Simulations of Radiative Transfer in Combustion Systems and Further Developments of High-Order Spherical Harmonics Methods

Wenjun Ge

Department of Mechanical Engineering
School of Engineering
University of California, Merced
Merced, CA 95343, USA
wge@ucmerced.edu

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Outline

1. Introduction
2. Spectral Models and FSK Look-Up Table
3. RTE Solvers and Spherical Harmonics ($P_N$) Methods
4. Gray Examples
5. Applications in Combustion Simulations
Combustion is a chemical process in which a fuel reacts rapidly with oxygen and gives off heat.

High-fidelity simulations: chemistry, turbulence, radiation and their interactions.

Source: left from SpaceX, top-right from internet, bottom-right from Imamori, Y. et al., 2011

Source: left from Sandia NL, right from Pitsch, H., 2006
Radiative transfer

- Radiative transfer $\rightarrow$ electromagnetic waves $\rightarrow$ spectral dependence and travelling at $3 \times 10^8$ m/s in vacuum
- The radiative energy emitted by a blackbody is proportional to the fourth power of temperature $\rightarrow$ importance in high-temperature applications, nonlinearity
- Radiative transfer in participating/particulate media $\rightarrow$ emission, absorption and scattering $\rightarrow$ directional dependence

$$E_b(T) = \int E_{b\lambda} d\lambda = n^2 \sigma_{SB} T^4.$$

- Combustion problems generally involve temperature levels between 500 K and 2800 K so that the spectral ranges of interest in combustion applications are from 0.7 $\mu$m to 30 $\mu$m (or 300~14000 cm$^{-1}$ in wavenumber).

Figure: Blackbody emissive power spectrum.
Radiative properties of molecular gases

- Vibration-rotation bands from bound-bound transitions
- The broadening of the spectral lines due to collisions and Doppler effect
- Modern databases: HITEMP, HITRAN, CDSD.
- \( \kappa_\eta(Y, T, p) \)
Radiative transfer in an absorbing, emitting and scattering medium is formulated by considering conservation of radiative energy, known as the **radiative transfer equation** (RTE).

**RTE:**

\[
\hat{s} \cdot \nabla_\tau I_\eta + I_\eta = (1 - \omega_\eta)I_{b\eta} + \frac{\omega}{4\pi} \int_{4\pi} I_\eta(\hat{s}')\Phi_\eta(\hat{s} \cdot \hat{s}')d\Omega'
\]

The net energy balance at any location in the medium is obtained by integrating the spectral intensity over all directions and all wavenumbers. The **radiative heat source** \( S_{rad} \), is the difference between local absorption and emission:

**Radiative heat source:**

\[
S_{rad} = -\nabla \cdot \mathbf{q}_{rad} = -S_{emi} + S_{abs} = -4\kappa_P\sigma_{SB}T^4 + \int_0^{\infty} \kappa_\eta \int_{4\pi} I_\eta(\tau, \hat{s})d\Omega d\eta
\]
Coupling to the energy equation for turbulent reacting flows

DNS (direct numerical simulation):

\[
\frac{\partial \rho h}{\partial t} + \frac{\partial \rho h u_i}{\partial x_i} = -\frac{\partial J_i^h}{\partial x_i} + \frac{Dp}{Dt} + \tau_{ij}\frac{\partial u_j}{\partial x_i} + S_{rad}
\]

LES (large eddy simulation):

\[
\frac{\partial \rho \tilde{h}}{\partial t} + \frac{\partial \rho \tilde{h} u_i}{\partial x_i} = \frac{\partial (\rho \tilde{h} u_i - \rho \tilde{h} u_i)}{\partial x_i} - \frac{\partial J_i^h}{\partial x_i} + \frac{D\bar{p}}{Dt} + \bar{\tau}_{ij}\frac{\bar{u}_j}{x_i} + \bar{S}_{rad}
\]

