated medium result in isotropic intensity distributions that improves the accuracies of the P_1 radiation model. Further, the reasonable agreement between the WSGGM predictions in this study against benchmark predictions obtained from employing high fidelity models (EM2C SNB and SLW) across all the investigated scenarios demonstrates its potential for usage in fine resolution simulations of combustion phenomena.

4. Conclusions

The iterative convergence behavior associated with the P_1 radiation model can be very slow in optically thin media (or at certain spectral/gray gas windows in a non-gray calculation) when employing classical iterative methods such as the Gauss Seidel (GS) or Successive Over Relaxation (SOR). In order to remedy this shortcoming, an in-house P_1 radiation model was first interfaced with high performance, scalable, linear solver libraries (PETSc). This enabled easy access to a suite of linear solvers based on Krylov subspace (KSP) methods along with various preconditioning (PC) options. Next, the accuracies of the P_1 radiation model calculations were assessed by employing it in conjunction with a WSGGM and comparing its predictions against benchmark data and corresponding discrete ordinates (DO) model calculations in prototypical

problems representative of modern combustion systems. L_2 error norms of the radiative source term and the radiative fluxes were employed to compare the P_1 and DO model predictions and to quantify the comparisons in a compact form. Based on the results of this study, the following conclusions can be drawn:

1. Utilizing Pre-Conditioners (PC) to the Conjugate Gradients (CG) method, the convergence time of the P_1 radiation model reduced by a factor of 30 for modest problem sizes and a factor of 70 for larger sized problems when compared against classical Gauss Seidel sweeps. Further, PC provided 25-50% computational savings compared to employing CG in a standalone mode with the increased savings associated with larger sized problems.
2. When PC is employed to the CG method, the time to solution scaled linearly with an increase in problem size offering no significant bottlenecks. This scaling behavior offers the possibility of tackling really large LES calculations in a computationally efficient manner within a parallel computing environment.
3. The optimized calculation times with the P_1 model were about 25-30% of the corresponding DO model solve times which were undertaken employing classical Gauss Seidel sweeps.
4. The weighted sum of gray gases model employed in this study in conjunction with the P_1 radiation model provided reasonably good agreement against both benchmark data and the corresponding DO calculations.
5. In order to quantify and express the accuracies of the radiative source term and heat flux predictions in a compact form, L_2 error norms for the P_1 predictions were computed relative to the corresponding DO predictions. The L_2 error norms in general were seen to improve when isotropic intensity distributions were prevalent as a result of higher opacities, lower thermal gradients in emission-dominated media conditions.

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Table 1. Summary of gas compositions, temperature profiles and boundary conditions employed in cases 1-6

Case (Fuel, combustion mode)	Gas composition	Temperature profile	Boundary conditions	Dimensions and mesh count
1 (Methane, air) [47]	10% CO ₂ , 20% H ₂ O, 70% N ₂ (1 atm)	Polynomial temperature profile [47]	Black walls at 300K	2 m × 2 m × 4 m 41 × 41 × 80
2 (Methane, dry FGR) [9]	85% CO ₂ , 10% H ₂ O, 5% N ₂ (1 atm)	Polynomial temperature profile [9]	Black walls at 300K	2 m × 2 m × 4 m 41 × 41 × 80
3 (Methane, dry FGR with 40% CO ₂ in fuel/oxidizer mixture, high Pressure) [21]	Polynomial species profile [21] (20 atm)	Polynomial temperature profile [21]	Black walls at 700K	0.4 m × 0.2 m × 0.2 m 63 × 33 × 33
4 (Methane, dry FGR with 62.5% CO ₂ in fuel/oxidizer mixture, high pressure) [21]	Polynomial species profile [21] (20 atm)	Polynomial temperature profile [21]	Black walls at 700K	0.4 m × 0.2 m × 0.2 m 63 × 33 × 33
5 (Biomass, air) [48]	11.7 % CO ₂ , 28.7 % H ₂ O, 59.6% N ₂ , particle absorption coefficient of 0.05 m ⁻¹	Polynomial temperature profile [48]	Black as well as reflective walls	2 m × 2 m × 4 m 41 × 41 × 80
6 (Biomass, dry FGR)	85% CO ₂ , 10% H ₂ O, 5% N ₂ , particle absorption coefficient of 0.05 m ⁻¹	Polynomial temperature profile [48]	Black as well as reflective walls	2 m × 2 m × 4 m 41 × 41 × 80

Table 2. Time (in seconds) and the number of iterations (in brackets) to achieve convergence across gray gases when solving the P_1 radiation model equation using classical Gauss Seidel sweeps (Case 2).

Degrees of Freedom	Gray Gas 1	Gray Gas 2	Gray Gas 3	Gray Gas 4	Gray Gas 5 (Clear Gas)
134K	66.4 (7156)	19.4 (2077)	0.84 (77)	0.17 (7)	77.9 (8380)
537K	824.3 (20693)	241 (6042)	8.4 (208)	0.5 (10)	968 (24298)

Table 3. Scaled timing results to achieve convergence when employing different solvers and preconditioners (in brackets) to solve the P_1 radiation model equation during the simulation of Case 2.

Degrees of Freedom	Gauss Seidel	CG (No preconditioning)	CG (SOR)	CG (ILU)	Discrete Ordinates with Gauss Seidel sweeps	Discrete Ordinates GMRES (SOR/ILU)
134K	35.7	1.2	1.0	1.1	6.4	22.8
537K	443.0	8.0	5.8	5.6	27.1	325.0
1076K	N/A	18.2	12.9	12.4	52.3	N/A

Table 4. The % RMS Error Norm (Eq. 29) for the different cases investigated in this study

Case	Radiative Source	Net Radiative Flux
1	4	6
2	4	5
3	20	10
4	13	12
5	4	7
6	4	6

Table 5. Variation of the L_2 Error Norm (Eq. 29) with $T_{\max}$ when employing the P_1 radiation model to solve Case 2

Case	Radiative Source	Net Radiative Flux
$T_{\max} = 1800 \text{ K}$	4	5
$T_{\max} = 2400 \text{ K}$	14	8
$T_{\max} = 3000 \text{ K}$	34	18

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Figure 6. Predictions of (a) Radiative source distributions along the centerline of the enclosure for case 6; (b) Incident wall heat flux distributions along (2 m, 1 m, z) for case 6.

(a)

(b)

Figure 1. Predictions of (a) Radiative source distributions along the centerline of the enclosure for case 1; (b) Incident wall heat flux distributions along $(2 \text{ m}, 1 \text{ m}, z)$ for case 1.

Figure 2. Predictions of (a) Radiative source distributions along the centerline of the enclosure for case 2; (b) Incident wall heat flux distributions along (2 m, 1 m, z) for case 2.

(a)

(b)

Figure 3. Predictions of (a) Radiative source distributions along the centerline of the enclosure for case 3; (b) Incident wall heat flux distributions along $(x, 0.2 \text{ m}, 0.1 \text{ m})$ for case 3.

(a)

(b)

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(a)

(b)

Figure 6. Predictions of (a) Radiative source distributions along the centerline of the enclosure for case 6; (b) Incident wall heat flux distributions along (2 m, 1 m, z) for case 6.