Aalto University

Thermal radiation

Summer School on Fire Dynamics Modeling 2017
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Objectives

1. Know the phenomena and parameters affecting Radiation Transport Equation (RTE).
2. Can explain the RTE discretization principles in FVM/DOM models.
3. Can investigate the sensitivity of results on the numerical parameters.
4. Can specify FDS inputs for radiation model.
5. Can modify the FDS verification tests.
6. *Understand the difference between gray gas and spectrally resolved calculations.*
7. *Can describe the challenges of predicting the radiative fraction.*
8. *Know the relationship between gas species/soot concentration and the calculated absorption coefficient.*
9. *Can identify the role of radiation modelling in validation.*
10. *Can tune the time-related solver parameters for* verification tests.

Contents

1	Part 1. Radiation fundamentals
2	Part 2. Radiation transport equation
3	Derivation of discrete form of Finite Volume Method
4	Exercise 1. Radiation in a box
5	Part 3. Radiation properties
6	Source term modelling in FDS
7	Exercise 2. Hottel’s charts

Recommended reading

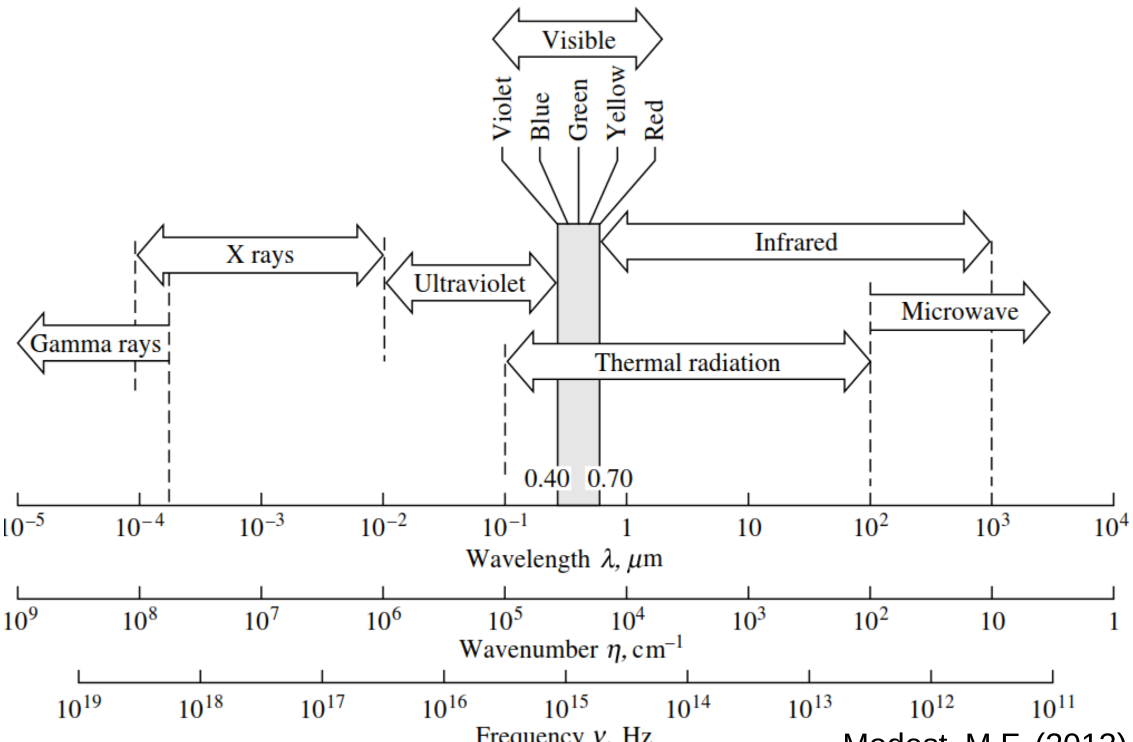
Howell, J.R., Pinar Menguc, M., Siegel, R. Thermal Radiation Exchange, (6. ed), CRC Press, 2015.