RANS (Raynolds-Averaged Navier-Stokes):

\[
\frac{\partial \langle \rho \rangle \tilde{h}}{\partial t} + \frac{\partial \langle \rho \rangle \tilde{h} u_i}{\partial x_i} = \frac{\partial (\langle \rho \rangle \tilde{h} u_i - \langle \rho \rangle \tilde{h} u_i)}{\partial x_i} - \frac{\partial \langle J_i^h \rangle}{\partial x_i} + \frac{D\langle p \rangle}{Dt} + \langle\tau_{ij}\rangle\frac{\bar{u}_j}{x_i} + \langle S_{rad} \rangle
\]
Turbulence-radiation interaction (TRI)

Time-averaged radiative source \( \langle S_{rad} \rangle \) accounting for turbulence effects:

\[
\langle S_{rad} \rangle = -\langle S_{emi} \rangle + \langle S_{abs} \rangle = -4\pi \sigma_{SB} \langle \kappa_P I_b \rangle + \int_0^\infty \int_{4\pi} \langle \kappa_\eta I_\eta \rangle d\Omega d\eta
\]

Emission TRI and absorption TRI:

Emission TRI: \( \langle \kappa_P I_b \rangle \neq \kappa_P \langle \phi \rangle I_b (\langle T \rangle) \)

Absorption TRI: \( \langle \kappa_\eta I_\eta \rangle \neq \kappa_\eta \langle \phi \rangle I_\eta (\langle \phi \rangle) \)

e.g. autocorrelation of \( I_b \):

\[
\mathcal{R}_{I_b} = \frac{I_b (\langle T \rangle)}{\langle I_b (T) \rangle} = \frac{(\langle T \rangle)^4}{\langle T^4 \rangle} \neq 1
\]
Interactions between radiation and reacting flow

Figure: Schematic of the coupling between radiation and other sub-models
Example: Sandia Flame D×4 - RANS Simulation

- Not considering radiation will overpredict the peak temperature by up to 300 K
- Optically-thin model will underpredict the temperature about 200 K
Figure: Droplet dist. sized by droplet mass and temp. dist. Source: CTR Stanford and NASA, 2014

- No Rad. v.s. O.T. (gas phase)
- $T_{\text{peak}}$ from O.T. is 400 K lower
- lower evaporation rates from O.T
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Summary of spectral models

- Gray model (Planck-mean)
  - Weighted average over the entire spectrum
  - Cheap, but inaccurate; Underpredict the absorption
  - In practice: most popular

- Band models
  - Constant properties over narrow or wide bands
  - Case dependent accuracy
  - In practice: popular, becoming less popular

- Full-spectrum $k$-distribution (FSK) or similar models (WSGG)
  - Reordering reoccuring spectral absorption coefficients
  - Very accurate; implementation dependent
  - In practice: less popular, becoming more popular

- Line-by-line (LBL) Calculations
  - The most accurate
  - Only practical for stochastic solution methods (PMC)
  - In practice: becoming more popular with Monte Carlo solution method
Gray model: constant absorption coefficient

Weighting the spectral absorption coefficient $\kappa_\eta$ with the Planck function $I_{b\eta}$:

**Planck-mean absorption coefficient:**

$$\kappa_P = \frac{\int_0^\infty \kappa_\eta I_{b\eta} d\eta}{\int_0^\infty I_{b\eta} d\eta} = \frac{\int_0^\infty \kappa_\eta I_{b\eta} d\eta}{\sigma_{SB} T^4}$$

![Figure: Planck-mean absorption coefficients of CO$_2$, H$_2$O, CO, CH$_4$ and C$_2$H$_4$](image)

**Figure**: Planck-mean absorption coefficients of CO$_2$, H$_2$O, CO, CH$_4$ and C$_2$H$_4$
Full-spectrum $k$-distribution (FSK) model: reordering reoccurring $\kappa \eta$

- Reduce the number of evaluations of the RTE required from 1 million to $8 \sim 16$.

\[ \eta - \kappa \eta \]
\[ k - f(k), f(k) \text{ is a weighted sum of the number of points where } \kappa \eta = k \]
\[ g - k, g \text{ is the cumulative distribution function of } f(k) \]

Figure: (a) Spectral absorption coefficient (b) PDF and (c) $k$-distribution for 4.5 $\mu$m CO$_2$ band at $T=1000$ K and $p=1$ bar.
Comparison of different FSK implementations

- generate \( k \)-distributions for individual species
  - Narrowband database - very accurate, less memory, more runtime computing
  - Correlations - less accurate, less memory, less runtime computing

- generate \( k \)-distributions for the mixture
  - Look-up table - very accurate, more memory, less computing

Table: CPU time comparisons of generating 10,000 arbitrary \( k \)-distributions of mixtures.

