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A simplified CFD model for spectral radiative heat transfer in high-pressure hydrocarbon–air combustion systems

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Abstract

Detailed radiation modeling in piston engines has received relatively little attention to date. Recently, it is being revisited in light of current trends towards higher operating pressures and higher levels of exhaust-gas recirculation (EGR), both of which enhance molecular gas radiation. Advanced high-efficiency engines also are expected to function closer to the limits of stable operation, where even small perturbations to the energy balance can have a large influence on system behavior. Detailed radiation modeling using sophisticated tools like photon Monte Carlo/line-by-line (PMC/LBL) is computationally expensive. Here, guided by results from PMC/LBL, a simplified stepwise-gray spectral model in combination with a first-order spherical harmonics (P1 method) radiative transfer equation (RTE) solver is proposed and tested for engine-relevant conditions. Radiative emission, reabsorption and radiation reaching the walls are computed for a heavy-duty compression-ignition engine at part-load and full-load operating conditions with different levels of EGR and soot. The results are compared with those from PMC/LBL, P1/FSK (P1 with a full-spectrum k -distribution spectral model) and P1/Gray radiation models to assess the proposed model's accuracy and computational cost. The results show that the proposed P1/StepwiseGray model can calculate reabsorption locally and globally with less than 10% error (with respect to PMC/LBL) at a small fraction of the computational cost of PMC/LBL (a factor of 30) and P1/FSK (a factor of 15). In contrast, error in computed reabsorption by the P1/Gray model is as high as 60%. It is expected that the simplified model should be broadly applicable to high-pressure hydrocarbon–air combustion systems, with or without soot.

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Keywords: Radiation modeling; Stepwise-gray spectral model; Compression-ignition engine

1. Introduction

Conventional wisdom has been that radiation can account for a significant fraction of the total heat losses in very large bore, heavy-duty diesel engines, and that radiation was of secondary

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importance in road-vehicle-scale (cars and trucks) engines [1]. Few in-cylinder CFD modeling studies have considered radiative heat transfer, and only a subset of those has considered radiatively participating medium effects by solving a radiative transfer equation (RTE); exceptions are [2–5].

In the meantime, higher operating pressures and higher levels of exhaust-gas recirculation (EGR) in advanced high-efficiency engines make molecular gas radiation (absorption coefficient proportional to participating species concentration) more prominent. Recent applications of high-fidelity spectral radiation models in engines [6,7] (including photon Monte Carlo/line-by-line – PMC/LBL – and full-spectrum k -distribution – FSK) show that radiation redistributes energy (through reabsorption) in the combustion chamber, in addition to contributing to heat losses. Soot emits over a broad wavenumber spectrum, while gas molecules emit over discrete wavenumber bands. It is therefore necessary to account for spectral properties of the medium using detailed radiation models to accurately compute reabsorption. It has been found that CO_2 dominates the total radiative emission in engines, but most of the emitted CO_2 radiation is reabsorbed before reaching the walls. On the other hand, most soot radiation reaches walls, but for the levels of soot in modern engines, H_2O dominates radiation reaching walls [6,7].

Detailed radiation models like PMC/LBL and FSK are very powerful and provide useful insight, but are computationally expensive. It is desirable to have a less computationally intensive model that captures the essential redistribution of in-cylinder energy and radiative heat loss and that can be used in routine engineering CFD for engine development/design.

In this paper, we exploit what we have learned from PMC/LBL [6,7] to propose a simple stepwise-gray model for spectral radiative heat transfer in engines (and other high-pressure hydrocarbon–air combustion systems) that gives results that are within 10% of those from a high-fidelity spectral radiation model at a small fraction of the computational cost. Key features to capture are broadband soot radiation and two key spectral bands for CO_2 - and H_2O -dominated molecular gas radiation. These are bands at which the system is relatively optically thick at engine-relevant pressures, so we expect that a simple radiative transfer equation (RTE) solver (a P1 method [8]) should be satisfactory.

