Numerical Implementation of Models for Radiative Properties of Gases and Particles in Combustion Applications

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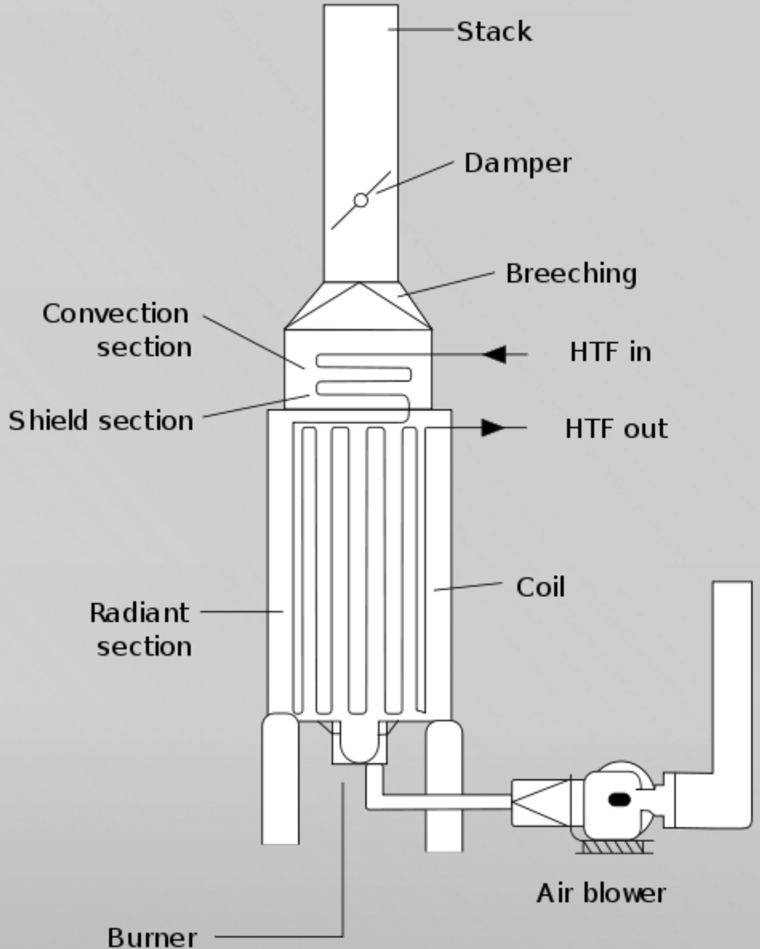
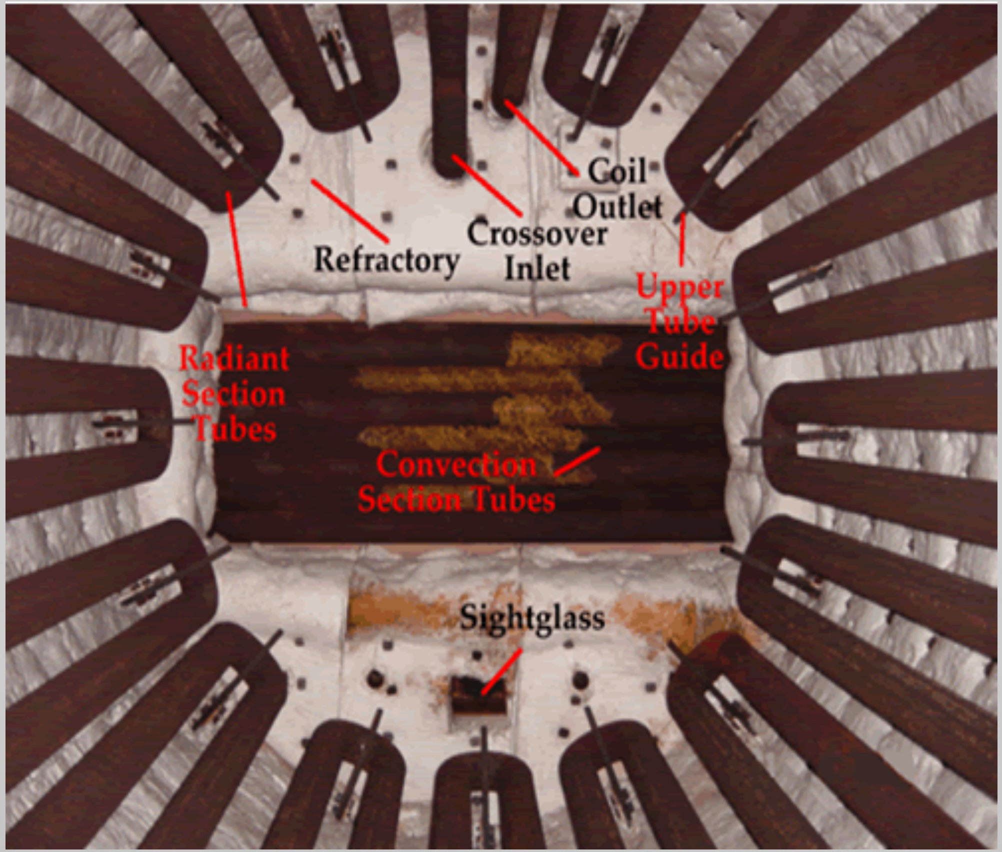
OUTLINE

- Overview of Radiation Heat Transfer
- Pertinence to Combustion Simulations
- Models for Radiative Properties of Molecular Gases
- Models for Radiative Properties of Particulate Media

Radiation Heat Transfer in Industrial Furnaces





Heat Transfer

Conservation of Energy Equation:

$$\partial \rho e/\partial t = -\boldsymbol{\nabla}\cdot \rho e\boldsymbol{v} - \boldsymbol{\nabla}\cdot P\boldsymbol{v} - \boldsymbol{\nabla}\cdot \boldsymbol{q} + S$$

where the heat flux vector, $\boldsymbol{q}$, is defined as

$$\boldsymbol{q} = -k\boldsymbol{\nabla}T + \boldsymbol{q}_r + \sum_j n_j h_j \boldsymbol{V}_j + \boldsymbol{q}_{d-1}.$$

ρ - total mass;

ρe - energy density;

$\boldsymbol{v}$ - fluid velocity;

P - pressure;

$\boldsymbol{q}_r$ - radiation heat flux;

n_i - number density of chemical species;

$\boldsymbol{V}_i$ - diffusion velocity;

S - local volumetric heat source/sink.