<table>
<thead>
<tr>
<th>Database</th>
<th>Mixing model</th>
<th>CPU Time (s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Narrowband</td>
<td>Multiplication</td>
<td>1389.65</td>
</tr>
<tr>
<td></td>
<td>MRmixing</td>
<td>5904.59</td>
</tr>
<tr>
<td>Correlations</td>
<td>Multiplication</td>
<td>0.41</td>
</tr>
<tr>
<td></td>
<td>MRmixing</td>
<td>8.97</td>
</tr>
<tr>
<td>Look-up table</td>
<td>-</td>
<td>0.26</td>
</tr>
</tbody>
</table>
## Table: Precalculated thermodynamic states of the FSK look-up table.

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Range</th>
<th>Values</th>
<th>Number of points</th>
</tr>
</thead>
<tbody>
<tr>
<td>Species</td>
<td>CO&lt;sub&gt;2&lt;/sub&gt;, H&lt;sub&gt;2&lt;/sub&gt;O and CO</td>
<td></td>
<td>3</td>
</tr>
<tr>
<td>Pressure (total)</td>
<td>0.1 ~ 0.5 bar</td>
<td>Every 0.1 bar</td>
<td>34</td>
</tr>
<tr>
<td></td>
<td>0.7 bar</td>
<td>0.7 bar</td>
<td></td>
</tr>
<tr>
<td></td>
<td>1.0 ~ 14.0 bar</td>
<td>Every 1.0 bar</td>
<td></td>
</tr>
<tr>
<td></td>
<td>15.0 ~ 80.0 bar</td>
<td>Every 5.0 bar</td>
<td></td>
</tr>
<tr>
<td>Gas temperature</td>
<td>300~ 3000 K</td>
<td>Every 100 K</td>
<td>28</td>
</tr>
<tr>
<td>Reference temperature</td>
<td>300~ 3000 K</td>
<td>Every 100 K</td>
<td></td>
</tr>
<tr>
<td>Mole fraction of CO&lt;sub&gt;2&lt;/sub&gt;</td>
<td>0.0 ~ 0.05</td>
<td>Every 0.01</td>
<td>10</td>
</tr>
<tr>
<td></td>
<td>0.25 ~ 1.0</td>
<td>Every 0.25</td>
<td></td>
</tr>
<tr>
<td>Mole fraction of H&lt;sub&gt;2&lt;/sub&gt;O</td>
<td>0.0 ~ 0.05</td>
<td>Every 0.01</td>
<td>13</td>
</tr>
<tr>
<td></td>
<td>0.1 ~ 0.2</td>
<td>Every 0.05</td>
<td></td>
</tr>
<tr>
<td></td>
<td>0.25 ~ 1.0</td>
<td>Every 0.25</td>
<td></td>
</tr>
<tr>
<td>Mole fraction of CO</td>
<td>0.0 ~ 0.5</td>
<td>{0.0, 0.01, 0.05, 0.1, 0.25, 0.5}</td>
<td>6</td>
</tr>
</tbody>
</table>

- The size of the table is about 5 GB.
- Apply dynamic loading to reduce memory demand.
- The look-up table can be customized for specific needs.
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Summary of RTE solvers

- **Optically Thin (O.T.)**
  - No absorption, only consider emission
  - Cheap, only useful for optically thin media
  - *In practice: currently most popular*