2. Physical model and numerical methods

2.1. Radiation modeling

An up-to-date review of the theory and applications of radiative heat transfer in turbulent combustion systems can be found in [9]. In engines, principal participating species are CO_2 ,

H_2O and CO along with soot (particulate matter). Spectral properties of CO_2 , H_2O and CO are obtained from the HITEMP2010 [10] database for pressures from 0.1 bar to 80 bar, temperatures from 300 K to 3000 K, and for various mole fractions of the participating species. Simple pressure-based scaling is used to extrapolate to higher pressures, where needed. The spectral absorption coefficient for soot is evaluated using the small-particle limit (Rayleigh theory) [8] with the complex index of refraction from [11]; scattering is neglected. Spray radiation is negligible for the conditions that are of interest here [9]. From the spectral molecular-gas databases and the presumed soot radiation properties, a hierarchy of spectral models is constructed. These range from full line-by-line (LBL), to high-fidelity full-spectrum k -distributions (FSK), to gray-gas models with Planck-mean absorption coefficients [8]. Along with these, in this study a new stepwise-gray spectral model is proposed (Section 2.2) that provides results within 10% of those from high-fidelity models at a fraction of the computational cost, under engine-relevant conditions.

Multiple RTE solvers have been implemented to calculate the local radiative intensity in situations where reabsorption is important. These include the stochastic photon Monte Carlo (PMC) method where no intrinsic assumptions are invoked regarding the directional distribution of radiative intensity, spherical-harmonics methods (SHM), and discrete-ordinates methods (DOM) [8,9]. In the lowest-order SHM implementation (the P1 method), a single elliptic PDE must be solved (see below). While DOM and variants probably have been used more widely than the others in combustion applications, recent work has shown that SHM methods (P1, P3, etc.) provide a more favorable tradeoff between computational effort and accuracy as one goes to higher-order implementations [12].

PMC/LBL provides a benchmark against which the performance of simpler RTE solvers and/or spectral models can be compared. The intent of this work is to compare the accuracy and computational cost of the proposed stepwise-gray spectral model, in combination with a P1 RTE solver (P1/StepwiseGray), against PMC/LBL, P1/FSK and P1/Gray models (in order of decreasing computational cost and accuracy).

2.2. Stepwise-gray spectral model

A stepwise-gray model is a simple and convenient wide-band spectral model where the entire wavenumber spectrum is divided into discrete bands, and an average absorption coefficient is calculated for each band. Various forms of stepwise-gray spectral models have been used to solve non-gray radiation problems [13–16].

Fig. 1. Stepwise-gray model bands. Here κ_η and $I_{b\eta}$ are the absorption coefficient and blackbody intensity at wavenumber η . For gas species, κ_η is calculated using unity mole fraction. For soot, κ_η is calculated using soot volume fraction of 10^{-5} (10 ppm). Here $\kappa_\eta I_{b\eta}$ is plotted for pressures from 1 bar to 80 bar and temperatures from 300 K to 3000 K.

Figure 1 shows the product of the spectral absorption coefficient κ_η and the Planck function $I_{b\eta}$ over a range of engine-relevant pressures and temperatures for three participating molecular gases and for soot particles. CO_2 has a strong emission peak at approximately 2300 cm^{-1} ($4.3 \text{ }\mu\text{m}$), and there is a strong overlap of CO_2 and H_2O emission spectra near 3700 cm^{-1} ($2.7 \text{ }\mu\text{m}$). Other emission peaks are relatively small compared to these two. Hence, the idea behind the proposed model is to divide the wavenumber spectrum into five bands, giving special attention to these two peaks (Fig. 1), and then to solve the RTE's assuming constant absorption coefficient (calculated by Planck-function weighted averaging [8]) in each of the bands.

In modern engines the in-cylinder soot volume fraction typically remains under 10 ppm [17,18], and at engine-relevant temperatures the radiative emission from soot occurs mainly in band b5 of Fig. 1. In this case, it is clear from Fig. 1 that radiative emission from molecular gases should be more important than radiative emission from soot.

For each band, the Planck-mean absorption coefficient ($\tilde{\kappa}_i$) and average black-body intensity ($\tilde{I}_{bi}$) are calculated using the following equations respectively:

$$\tilde{\kappa}_i = \frac{\int_{\Delta\eta_i} \kappa_\eta I_{b\eta} d\eta}{\int_{\Delta\eta_i} I_{b\eta} d\eta}, \quad i = 1, 2, \dots, 5, \quad (1)$$

$$\tilde{I}_{bi} = \frac{1}{\Delta\eta_i} \int_{\Delta\eta_i} I_{b\eta} d\eta, \quad i = 1, 2, \dots, 5. \quad (2)$$

Here subscript i corresponds to one of the five bands. For example, $\Delta\eta_i$ is the bandwidth (in units of wavenumber) of the i 'th band.