Radiative Transfer Equation

Derived through energy balance on the radiative energy traveling in the direction of $\boldsymbol{s}$ within a small pencil of rays:

$$\frac{\partial I_\eta}{\partial s} = k_\eta I_{b\eta} - k_\eta I_\eta - \sigma_{s\eta} I_\eta + \frac{\sigma_{s\eta}}{4\pi} \int_{4\pi} I_\eta(\boldsymbol{s}_i)\Phi(\boldsymbol{s}_i, \boldsymbol{s})\, d\Omega_i .$$

Divergence of the radiative heat flux:

$$\nabla\cdot\boldsymbol{q}_\eta = 4\pi k_\eta I_{b\eta} - (k_\eta + \sigma_{s\eta}) \int_{4\pi} I_\eta(\boldsymbol{s})\, d\Omega + \sigma_{s\eta} \int_{4\pi} I_\eta(\boldsymbol{s}_i)\, d\Omega_i .$$

I_η - spectral intensity of radiation;

$I_{b\eta}$ - blackbody spectral intensity;

Ω - solid angle;

k_η - spectral absorption coefficient

$\sigma_{s\eta}$ - spectral scattering coefficient

Considerations

- Computationally expensive and time-consuming to solve (60-70% of computational time);
- The accuracy of radiative transfer predictions in combustion systems cannot be better than the radiative properties of the combustion products used in the analysis:
  - water vapor
  - carbon dioxide
  - carbon monoxide
  - sulfur dioxide
  - nitrous oxide
  - soot
  - fly-ash
  - pulverized coal
  - char
  - fuel droplets

Radiation Transfer Equation in **ARCHES**:

- Current Method: *Discrete Ordinates Method* – discretizing the entire solid angle (Ω=4π) using a finite number of ordinate directions and corresponding weight factors. The RTE is written for each ordinate and the integral terms are replaced by a quadrature summed over each coordinate.
- New Method in development: *Monte Carlo Ray Tracing* – simulating a finite number of photon histories through a random number generator.
    - Each photon history is assigned initial energy, position, and direction;
    - The number of free paths that the photon propagates is determined stochastically;
    - The absorption and scattering coefficients are sampled to determine if the collided photon is absorbed or scattered by the gas molecules and particles in the medium.
    - If scattered, the distribution of scattering angles is sampled and a new direction is assigned to the photon. If elastic scattering – a new energy is determined by conservation of energy and momentum.

Radiative Properties of Molecular Gases

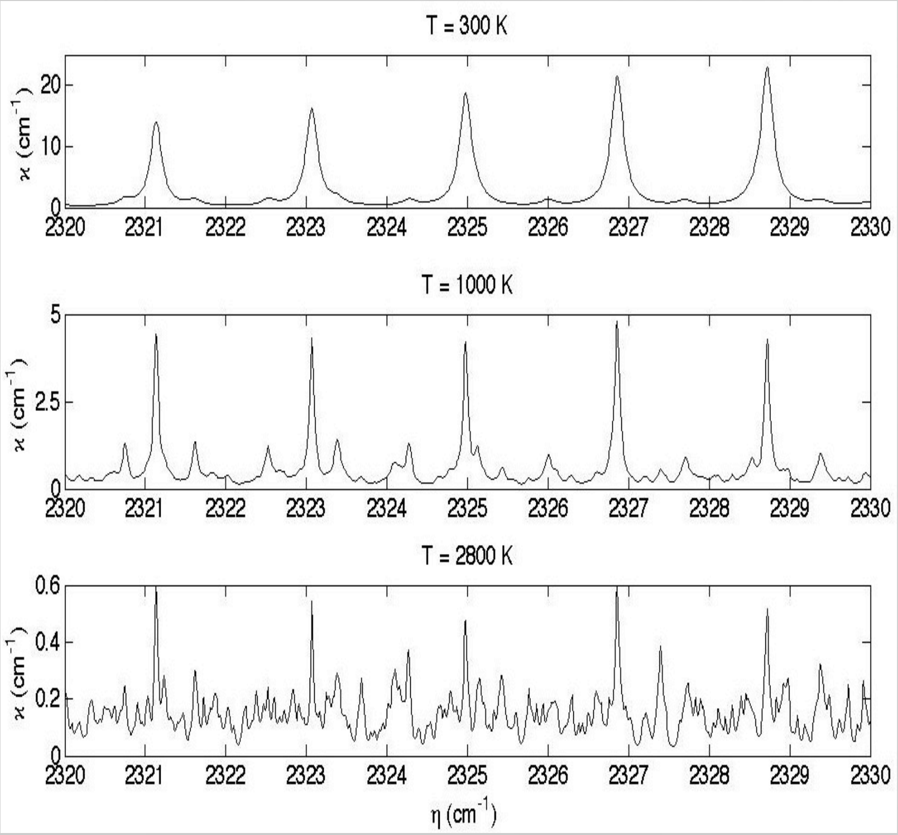
- Strong and rapid variation across the spectrum;
- Assumption of "grey gas" is almost never a good assumption;
- Line-by-line calculations, relying on detailed knowledge about the absorption coefficient for every spectral line, are infeasible for combustion computations:

SPECIES	SPECTRAL LINES
H_2O	114,241,164
CO_2	11,193,608
N_2	105,356
CO	113,631
NO	115,610

- Scattering in gases is negligible and is neglected for combustion applications.

Radiative properties of molecular gases

- Absorption coefficient gyrates violently across the band.
- Spectral integration for total intensity, total radiative heat flux, or the divergence of heat flux, is extremely difficult.
- At the high temperatures the spectral lines narrow considerably, decreasing line overlap; the strengths of the lines that were most important at low temperature decrease, and “hot lines” that were negligible at room temperature become important.
- Integration across the entire spectrum of such erratic functions is a formidable task. This prompted the development of approximate narrow models.