- **Discrete Ordinates Method (DOM) or similar concepts**
  - Discretize the angular profile of intensity by several finite directions
  - Cheap and accurate for non-scattering media, suffers from ray effects and false scattering for scattering media or reflecting surfaces
  - *In practice: very popular, available in most commercial CFD softwares, DOM_{8\times8} is usually good enough*

- **Spherical Harmonics (P_N) Method**
  - Approximate the angular profile of intensity by a truncated series of spherical harmonics (a spectral method)
  - Very accurate for optically thick media; not accurate when intensity is directionally anisotropic
  - *In practice: P_1 is very popular, high-order P_N needs more research*

- **Photon Monte Carlo (PMC)**
  - The most accurate and robust
  - Used to be considered impractical
  - *In practice: becoming more and more popular*
Spherical harmonics ($P_N$) method

Truncated series of spherical harmonics of order $N$:

$$I(\tau, \hat{s}) = \sum_{n=0}^{N} \sum_{m=-n}^{n} I_n^m(\tau) Y_n^m(\hat{s}), \quad Y_n^m(\psi, \theta) = \begin{cases} 
\cos(m\psi) P_n^m(\cos \theta) & \text{for } m \geq 0 \\
\sin(|m|\psi) P_n^m(\cos \theta) & \text{for } m < 0
\end{cases}$$

- Use spherical harmonics as bases for the angular profile of intensity
- Transform the RTE into equations of the intensity coefficients $I_n^m$
The 3-D formulation

Governing equations

- Substitute the spherical harmonics series into the RTE;

- Multiply the resulting equation by $Y_n^m$ and integrate the whole equation over a solid angle of $4\pi$; One obtains $(N + 1)^2$ first-order PDEs;

- The second-order elliptic formulation is obtained by eliminating the odd order intensity coefficients ($I_n^m$ with odd $n$) by their relation to the gradients of $I_{n+1}^m$ and $I_{n-1}^m$; This will reduce the number of governing equations to $N(N + 1)/2$.

<table>
<thead>
<tr>
<th>$n$</th>
<th>Intensity Coefficients</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>$I_0^0$</td>
</tr>
<tr>
<td>2</td>
<td>$I_2^{-2}$ $I_4^{-1}$ $I_4^0$ $I_4^1$ $I_4^2$</td>
</tr>
<tr>
<td>4</td>
<td>$I_4^{-4}$ $I_6^{-3}$ $I_6^{-2}$ $I_6^{-1}$ $I_6^0$ $I_6^1$ $I_6^2$ $I_6^3$ $I_6^4$ $I_6^5$ $I_6^6$</td>
</tr>
<tr>
<td>6</td>
<td>$I_6^{-6}$ $I_6^{-5}$ $I_6^{-4}$ $I_6^{-3}$ $I_6^{-2}$ $I_6^{-1}$ $I_6^0$ $I_6^1$ $I_6^2$ $I_6^3$ $I_6^4$ $I_6^5$ $I_6^6$</td>
</tr>
<tr>
<td>$n$</td>
<td>$I_n^{-n}$ $\ldots$ $I_n^{-3}$ $I_n^{-2}$ $I_n^{-1}$ $I_n^0$ $I_n^1$ $I_n^2$ $I_n^3$ $\ldots$ $I_n^n$</td>
</tr>
</tbody>
</table>

Table: Intensity coefficients employed for 3-D Cartesian formulation
Governing equations

For each $Y^m_n : n = 0, 2, \ldots, N - 1, 0 \leq m \leq n$:

$$
\sum_{k=1}^{3} \left\{ \left( L_{xx} - L_{yy} \right) \left[ (1 + \delta_{m2}) a_{k}^{nm} I_{n+4-2k}^m - \frac{\delta_{m1}}{2} c_{k}^{nm} I_{n+4-2k}^m + e_{k}^{nm} I_{n+4-2k}^{m+2} \right] \\
+ \left( L_{xz} + L_{zx} \right) \left[ (1 + \delta_{m1}) b_{k}^{nm} I_{n+4-2k}^{m-1} + d_{k}^{nm} I_{n+4-2k}^{m+1} \right] \\
+ \left( L_{xy} + L_{yx} \right) \left[ -(1 - \delta_{m2}) a_{k}^{nm} I_{n+4-2k}^{-(m-2)} + \frac{\delta_{m1}}{2} c_{k}^{nm} I_{n+4-2k}^{-(m-1)} + e_{k}^{nm} I_{n+4-2k}^{-(m+2)} \right] \\
+ \left( L_{yz} + L_{zy} \right) \left[ -(1 - \delta_{m1}) b_{k}^{nm} I_{n+4-2k}^{-(m-1)} + d_{k}^{nm} I_{n+4-2k}^{-(m+1)} \right] \\
+ \left( L_{xx} + L_{yy} - 2L_{zz} \right) c_{k}^{nm} I_{n+4-2k}^{m} \right\} \\
+ \left[ L_{zz} - (1 - \omega \delta_{0n}) \right] I_{n}^{m} = -(1 - \omega) I_{b} \delta_{0n}
$$

where the operators: $L_{xy} = \frac{1}{\beta} \frac{\partial}{\partial x} \left( \frac{1}{\beta} \frac{\partial}{\partial y} \right)$

Each governing equation is characterized by the spherical harmonics $Y^m_n$. 
Marshak’s boundary conditions

For each $\bar{Y}_{2i-1}^{\pm m}$, $i = 1, 2, \cdots, (N + 1)/2$:

\[
0 = \sum_{l=0}^{N-1/2} \sum_{m'=-2l}^{2l} p^m_{2l,2i-1} \bar{\Delta}^{2l}_{\pm m,m'} I^{m'}_{2l} \\
- \frac{\partial}{\partial \tau^x} \sum_{l=l_1}^{N-1/2} \sum_{m'=-2l}^{2l} \left[ (1 \pm \delta_{m,1}) u^m_{l,i} \bar{\Delta}^{2l}_{\mp(m-1),m'} - v^m_{l,i} \bar{\Delta}^{2l}_{\mp(m+1),m'} \right] I^{m'}_{2l} \\
\pm \frac{\partial}{\partial \tau^y} \sum_{l=l_2}^{N-1/2} \sum_{m'=-2l}^{2l} \left[ (1 \mp \delta_{m,1}) u^m_{l,i} \bar{\Delta}^{2l}_{\pm(m-1),m'} + v^m_{l,i} \bar{\Delta}^{2l}_{\pm(m+1),m'} \right] I^{m'}_{2l} \\
- \frac{\partial}{\partial \tau^z} \sum_{l=0}^{N-1/2} \sum_{m'=-2l}^{2l} w^m_{l,i} \bar{\Delta}^{2l}_{\pm m,m'} I^{m'}_{2l}
\]

Each boundary condition is characterized by the local spherical harmonics $\bar{Y}_{2i-1}^{m}$. 

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2-D axisymmetric formulation

$I$ varies with $r$ and axially with $z$, but not azimuthally with $\phi$

\[
I (r, \phi, z; \theta, \psi + \phi) = I (r, 0, z; \theta, \psi)
\]

\[
I^m_n (r, \phi, z) = I^m_n (r, 0, z) \cos m\phi = \hat{I}^m_n \cos m\phi
\]

\[
I^{-m}_n (r, \phi, z) = I^m_n (r, 0, z) \sin m\phi = \hat{I}^m_n \sin m\phi
\]

Employing the above relations to the general 3-D formulation, the number of governing equations is reduced to $(N + 1)^2 / 4$ for axisymmetric geometry.

### Table: Intensity coefficients employed for 2-D axisymmetric formulation

<table>
<thead>
<tr>
<th>$n$</th>
<th>Intensity Coefficients</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>$\hat{I}^0_0$</td>
</tr>
<tr>
<td>2</td>
<td>$\hat{I}^2_2$, $\hat{I}^1_2$, $\hat{I}^2_2$</td>
</tr>
<tr>
<td>4</td>
<td>$\hat{I}^4_4$, $\hat{I}^1_4$, $\hat{I}^2_4$, $\hat{I}^3_4$, $\hat{I}^4_4$</td>
</tr>
<tr>
<td>6</td>
<td>$\hat{I}^6_6$, $\hat{I}^1_6$, $\hat{I}^2_6$, $\hat{I}^3_6$, $\hat{I}^4_6$, $\hat{I}^5_6$, $\hat{I}^6_6$</td>
</tr>
</tbody>
</table>

$\hat{I} = \text{Intensity Coefficients}$

$\hat{I}^m_n$ = Coefficients for terms in $r$, $\phi$, and $z$.