Michael F. Modest. Radiative Heat Transfer (3. ed) Academic Press. (1993, 2003, 2013)

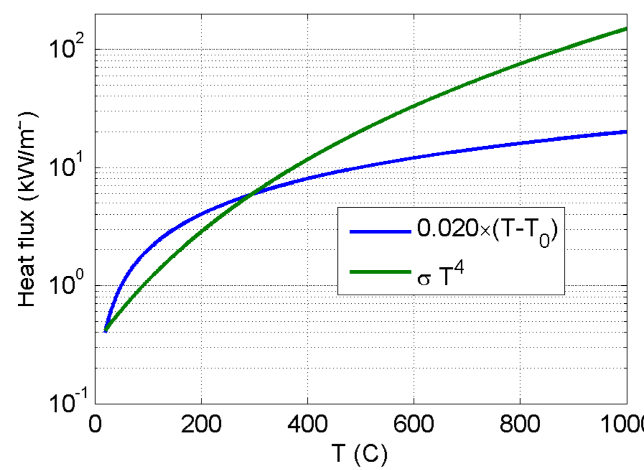
Part 1: Fundamentals

Thermal radiation

- Thermal radiation is electromagnetic radiation (at infrared (IR) range).
- What radiates?
- Radiation dominates fire heat transfer when
  - Flame diameter > ~ 0,3 m
  - Temperature > 400 °C



Modest, M.F. (2013)



Black body -radiation

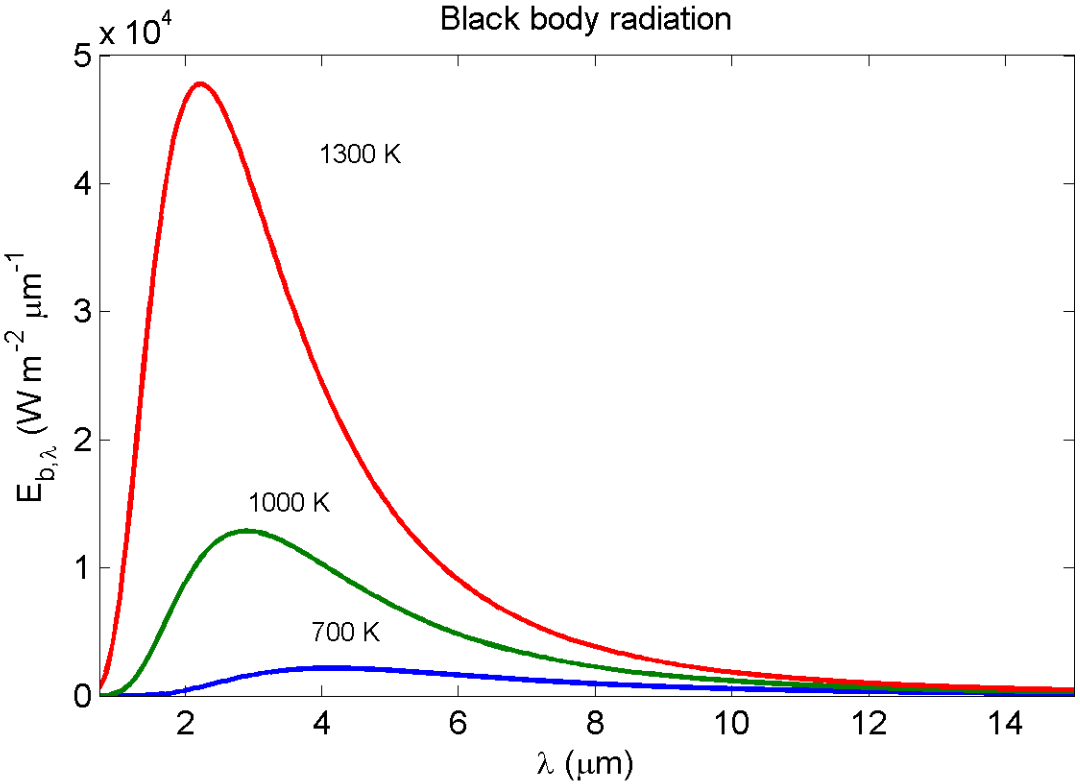
- Energy density depends on the wavelength and the temperature of the radiating body.
- Qualitatively