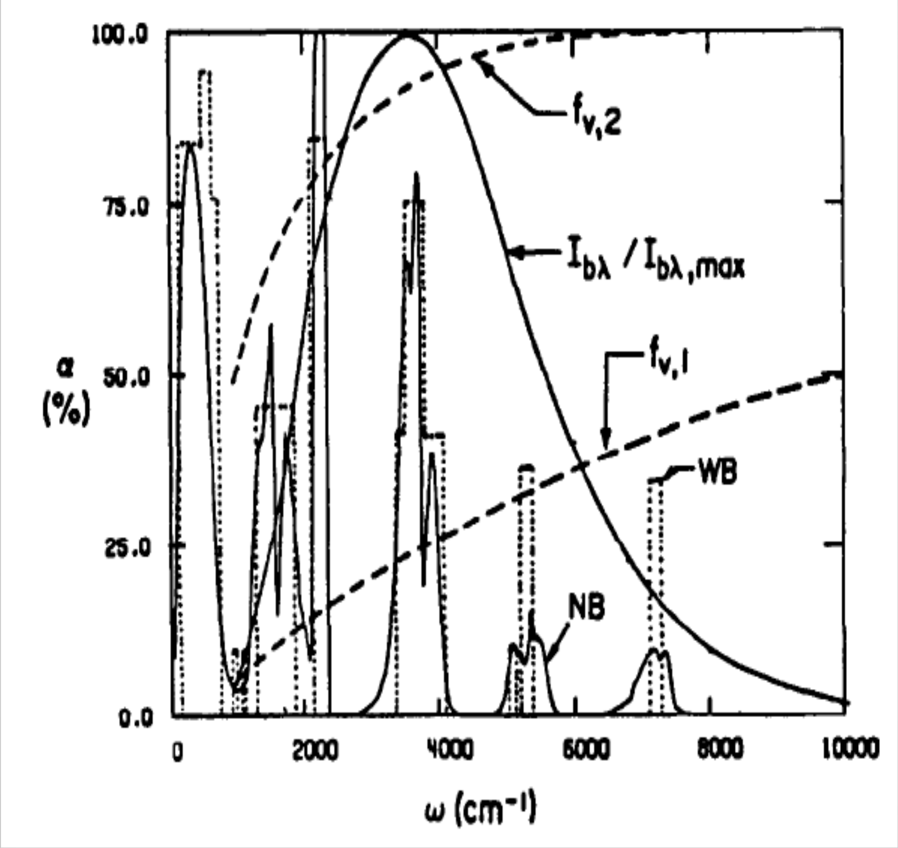
Spectral absorption coefficient, κ, for small amounts of CO_2 in nitrogen, across a small portion of the CO_2 4.3 μm band (Modest and HITRAN database).

Current method

- Simple models for predicting the radiative properties of gases;
- Based on Hottel's charts for gas properties as functions of temperatures, pressure and concentration of a gas;
- Appropriate polynomials are curve-fitted for a given temperature and pressure (=1atm);
- The gray absorption coefficient is obtained for a given mean beam length L_m:

$$k = -1/L_m \ln(1-\varepsilon)$$

- Uniform gas mixture (uniform composition, temperature, and pressure);
- Inappropriate if scattering particles are present.



Spectral absorptivities of H2O-CO2-air mixture (Viskanta, Menguc).

Total Properties and Implementation (of existing models)

$$k_{\eta,tot} = \sum_{i} k_{\eta,poly-i} + k_{\eta,soot} + \sum_{j} k_{\eta,gas-i}\, x_{gas-i} \ .$$

- Soot absorption coefficient (Rayleigh's theory), given a complex index of refraction ($m = n - ik$) and volume fraction, f_v:

$$k_{\eta,soot} = \frac{36\pi n k}{(n^2 - k^2 + 2)^2 + 4n^2 k^2}\, f_v\, \eta.$$

"Grey gas" absorption coefficients

- As the characteristic dimension of the enclosure decreases the gas becomes thinner, and eventually in the limit of optically thin gas the mean absorption coefficient becomes identical to the Planck's mean absorption coefficient:

$$k_P = \int_0^\infty I_{b\eta} k_\eta \, d\eta \Big/ \int_0^\infty I_{b\eta} \, d\eta = \frac{\pi}{\sigma T^4} \int_0^\infty I_{b\eta} k_\eta \, d\eta \, .$$

- With increasing size of the enclosure, the gas becomes optically thicker and the mean absorption coefficient approaches Rosseland's mean absorption coefficient:

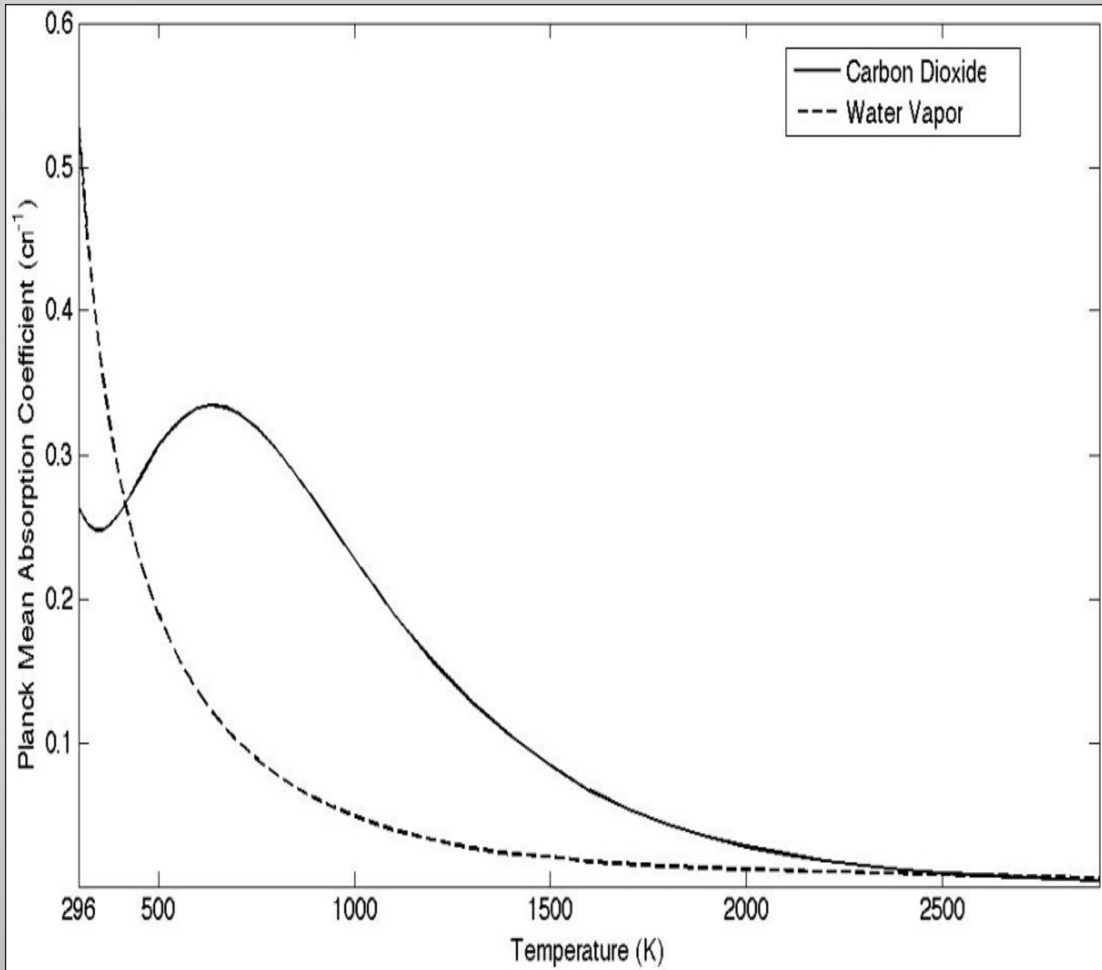
$$\frac{1}{k_R} = \int_0^\infty \frac{1}{k_\eta} \frac{dI_{b\eta}}{dT} \, d\eta \Big/ \int_0^\infty \frac{dI_{b\eta}}{dT} \, d\eta = \frac{\pi}{4\sigma T^3} \int_0^\infty \frac{1}{k_\eta} \frac{dI_{b\eta}}{dT} \, d\eta \, .$$