$N = \text{Number of terms considered}$.
Development of special boundary conditions

- Specified radiative flux at the wall;
- Symmetry/specular reflection boundaries;
- Mixed diffuse-specular reflection surfaces;
- Cyclic boundaries.
Implementation

- Implementation platform → OpenFOAM® 2.2.x
- The spatial discretization → standard second-order finite volume method
- Solution method → segregated iterative method
- Solution of each governing equation (inner iterations) → the incomplete Cholesky preconditioned conjugated gradient method (PCG)
- Resolving the coupling between governing equations and Robin-type BCs (outer iterations) → Gauss Seidel method
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Problem 1: 1-D slab with homogeneous radiative properties

1-D Cartesian examples represent the radiative transfer between two infinitely long parallel plates;

Geometry: 1-D Slab (1×1×101);

All properties are normalized so that the only difference is the optical thickness;

\[ -\nabla \cdot \mathbf{q} \quad \text{and} \quad G \quad \text{from} \quad P_1 \quad \text{to} \quad P_7 \quad \text{are compared to exact solution}; \]

Intensity \( I \) is reconstructed at the center \( (z/L = 0.5) \) and is also compared with the exact intensity.
Results of $\tau=10.0$ and $\tau=1.0$

$\tau=10$ (Optically thick):

$\tau=1$ (Optically intermediate):
Results of $\tau=0.5$ and $\tau=0.001$

$\tau=0.5$ (Optically intermediate):

$\tau=0.001$ (Optically thin):
Problem 2: 1-D slab with flame-like variable radiative properties

Geometry: 1-D Slab (200 cells), $L=0.52\times2$ m;
Rotational invariance and comparison with PMC

Table: Comparison of CPU time (s)

<table>
<thead>
<tr>
<th>Num. of cells</th>
<th>$\tau_L$</th>
<th>$P_1$</th>
<th>$P_3$</th>
<th>$P_5$</th>
<th>$P_7$</th>
<th>PMC (0.1M×10)</th>
<th>PMC (5M×10)</th>
</tr>
</thead>
<tbody>
<tr>
<td>200</td>
<td>0.886</td>
<td>0.01</td>
<td>0.10</td>
<td>0.52</td>
<td>1.34</td>
<td>45.7</td>
<td>2532.1</td>
</tr>
</tbody>
</table>

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Problem 3: 2-D square geometry

Table: Comparison of CPU time (s)

<table>
<thead>
<tr>
<th>No. of cells</th>
<th>$C_k$</th>
<th>$\tau_R$</th>
<th>$P_1$</th>
<th>$P_3$</th>
<th>$P_5$</th>
<th>$P_7$</th>
<th>PMC</th>
</tr>
</thead>
<tbody>
<tr>
<td>2,601 (51×51)</td>
<td>$C_k$=1</td>
<td>12.7</td>
<td>0.02</td>
<td>0.75</td>
<td>4.71</td>
<td>7.0</td>
<td>459 (5M×10)</td>
</tr>
<tr>
<td></td>
<td>$C_k$=0.1</td>
<td>1.27</td>
<td>0.02</td>
<td>0.87</td>
<td>5.05</td>
<td>9.33</td>
<td>125.5 (0.5M×10)</td>
</tr>
<tr>
<td></td>
<td>$C_k$=0.01</td>
<td>0.127</td>
<td>0.02</td>
<td>1.78</td>
<td>7.09</td>
<td>19.2</td>
<td>21.2 (0.05M×10)</td>
</tr>
</tbody>
</table>
Problem 4: A 45-degree wedge and a full cylinder