550 °C: reddish

900 °C: bright red

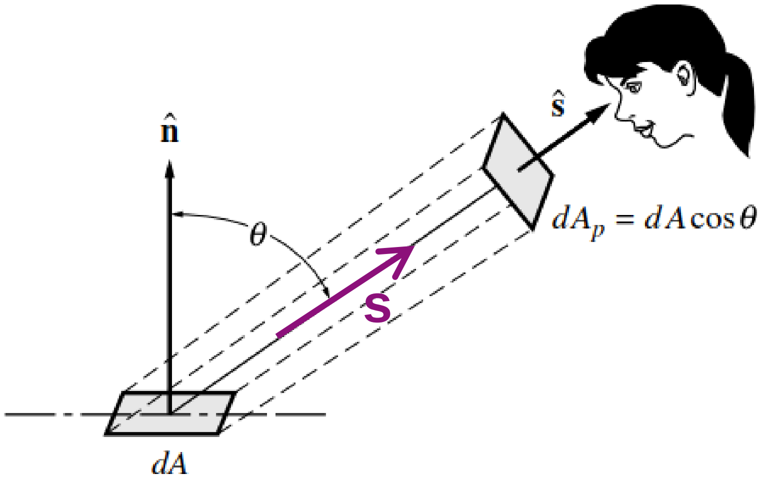
1100 °C: orange

1500 °C: white



Definitions

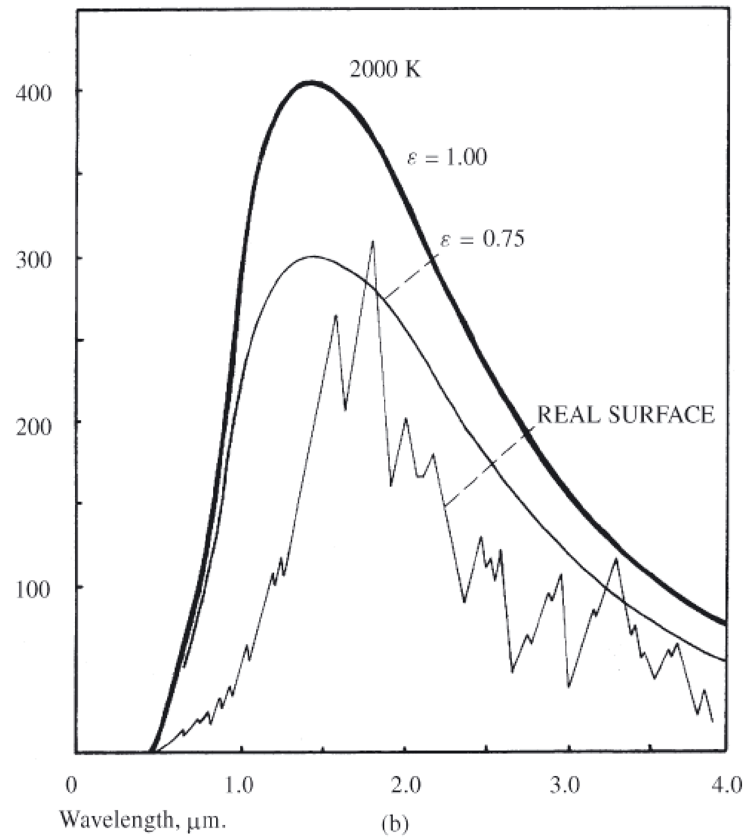
- **Spectral emissive power** E_λ (or E_ν)
  $\equiv$ radiative energy / time / surface area / wavelength (W m^{-2} μm^{-1})
- **Total emissive power** E (W m^{-2})
- **Spectral intensity** (*or radiance*) I_λ
  $\equiv$ radiative energy / time / area normal to rays / solid angle / wavelength (W m^{-2} sr^{-1} μm^{-1})
- **Total intensity** (W m^{-2} sr^{-1})
- Blackbody emissive power E_b
- Blackbody emissive intensity I_b
- Direction vector **s**



Stefan-Boltzmann law

$$\frac{P}{A} = E_b = \dot{q}_b'' = \sigma T^4$$

- Power *P* emitted by black surface with area *A*
- σ = Stefan-Boltzmann constant 5.67×10^{-8} W m^{-2} K^{-4}
- Real surfaces are not black, but emit less than the ideal surfaces.