- Effective mean absorption coefficient, which is a function of path length:

$$k_e(L) = \int_0^\infty I_{b\eta} k_\eta e^{-k_\eta L} \, d\eta \Big/ \int_0^\infty I_{b\eta} e^{-k_\eta L} \, d\eta \, .$$

“Grey gas” absorption coefficients computation

"Grey gas" absorption coefficients



Error from interpolation:

$$\epsilon = \max_{k} |k_{interp} - k| / k$$

N_T	10	20	45
ϵ	$1.85e^{-2}$	$3.3e^{-3}$	$1.5e^{-3}$

Planck mean absorption coefficient for carbon dioxide and water vapor

k-Distribution method (Taine et al., Modest)

- Gas absorption coefficient varies wildly even across a very narrow spectrum, attaining the very same values of k_η many times, each time producing identical intensity field with the medium;
- Re-order absorption coefficient field into a smooth, monotonously increasing function, assuring that each field intensity calculation is performed only once.
- Full-spectrum k-distribution:

$$f(T,k)=\frac{1}{I_b}\int_0^\infty I_{b\eta}(T)\delta(k-k_\eta)\,d\eta .$$

- k-Distributions at different Planck function temperatures are different.
- However, the sharp peaks of $f(T,k)$ are due to maxima and minima of k_η, which remain the same for all Planck function temperatures.
- The ratio of any two full-spectrum k-distributions will produce a smooth function.

Transformation of the RTE

$$\frac{\partial I_g}{\partial s} = k\left(I_b(T) - I_g\right) - \sigma_{s\eta}\left(I_g - \frac{1}{4\pi}\int_{4\pi} I_g(\mathbf{s}_i)\Phi(\mathbf{s}_i, \mathbf{s})\, d\Omega_i\right),$$

where

$$I_g = \int_0^\infty I_\eta(T)\delta(k - k_\eta)\, d\eta \,/\, f(T,k),$$

$$g(T,k) = \int_0^k f(T,k)\, dk,$$

$$I = \int_0^\infty I_\eta\, d\eta = \int_0^1 I_g\, dg.$$

k-distribution Model

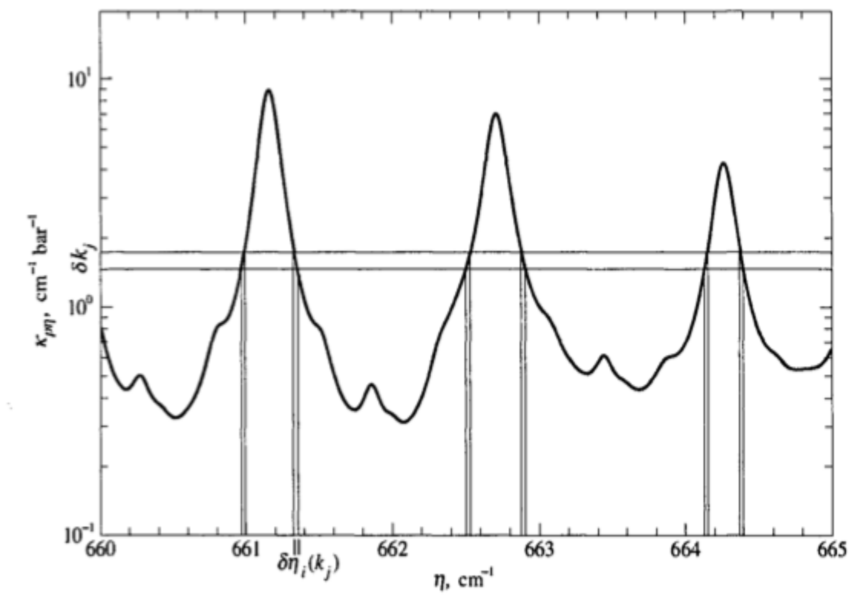
$$f(T,k_j)\delta k_j \cong \sum_i \frac{I_{b\eta i}(T)}{I_b(T)} \left|\frac{\delta\eta}{\delta k_\eta}\right|_i \left[H(k_j+\delta k_\eta-k_\eta)-H(k_j-k_\eta)\right]$$

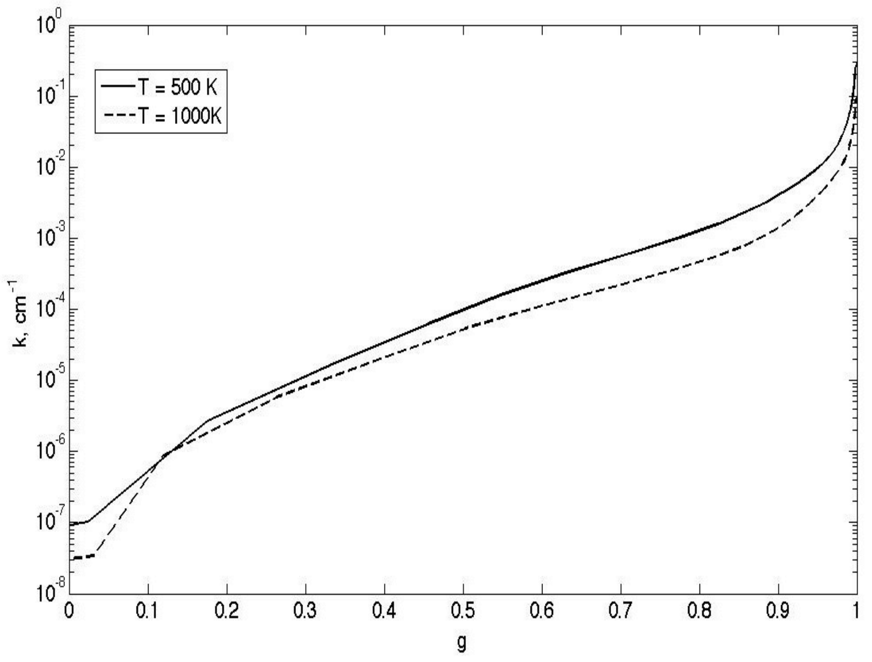
ALGORITHM: For any number of temperatures T_i:

1. The total spectrum is broken up into N

   logarithmically spaced subintervals δ_η
2. The absorption coefficient is evaluated at the center of each interval
3. If $k_j \le k_\eta \le k_{j+1}$, the value of each $f(T_i,k_j)\delta k_j$ is incremented by $\delta i(T_i)=I_{b\eta}(T_i,\eta_n)\delta_\eta/I_b(T_i)$, respectively.
4. Cumulative function $g(T,k)$ is calculated:

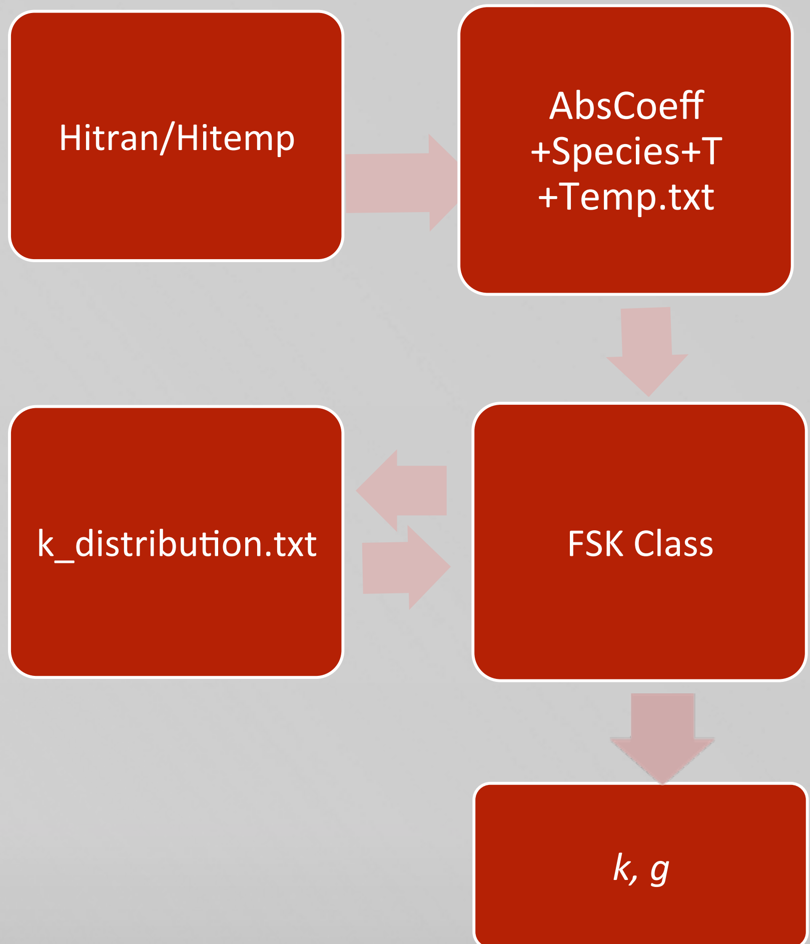
$$g(T_i,k_{j+1})=\sum_{j'=1}^{j} f(T_i,k_{j'})\,\delta k_{j'}$$
$$=g(k_j)+f(T_i,k_j)\delta k_j.$$

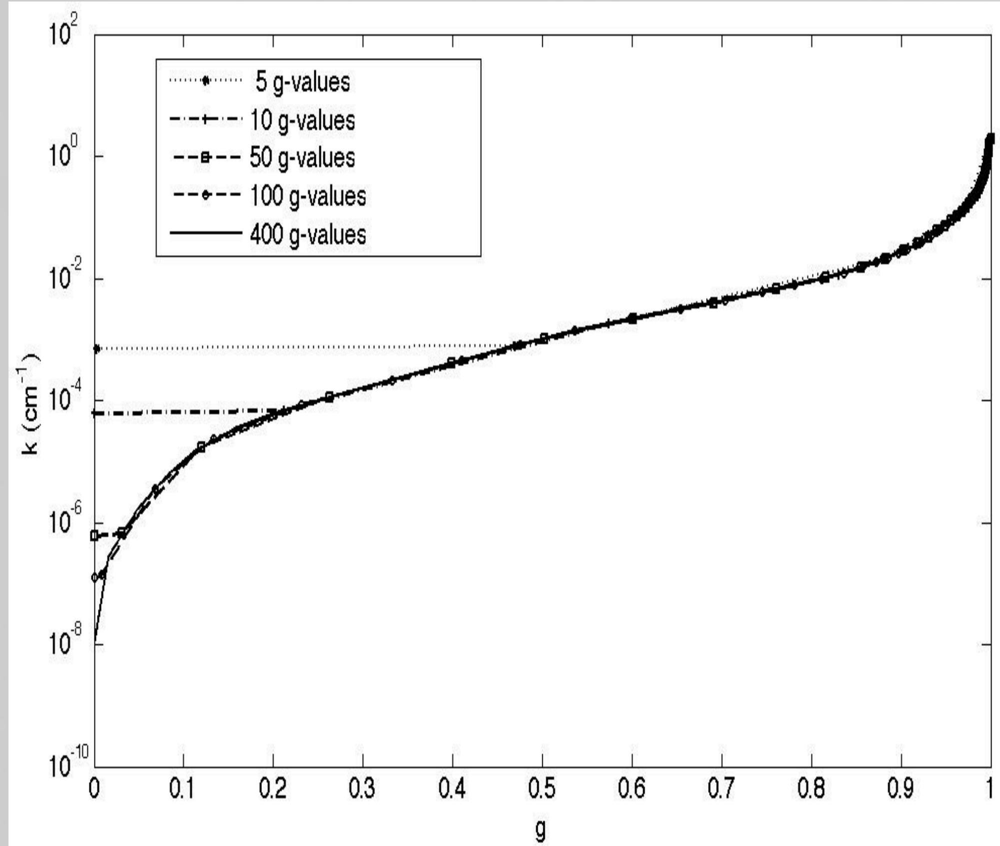




k-distribution for 10% CO_2 in nitrogen

k-distribution Model Numerical Implementation





The dependence of the *k*-distribution approximation on the number of *g*-values for a mixture of 20% H_2O, 40% CO_2, 5% CO, 0.03% NO, 5% OH

Radiative Properties of Particulate Media

When an electromagnetic wave (or a photon) interacts with a medium containing particles the radiative properties may be changed by absorption and/or scattering. How much and in which direction a particle scatters an electromagnetic wave depends on:

- the shape of the particle
- the material of the particle (i.e. the refractive index of refraction, $m = n - ik$)
- its relative size
- the clearance between the particles.