\[ I_b = 1 + \frac{20}{R^4} r^2 (R^2 - r^2) \quad \text{W} \cdot \text{m}^{-3} \]

\[ \kappa = \left[ 1 + \frac{15}{R^4} (R^2 - r^2)^2 \right] \left( 1 + 0.5 \frac{r}{R} \cos 8\theta \right), \quad \text{m}^{-1} \]

\[ 0 \leq r \leq R = 0.5, \quad \text{m} \]
Sandia Flame D is a turbulent piloted jet flame with a Reynolds number of $Re_D = 22,400$

Fuel: Methane

Diameter of main jet: $d_j = 7.2$ mm

The flame is scaled up to show radiation effects.

<table>
<thead>
<tr>
<th></th>
<th>Sandia Flame D</th>
<th>Sandia Flame D×4</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$d$ (mm)</td>
<td>$u$ (m/s)</td>
</tr>
<tr>
<td>main jet</td>
<td>7.2</td>
<td>49.89</td>
</tr>
<tr>
<td>pilot</td>
<td>18.864</td>
<td>10.57</td>
</tr>
<tr>
<td>co-flow</td>
<td>258.2</td>
<td>0.90</td>
</tr>
</tbody>
</table>

$Re_D = 22,400$

Chemistry model: GRI-Mech 2.11 (49 species and 277 reactions), PaSR (partially-stirred reactor)

Turbulence model: Standard two-equation $k-\epsilon$ model

Radiation models: O.T., PN+FSK, DOM+FSK, PMC+LBL

Source: Sandia NL
Adding radiation models cools down the flame and results in around 3% less-complete combustion.

Nearly 30% of the combustion heat release is transferred to the environment through radiation.
Computational cost

Table: Average CPU time per time step (radiation is evaluated once per 1/10/100/250 time steps for the PN/DOM+FSK solvers and the average $t_{RTE} + t_{overhead}$ and $t_{FSK}$ are only shown for runs with radiation evaluated once per time step)

<table>
<thead>
<tr>
<th>Radiation Solver</th>
<th>Average CPU Time (s)</th>
<th>$t_{RTE} + t_{overhead}$ (s)</th>
<th>$t_{FSK}$ (s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>No Rad</td>
<td>0.82</td>
<td>/</td>
<td>/</td>
</tr>
<tr>
<td>P1+FSK</td>
<td>0.97/0.85/0.82/0.82</td>
<td>0.09</td>
<td>1 second-order PDE</td>
</tr>
<tr>
<td>P3+FSK</td>
<td>1.05/0.87/0.83/0.83</td>
<td>0.17</td>
<td>4 second-order PDE</td>
</tr>
<tr>
<td>P5+FSK</td>
<td>1.36/0.88/0.84/0.84</td>
<td>0.48</td>
<td>9 second-order PDE</td>
</tr>
<tr>
<td>P7+FSK</td>
<td>1.64/0.90/0.85/0.85</td>
<td>0.76</td>
<td>16 second-order PDE</td>
</tr>
<tr>
<td>DOM 2×4+FSK</td>
<td>1.11/0.86/0.85/0.84</td>
<td>0.23</td>
<td>8 first-order PDE</td>
</tr>
<tr>
<td>DOM 4×4+FSK</td>
<td>1.20/0.87/0.85/0.84</td>
<td>0.32</td>
<td>16 first-order PDE</td>
</tr>
<tr>
<td>DOM 4×8+FSK</td>
<td>1.42/0.91/0.86/0.86</td>
<td>0.54</td>
<td>32 first-order PDE</td>
</tr>
<tr>
<td>DOM 8×8+FSK</td>
<td>1.78/0.94/0.87/0.87</td>
<td>0.9</td>
<td>64 first-order PDE</td>
</tr>
<tr>
<td>PMC+LBL</td>
<td>0.87</td>
<td>0.05</td>
<td>5,000 with time-blending</td>
</tr>
<tr>
<td>PMC+LBL</td>
<td>0.92</td>
<td>0.10</td>
<td>10,000 with time-blending</td>
</tr>
</tbody>
</table>