A key feature of the proposed model is the use of a simple P1 RTE solver. This essentially

assumes local isotropy of the radiative intensity distribution. Radiative intensity then evolves according to an elliptic equation, with a local diffusivity that is proportional to the inverse of the local absorption coefficient. This is a reasonable approximation for relatively optically thick systems, such as high-pressure hydrocarbon–air combustion systems where CO_2 and H_2O radiation dominate. The validity of using P1 for in-cylinder radiation in engines is confirmed in the results presented later. The P1 RTE equation (neglecting scattering) is solved for each band:

$$\nabla \cdot \left(\frac{1}{\tilde{\kappa}_i} \nabla G_i \right) - 3\tilde{\kappa}_i G_i = -12\pi \tilde{\kappa}_i \tilde{I}_{bi}, \quad (3)$$

where $\tilde{\kappa}_i$ is the sum of the absorption coefficients for all participating species and soot, subject to Marshak's boundary condition [8],

$$\frac{2 - \epsilon}{\epsilon} \frac{2}{3\tilde{\kappa}_i} \hat{n} \cdot \nabla G_i + G_i = 4\pi \tilde{I}_{bwi}. \quad (4)$$

Here G_i is the incident radiation for band i , ϵ is the wall emissivity, $\hat{n}$ is the surface normal vector and $\tilde{I}_{bwi}$ is the average blackbody intensity at the wall temperature for band i . In this work, walls are considered to be black ($\epsilon = 1$). The radiative heat flux is then calculated as:

$$\nabla \cdot \mathbf{q} = \sum_{i=1}^5 \tilde{\kappa}_i (4\pi \tilde{I}_{bi} - G_i) \Delta\eta_i. \quad (5)$$

Five RTE's need to be solved for the proposed P1/StepwiseGray model, compared to a single RTE for the P1/Gray model.

To implement the model, a table of $\tilde{\kappa}_i$'s is calculated for each gas species (CO_2 , H_2O and CO) considering unity mole fraction at nine pressures (1 bar, then 10–80 bar in steps of 10 bar) and 28 temperatures (300 K to 3000 K in steps of 100 K). Bandwise-average blackbody intensity ($\tilde{I}_{bi}$) and $\tilde{\kappa}_i$'s for soot (considering unity soot volume fraction) are also pre-tabulated at 28 temperatures. In a CFD simulation, local values of κ_i and $\tilde{I}_{bi}$ are interpolated from these tables.

2.3. Numerical methods

Here the proposed P1/Stepwise-gray radiation model is assessed in a post-processing mode (one-way coupling), where there is no radiative source term feedback to the CFD solver through the enthalpy equation. That is, radiative emission, reabsorption and radiation reaching the walls are computed using fields of participating molecular gases, soot and temperature from earlier engine simulations that did not use a radiation model (Section 3). This allows a cleaner comparison of the different radiation models over a wide range of conditions. For the cases considered here, the global influence of radiation on computed wall heat loss and on NO and soot emissions is less than 10%. It has been

confirmed that the key findings do not change with consideration of feedback of radiation to the CFD simulation (Table S2 of the Supplemental Material).

An unsteady Reynolds-averaged formulation is used for the engine simulations, with a standard two-equation turbulence model including wall functions, and conventional stochastic-Lagrangian-parcel fuel injection and spray models (using n-heptane liquid fuel properties). A 42-species chemical mechanism (40-species n-heptane [19], plus two additional species for thermal NO) is used to represent the gas-phase chemistry, and a semi-empirical two-equation model is used for soot [20].