For clouds of particles of nonuniform size, we use the particle distribution function:

$$n(a) = A a^{\gamma} \exp(-B a^{\delta}), \quad 0 \le a(radius) < \infty, \quad N_T = \int_0^{\infty} n(a)\,da.$$

Assuming all properties have the same optical properties:

$$k_{\lambda} = \pi \int_0^{\infty} Q_{abs}\, a^2\, n(a)\,da, \quad \sigma_{s\lambda} = \pi \int_0^{\infty} Q_{sca}\, a^2\, n(a)\,da.$$

Q_{abs} and Q_{sca} are the absorption and scattering efficiency factors, calculated using Mie theory

Algorithm

For given number of temperatures T_i (spaced logarithmically), given refractive index of coal and ash particles, number of particles and the particles radii (spaced logarithmically):

1. Calculate wavelength-dependent Q_{abs} and Q_{sca} (wavelengths spaced logarithmically).
2. Calculate the absorption and scattering coefficients for coal and ash particles:

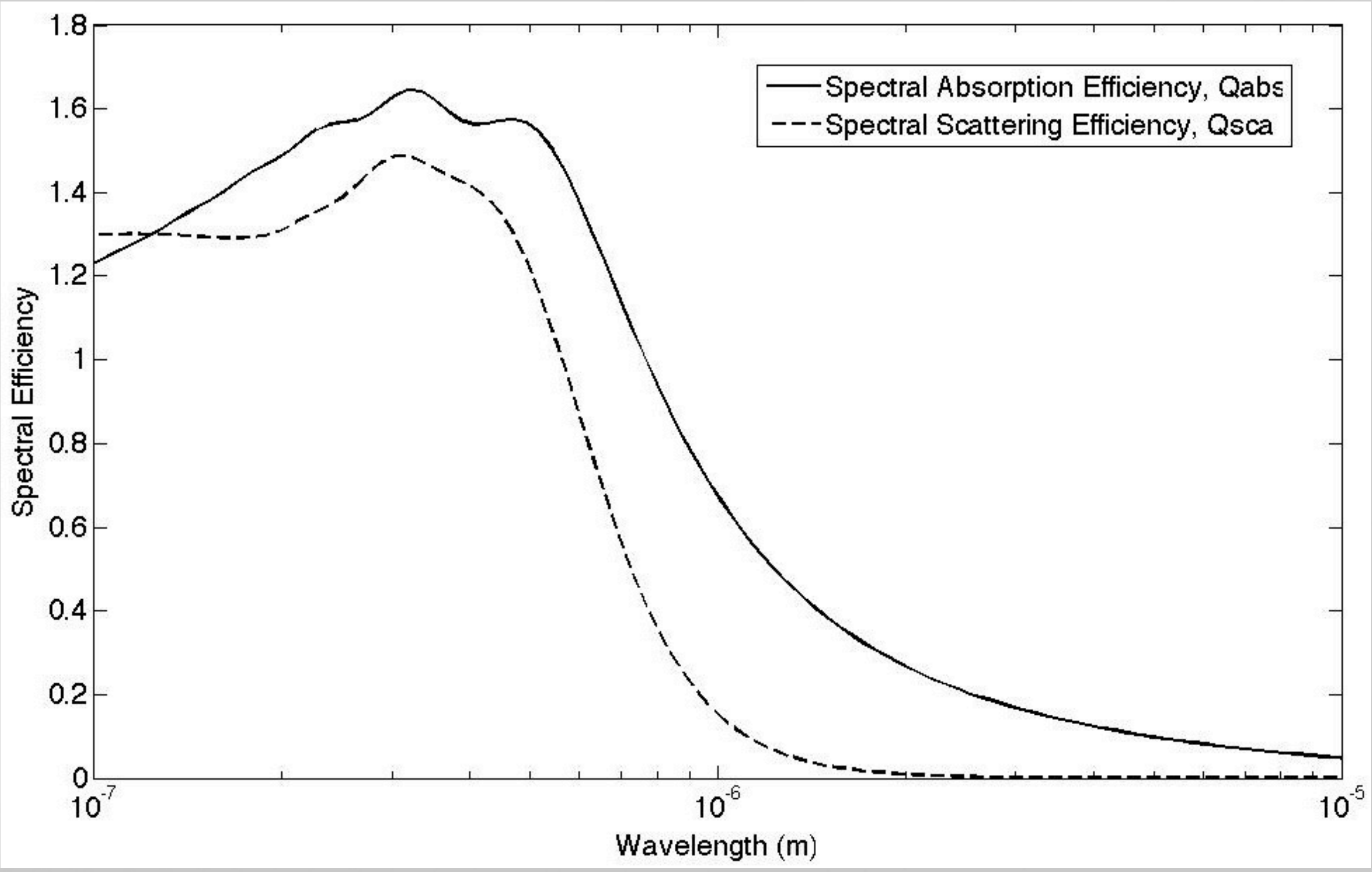
$$k_\lambda = \pi \sum_i Q_{abs}\, a_i^2\, n_i, \qquad \sigma_{s\lambda} = \pi \sum_i Q_{sca}\, a_i^2\, n_i.$$

3. Calculate spectrally integrated properties (Planck-mean and Rosseland-mean coefficients):

$$k_P = \frac{\pi}{\sigma T^4} \int_0^\infty I_{b\lambda}\, k_\lambda\, d\lambda, \qquad \frac{1}{k_R} = \frac{\pi}{4\sigma T^3} \int_0^\infty \frac{1}{k_\lambda} \frac{dI_{b\lambda}}{dT}\, d\lambda.$$

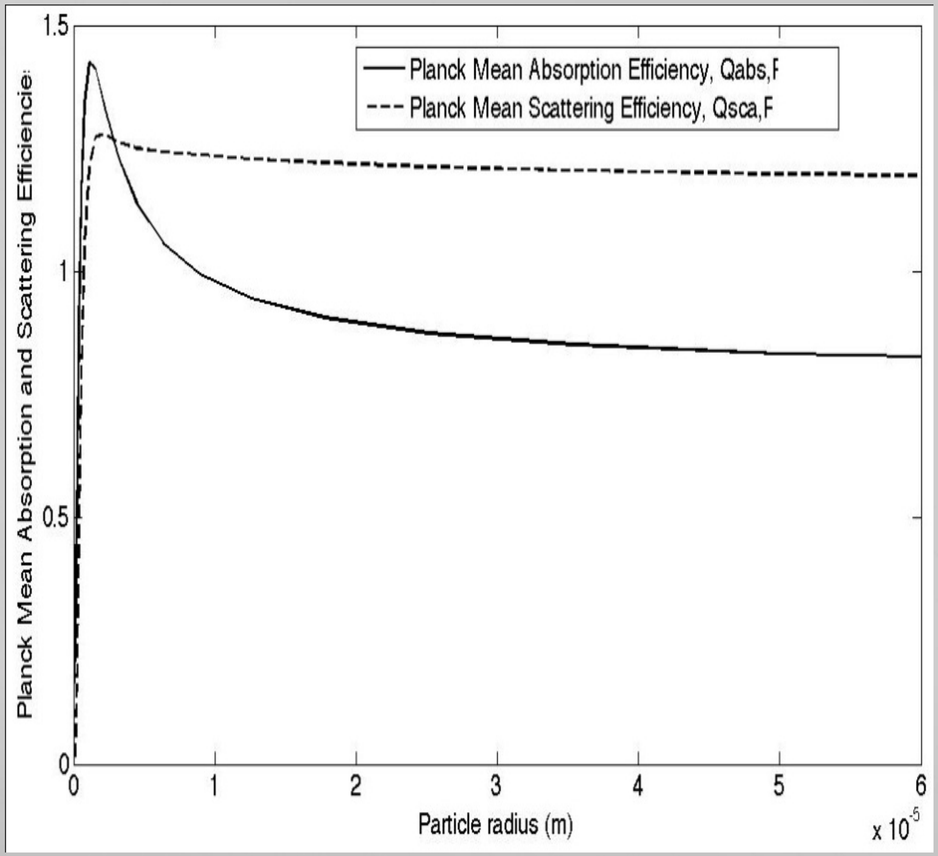
4. For nonhomogeneous particles, use regression, taking into account the coal and the ash mass fraction.