All computations are performed on twelve 2.66 GHz Intel Xeon X7460 processors.
Sandia Flame D×4, a frozen snapshot study

A mixture of hot CO₂, H₂O and CO:

Spectral model for $P_N$ and DOM: FSK-Table with eight quadrature points
Spectral model for for PMC: LBL
Grids

- Radiative calculations are conducted on a 2-D wedge, a 3-D cylinder and a 3-D cuboid
- The same axisymmetric distributions of temperature and mole fractions
Results from different meshes

$-q_r$ (m) at $z = 1.0$ m

Negative Radiative Heat Source $q_r$ (kW/m$^3$)

0 0.05 0.1 0.15 0.2 0.25

0
500
1000

2D Wedge P7+FSK
2D Wedge DOM8x8+FSK
2D Wedge PMC-LBL
3D Cylinder P7+FSK
3D Cylinder DOM8x8+FSK
3D Cylinder PMC-LBL
3D Cuboid P7+FSK
3D Cuboid DOM8x8+FSK
3D Cuboid PMC+LBL
Negative radiative heat source $\nabla \cdot \mathbf{q}$ from different RTEs
The most important quadratures

Table: Optical thickness $\tau_{R,g}$ along radius at $z = 1.0$ m for each quadrature point

<table>
<thead>
<tr>
<th>Index</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
<th>6</th>
<th>7</th>
<th>8</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\tau_{R,g}$</td>
<td>0.0006</td>
<td>0.0035</td>
<td>0.0120</td>
<td>0.03348</td>
<td>0.08081</td>
<td>0.2112</td>
<td>0.8327</td>
<td>3.5118</td>
</tr>
</tbody>
</table>

![Graph showing negative radiative heat source versus radius for 8th and 7th quadrants.](image)
High-temperature oxy-natural gas flame

Oxy-fuel combustion is the process of burning a fuel using pure oxygen instead of air as the primary oxidant. A 0.8 MW oxy-natural gas burner (OXYFLAM-2A) from the OXYFLAME project:
Gray Spectral Model, $z = 1.42$ m

Table: Comparison of CPU time (s) of the RTE solvers for the gray case

<table>
<thead>
<tr>
<th></th>
<th>$P_1$</th>
<th>$P_3$</th>
<th>$P_5$</th>
<th>$P_7$</th>
<th>DOM$_{2\times4}$</th>
<th>DOM$_{4\times4}$</th>
<th>DOM$_{4\times8}$</th>
<th>DOM$_{8\times8}$</th>
<th>PMC</th>
</tr>
</thead>
<tbody>
<tr>
<td>Gray</td>
<td>0.22</td>
<td>2.95</td>
<td>10.2</td>
<td>27.8</td>
<td>4.53</td>
<td>5.45</td>
<td>6.66</td>
<td>13.9</td>
<td>223 (1M×10)</td>
</tr>
</tbody>
</table>
Table: Comparison of CPU time (s) of the RTE solvers for the nongray case

<table>
<thead>
<tr>
<th></th>
<th>P_1</th>
<th>P_3</th>
<th>P_5</th>
<th>P_7</th>
<th>DOM_{2\times4}</th>
<th>DOM_{4\times4}</th>
<th>DOM_{4\times8}</th>
<th>DOM_{8\times8}</th>
<th>PMC</th>
</tr>
</thead>
<tbody>
<tr>
<td>Nongray</td>
<td>0.95</td>
<td>12.8</td>
<td>49.7</td>
<td>111</td>
<td>13.1</td>
<td>25.8</td>
<td>39.4</td>
<td>77.5</td>
<td>1672 (10M\times10)</td>
</tr>
</tbody>
</table>
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RADIATIVE EQUILIBRIUM IN A RECTANGULAR ENCLOSURE BOUNDED BY GRAY WALLS

MICHAEL F. MODEST*
National Research Council, NASA-Lyndon B. Johnson Space Center, Houston, Texas 77058, U.S.A.

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