Gas-phase chemistry and soot are calculated at the notional particle level in a particle-based transported probability density function (tPDF) method [21] that accounts for turbulent fluctuations with respect to local mean values (turbulence–chemistry interactions – TCI). The models are essentially the same as those that were used in an earlier modeling study for a heavy-duty diesel engine [22]. There it was shown that the tPDF-based model gave better agreement with experimental measurements compared to a locally well-stirred-reactor (WSR) model over a range of operating conditions, especially for soot. In the radiation calculations, local cell-mean values of composition and temperature are used, thereby neglecting the influences of unresolved turbulent fluctuations on radiation (turbulence–radiation interactions – TRI). TRI effects have been found to be small at these conditions [6,7]. It has been confirmed that the key findings do not change when a simpler turbulent combustion model (WSR) is used (Table S1 of the Supplemental Material).

3. Engine configuration and operating conditions

A simplified model of a Volvo 13L production six-cylinder heavy-duty diesel truck engine has been built using OpenFOAM v2.3.x [23], and simulations have been performed for four operating conditions (Table 1). Here EGR is modeled by appropriate mass fractions of CO₂ and H₂O. For no-EGR cases, the O₂ mass fraction is kept the same as for the corresponding EGR case, and the rest of the in-cylinder gas is prescribed as N₂. The engine configuration (15.8:1 compression ratio, 1213 r/min, 0.3 swirl ratio) is same as that in an earlier modeling study [22]. Simulations begin after intake-valve closure at 60° before top-dead-center (bTDC), and continue until 120° after top-dead-center (aTDC): that is, before exhaust-valve opening. A 60-degree sector mesh with 85,650 cells is used, centered on one of the six spray plumes, with cyclic symmetry conditions on the lateral faces. A computational time step of 3.4 μs (0.025 crank-angle-degree – CAD) is used, in all cases. For radiation

post-processing, the solution fields (pressure, temperature, gas species concentrations and soot) are saved every 2.5 CAD. The peak pressure for the part-load and full-load EGR operating conditions are approximately 85 bar and 200 bar, respectively [22].

4. Results and discussion

Results are presented for two levels of in-cylinder soot. First, the “normal” engine operating conditions (Table 1) are explored. For these cases, computed engine-out soot levels closely match the experimentally measured values [22]. The computed maximum local (volume-averaged) soot volume fractions for the four operating conditions are: 3.3 ppm (0.14 ppm) for part-load EGR; 8.0 ppm (0.25 ppm) for full-load EGR; 5.2 ppm (0.14 ppm) for part-load no-EGR; and 10 ppm (0.33 ppm) for full-load no-EGR.

Second, for the EGR cases (Table 1), the computed soot volume fraction in each computational cell is multiplied by a factor of 100. The intent is to assess the performance of the P1/Stepwise-gray model for environments where the contribution of soot radiation is not negligible. The factor of 100 is somewhat arbitrary, but is sufficiently high to cover the levels of soot that would be expected in any engine or other combustion device.

4.1. Normal engine operating conditions

Computed cumulative radiative emission, reabsorption and radiation reaching walls for part-load EGR and no-EGR operating conditions are shown as functions of crank-angle degrees in Fig. 2, and the final values for all four cases are tabulated in Table 2. To simplify the plots, P1/FSK results are not shown there, but P1/FSK results are tabulated in Table 2. The computed radiative emission is essentially identical for all four radiation models. This is expected, as the same underlying spectral database has been used for all models and there is no feedback of radiation to the CFD.

Turning to reabsorption, P1/FSK is within approximately 1% of PMC/LBL in all cases. This confirms the appropriateness of using the P1 RTE solver. The maximum error in computed reabsorption by the P1/Gray model is as much as 61% for the part-load no-EGR case. For the same operating condition, the P1/StepwiseGray model error is only 8%. The P1/StepwiseGray model predicts reabsorption with significantly better accuracy in comparison to the P1/Gray model, and within 10% of PMC/LBL for all operating conditions. This illustrates the importance of accounting for spectral radiation properties, and demonstrates the validity of the specific spectral model proposed here.

The differences in bandwise reabsorption among PMC/LBL, P1/StepwiseGray and P1/Gray

Table 1
Initial conditions and fuel-injection parameters for four engine operating conditions. SOI: Start of injection ($^{\circ}$ aTDC); EOI: End of injection ($^{\circ}$ aTDC).