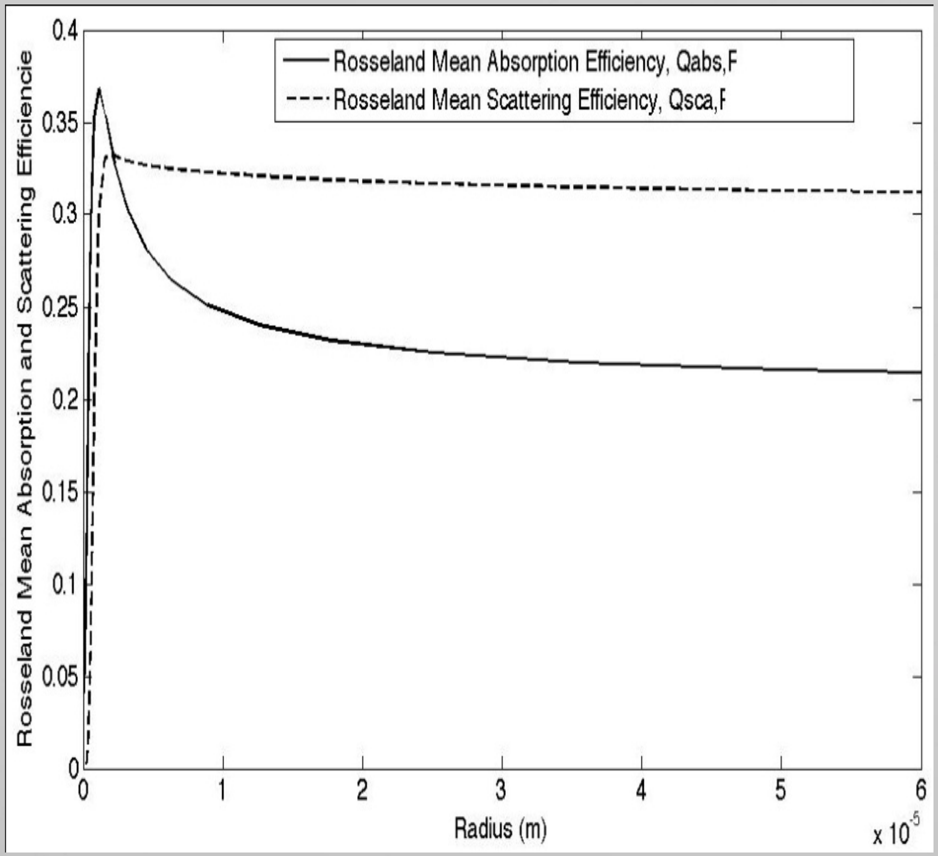
Spectral Absorption and Scattering Efficiencies



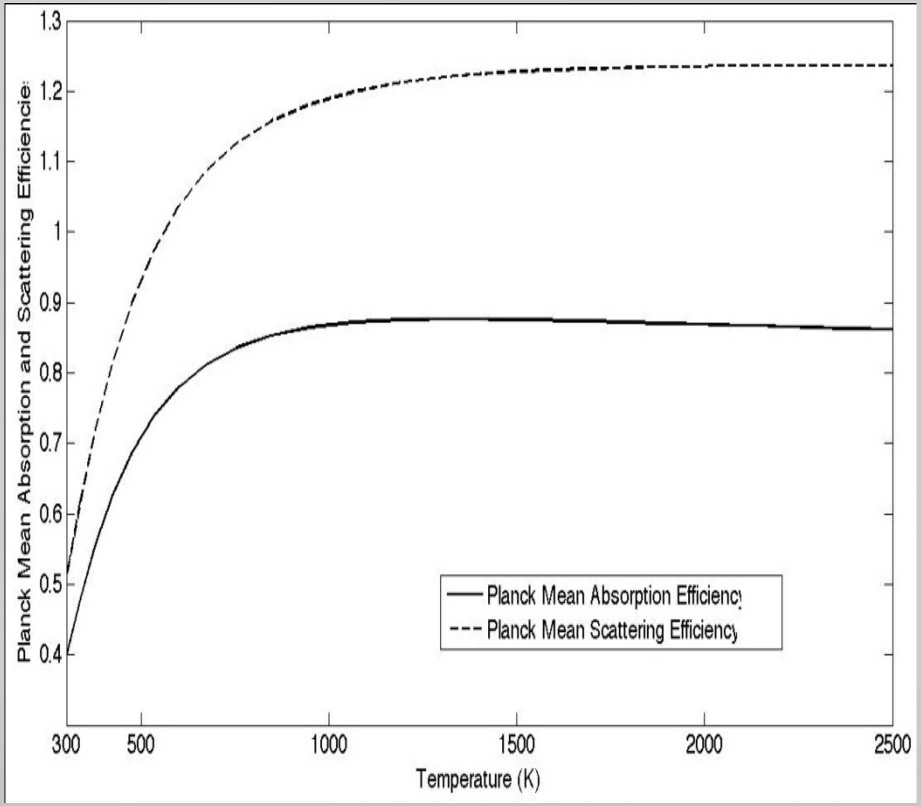
Spectral Efficiencies for 0.1 μm radius coal particle