	EGR		No-EGR	
	Part-load	Full-load	Part-load	Full-load
Initial pressure and temperature:				
p (bar)	5.65	14.28	5.65	14.28
T (K)	540.9	560.9	540.9	560.9
Initial composition (% mass):				
O ₂	18.68	18.84	18.68	18.84
N ₂	75.72	75.75	81.32	81.16
H ₂ O	4.06	3.92	0.0	0.0
CO ₂	1.54	1.49	0.0	0.0
Fuel injection parameters:				
SOI	-2.8°	-4.6°	-2.8°	-4.6°
EOI	3.5°	16.8°	3.5°	16.8°
Mass (mg)	13	47	13	47

Fig. 2. Cumulative radiative emission, reabsorption and radiation reaching walls as functions of crank angle degrees. (a) Part-load with EGR. (b) Part-load with no-EGR.

Table 2
Total radiative emission, reabsorption and radiation reaching walls. Total fuel energy and turbulent boundary-layer wall heat loss are also given. All values are for the 1/6 sector mesh, from intake-valve closing to exhaust-valve opening. The (%) in the reabsorption column is the percent difference with respect to PMC/LBL.

Case	Fuel energy (J)	BL wall heat loss (J)	Radiative emission (J)	Radiation model	Radiative reabsorption (J)	Radiation reaching walls (J)
Part-load EGR	572	82.0	27.3	PMC/LBL	22.1	5.2
				P1/FSK	22.1 (0%)	5.2
				P1/Gray	11.9 (46%)	15.4
				P1/StepwiseGray	20.7 (6.3%)	6.6
Full-load EGR	2068	232.6	107.3	PMC/LBL	94.2	13.1
				P1/FSK	94.9 (0.7%)	13.3
				P1/Gray	74.0 (21.4%)	33.2
				P1/StepwiseGray	91.0 (3.4%)	16.3
Part-load no-EGR	572	84.8	20.5	PMC/LBL	15.8	4.6
				P1/FSK	15.6 (1.4%)	4.8
				P1/Gray	6.2 (60.7%)	14.2
				P1/StepwiseGray	14.6 (7.9%)	5.9
Full-load no-EGR	2068	234.1	81.0	PMC/LBL	68.8	12.3
				P1/FSK	68.0 (1.2%)	13.0
				P1/Gray	46.2 (32.9%)	34.8
				P1/StepwiseGray	66.1 (4.0%)	15.0

Fig. 3. Cumulative band-wise reabsorption for PMC/LBL, P1/StepwiseGray and P1/Gray models. (a) Part-load with EGR. (b) and (c) Full-load with EGR.

are explored in Fig. 3. It is evident from Fig. 3a and b that band b2 ($4.3 \mu\text{m}$ band) is responsible for most of the reabsorption. The P1/StepwiseGray model predicts band b2 reabsorption quite accurately. Most of the discrepancies in reabsorption between P1/StepwiseGray and PMC/LBL are in bands b1 and b4; bands b3 and b5 contribute little to reabsorption. Band b1 is wider than bands b2 and band b4 (Fig. 1). Several small peaks of H_2O absorption coefficient in band b1 are smoothed out by the averaging (Eq. 1), and that causes the discrepancy in band b1. In band b4, H_2O emission spans from 3150 cm^{-1} to 4050 cm^{-1} , while CO_2 emission spans from 3400 cm^{-1} to 3800 cm^{-1} . Hence there is significant smoothing of the CO_2 absorption coefficient due to averaging, and that causes the discrepancy in band b4. To improve the accuracy, the number of bands could be increased to take into account other individual peaks. Here to keep the method simple and computationally inexpensive, only five bands are considered.

Figure 3(c) shows band-wise reabsorption for the P1/Gray model. Here the reabsorption amount is simply proportional to the bandwidth. Hence band b5 reabsorbs the most and band b2 the least, and the absorption differs significantly from the PMC/LBL results. In that respect, the P1/StepwiseGray model captures the essential characteristics of the spectral reabsorption distribution quite accurately.

4.2. Increased soot operating condition

For the four engine operating conditions considered, molecular gas radiation dominates. It is of interest to assess how well the proposed stepwise-gray model performs under conditions where soot radiation is more prominent. To that end, the computed soot volume fraction is increased by a factor of 100 during radiative post-processing for the part-load and full-load EGR cases. Results for the part-load case are plotted in Fig. 4, and results for both cases are summarized in Table 3. With the higher level of soot radiation, the P1/Gray model performs

somewhat better than before (maximum error of approximately 40% with respect to PMC/LBL for the part-load no-EGR case – not shown), but the P1/StepwiseGray model continues to outperform P1/Gray with a maximum error of approximately 10%.

Figure 4(b) shows the band-wise reabsorption for a high-soot case. Soot radiation dominates in band b5, and band b5 now contributes significantly to reabsorption. However, most of the soot has oxidized after approximately 45° aTDC , and the contribution of band b5 then becomes negligible.

Figure 5 shows computed contours of the local reabsorption at 12.5° aTDC for the full-load EGR case with normal and increased soot. Results from PMC/LBL, P1/StepwiseGray and P1/Gray models are shown. Here 12.5° is chosen because it is close to the instant when in-cylinder pressure, temperature and soot are at their peak values. Hence radiative emission and reabsorption are expected to be especially prominent, including interaction between molecular gas radiation and soot radiation. The P1/StepwiseGray model's local reabsorption contour matches the PMC/LBL contour quite closely, in contrast to the P1/Gray model. Therefore, the P1/Gray model gives significant errors in local radiation fields, in addition to global errors in computing reabsorption. In a coupled run, these errors may build over time and eventually lead to significant differences in local temperature and other flow variables.

4.3. Computational cost

Finally, the computational cost of the different radiation models in coupled runs is tabulated in Table 4. These runs have been carried out for the full-load EGR case with a WSR model, using 24 processors and a computational timestep of $3.4 \mu\text{s}$ (0.025 CAD). The P1/StepwiseGray requires 3.0 h, less than 10% of the time required for P1/FSK (43 h) and approximately 3% of the time required for PMC/LBL (96 h). This is a significant gain in efficiency, with less than 10% loss of accuracy. With

Fig. 4. Comparisons among radiation models for high-soot part-load case with EGR. (a) Cumulative radiative emission, reabsorption, radiation reaching walls. (b) Cumulative band-wise reabsorption.

Table 3

Total radiative emission, reabsorption and radiation reaching walls for increased soot cases.

Case	Fuel energy (J)	BL wall heat loss (J)	Radiative emission (J)	Radiation model	Radiative reabsorption (J)	Radiation reaching walls (J)
Part-load EGR	572	82.0	38.3	PMC/LBL	27.9	10.4
				P1/FSK	26.6 (4.5%)	11.5
				P1/Gray	20.1 (28%)	18.2
				P1/StepwiseGray	25.5 (8.5%)	12.8
Full-load EGR	2068	232.6	135.5	PMC/LBL	112.8	22.9
				P1/FSK	109.7 (2.7%)	25.4
				P1/Gray	100.9 (10.5%)	34.8
				P1/StepwiseGray	108.5 (3.8%)	27.5

Fig. 5. Instantaneous reabsorption contours at 12.5° aTDC on a cutting plane containing the injector axis for the normal (left) and high-soot (right) cases for the full-load EGR operating condition.

Table 4

Simulation time for coupled radiation runs for the full-load EGR case using a WSR model. The (%) after the radiation time is the percent of total simulation time required for the radiation calculation.

	Total time (h)	Rad. time (h)
PMC/LBL	107.5	96.7 (90%)
P1/FSK (16 RTE)	52.2	43.3 (80%)
P1/Gray	10.5	0.25 (2%)
P1/StepwiseGray	13.8	3.0 (22%)

the P1 method, the computational effort is dominated by property lookups/interpolations for the nongray spectral models, rather than by the RTE solver. Hence the simulation time does not scale simply with the number of RTEs solved. The Gray property table is an order of magnitude smaller than the StepwiseGray table, which in turn is orders of magnitude smaller than the FSK table, so that memory locality on modern processors plays a significant role.