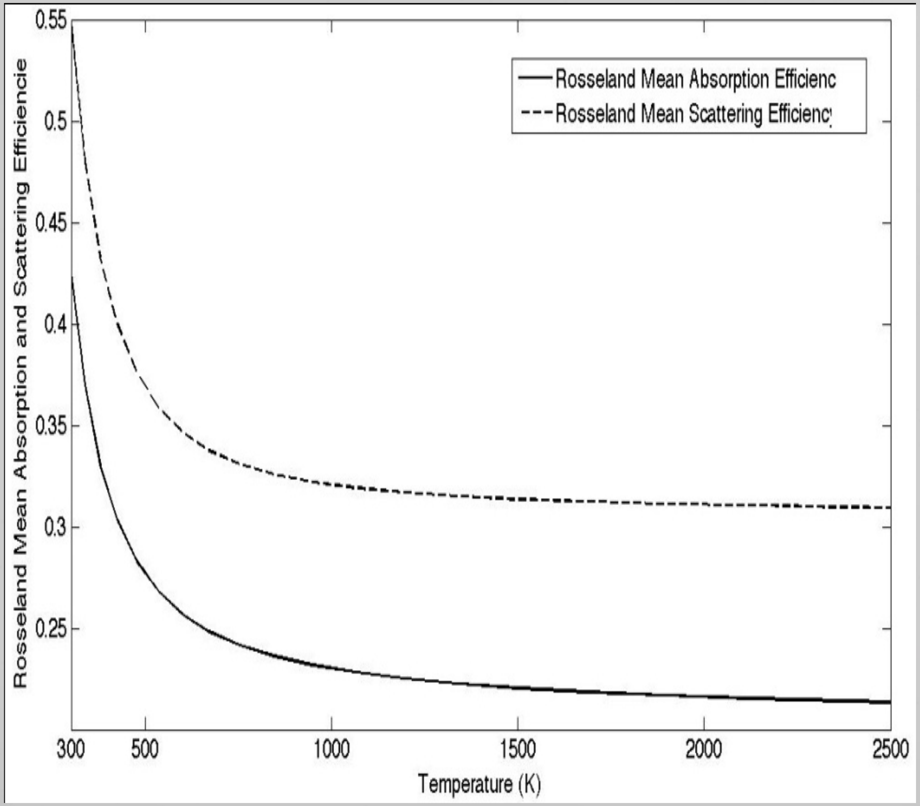
Dependence on Radius





Dependence on Temperature

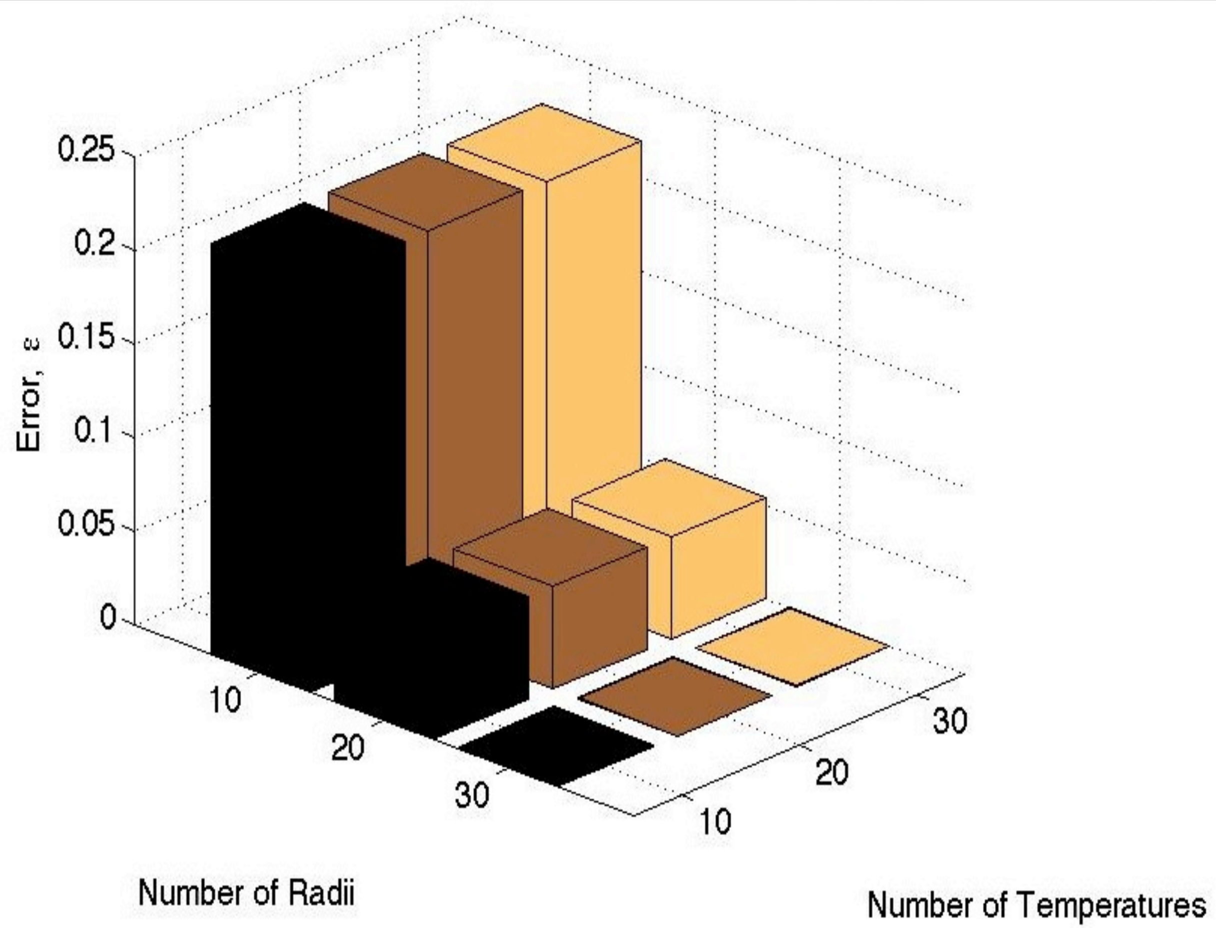




Accuracy

Error from interpolation:

$$\epsilon = \max_{k} |k_{interp} - k|/k$$



Error in the Planck Absorption Efficiencies due to interpolation. The temperature ranges from 296 K to 3000 K, and radius ranges from $1e^{-7}$ to $1e^{-4}$ m.

Acknowledgements

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THANK YOU!

Q&A

Radiation Heat Transfer in Combustion Systems

Goal: Develop Computational Models, which could be used for the design and optimization of more cost effective and environmentally friendly combustion systems with improved performance.

Constraint: Combustion is one of the most difficult processes to model since it involves:

- 3D two-phase fluid dynamics;
- Turbulent mixing;
- Fuel evaporation;
- Radiative and convective heat transfer;
- Chemical kinetics.

Thus, an adequate treatment of thermal radiation is essential to develop a model of the combustion system!

Software

ARCHES - a finite-volume large eddy simulation code developed by The Institute of Clean and Secure Energy at the University of Utah:

- predictive tools for highly turbulent, multiphase, reacting flows in industrial systems such as coal-fired boilers and furnaces;
- predicts the heat-flux from large buoyant pool fires with potential hazards immersed in or near a pool fire of transportation fuel;
- other industrially relevant problems such as industrial flares, oxy-coal combustion processes, and fuel gasification;
- an object-oriented C++ framework that enables parallelization to thousands of processors.