5. Conclusions

A P1/StepwiseGray radiation model is proposed and compared with simpler (P1/Gray) and more detailed (PMC/LBL and P1/FSK) radiation models for a diesel engine. In the stepwise-gray model, the wavenumber spectrum is divided into five bands, emphasizing the CO₂ peak at 4.3 μm and the strong CO₂ and H₂O overlap at 2.7 μm. The P1 RTE equation is solved for each band using the band's Planck-mean absorption coefficient. Radiative emission and reabsorption are computed in a post-processing mode at part-load and full-load operating conditions with different levels of EGR

and soot. The results show that band b2 (around 4.3 μm) is responsible for most of the reabsorption and that the P1/StepwiseGray model captures that quite accurately. With higher soot, band b5 reabsorption becomes important, and the model continues to perform well. The results show that the P1/StepwiseGray model can compute reabsorption for different engine-relevant operating conditions with less than 10% error, while the error for the P1/Gray model is as high as 60%. The computational cost of the P1/StepwiseGray model is approximately 15 times lower than that of P1/FSK and 30 times lower than that of PMC/LBL. Hence the proposed P1/StepwiseGray model has great potential to provide a computationally less expensive alternative to detailed radiation models for engine relevant conditions. While the focus here is diesel engines, it is expected that the model should be broadly applicable to other high-pressure hydrocarbon-air combustion systems, with or without soot.

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Supplementary material

Supplementary material associated with this article can be found, in the online version, at doi:10.1016/j.proci.2018.08.024.

References

[1] G. Borman, K. Nishiwaki, *Prog. Energy Combust. Sci.* 13 (1) (1987) 1–46.

[2] T. Yoshikawa, R. Reitz, *J. Thermal Sci. Technol.* 4 (2009) 86–97.

[3] J. Abraham, V. Magi, SAE Technical Paper No. 970888 (1997).

[4] M.P. Mengüç, R. Viskanta, C.R. Ferguson, SAE Technical Paper No. 850503 (1985).

[5] J.F. Wiedenhofer, R.D. Reitz, *Numer. Heat Transf. A* 44 (7) (2003) 665–682.

[6] S.F. Fernandez, C. Paul, A. Sircar, et al., *Combust. Flame* 190 (2018) 402–415.

[7] C. Paul, A. Sircar, S. Ferreyro-Fernandez, et al., in: 10th U. S. National Combustion Meeting, College Park, Maryland, USA, 2017.

[8] M.F. Modest, *Radiative Heat Transfer*, third, Academic Press, Boston, 2013.

[9] M.F. Modest, D.C. Haworth, *Radiative Heat Transfer in Turbulent Combustion Systems*, Springer, 2016.

[10] L.S. Rothman, I.E. Gordon, R.J. Barber, et al., *J. Quant. Spectrosc. Radiat.* 111 (15) (2010) 2139–2150.

[11] H. Chang, T.T. Charalampopoulos, *Proc. R. Soc. Lond. A: Math., Phys. Eng. Sci.* 430 (1880) (1990) 577–591.

[12] G. Pal, A. Gupta, M.F. Modest, D.C. Haworth, *Combust. Flame* 162 (6) (2015) 2487–2495.

[13] D.K. Edwards, L.K. Glassen, W.C. Hauser, J.S. Tuchscher, *ASME. J. Heat Transf.* 89 (3) (1967) 219–228.

[14] M.F. Modest, K.K. Sikka, *J. Quant. Spectrosc. Radiat.* 48 (2) (1992) 159–168.

[15] D.A. Kaminski, X.D. Fu, M.K. Jensen, *Int. J. Heat Mass Transf.* 38 (17) (1995) 3161–3169.

[16] S. Mazumder, M.F. Modest, *Int. J. Heat Mass Transf.* 42 (1999) 971991.

[17] C.J. Du, D.B. Kittelson, SAE Technical Paper No. 830243 (1983).

[18] B. Menkiel, A. Donkerbroek, R. Uitz, R. Cracknell, L. Ganippa, *Combust. Flame* 159 (9) (2012) 2985–2998.

[19] V.I. Golovitchev, Chalmers University of Technology, Gothenburg, Sweden, 2000, <http://www.tfd.chalmers.se/%7Evaleri/MECH.html>.

[20] K.M. Leung, R.P. Lindstedt, W.P. Jones, *Combust. Flame* 87 (3) (1991) 289–305.

[21] D.C. Haworth, *Prog. Energy Combust. Sci.* 36 (2) (2010) 168–259.

[22] V.R. Mohan, D.C. Haworth, *Proc. Combust. Inst.* 35 (3) (2015) 3053–3060.

[23] OpenFOAM, <https://openfoam.org/>.