- Surface emissivity (and absorptivity) $\varepsilon(\lambda) = \dfrac{E_\lambda}{E_{b,\lambda}}$
- For *gray bodies* ε = constant $\Rightarrow$

$$\dot{q}'' = \varepsilon \sigma T^4$$

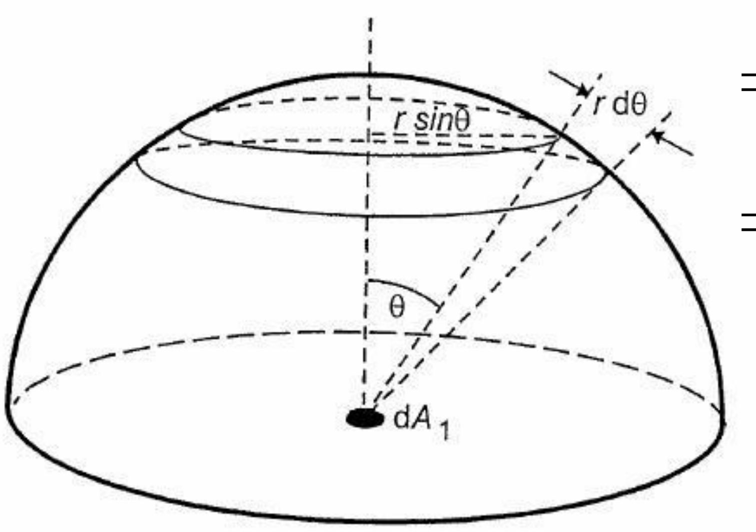
Intensity vs. emissive power

- Black body radiates at same intensity to all directions $I(\theta) = I_n$.
- The projected area of the radiating surface decreases when the observer goes away from the surface normal.
- Surfaces like this are called Lambert radiatiors or *diffuse radiators*, and they obey the cosine law

$$E_{\lambda,b}(\theta)d\lambda = I_{\lambda,b}\cos\theta d\lambda = I_{\lambda,n}\cos\theta d\lambda$$

$$\Rightarrow E_b = \int_0^\infty E_{\lambda,b}d\lambda = I_b \int_0^{2\pi}\int_0^{\pi/2} \cos\theta \sin\theta \, d\theta \, d\phi = I_b \cdot \pi$$

$$\Rightarrow I_b = E_b / \pi$$



Attenuation in participating media

Intensity of monochromatic radiation attenuates as

$$\mathrm{d}I_\lambda = \kappa_\lambda C I_{\lambda x}\,\mathrm{d}x$$

where κ_λ is specific absorption coefficient and *C* is concentration.

Integrating in domain *x* = 0…*L we get* $I_{\lambda L} = I_{\lambda 0}\exp(-\kappa_\lambda C L)$

Monocromatic absorptivity $a_\lambda = \dfrac{I_{\lambda 0} - I_{\lambda L}}{I_{\lambda 0}} = 1 - \exp(-\kappa_\lambda C L)$

Part 2. Radiation transport

Radiation Transport Equation (RTE)

General equation for radiation intensity at point **x** to direction **s**

$$\frac{1}{c}\frac{\partial I_\lambda(\mathbf{x},\mathbf{s},t)}{\partial t} + \mathbf{s}\cdot\nabla I_\lambda(\mathbf{x},\mathbf{s}) = \underbrace{-\kappa(\mathbf{x},\lambda)\,I_\lambda(\mathbf{x},\mathbf{s})}_{\text{Energy loss by absorption}} - \underbrace{\sigma_s(\mathbf{x},\lambda)\,I_\lambda(\mathbf{x},\mathbf{s})}_{\text{Energy loss by scattering}} +$$

$$\underbrace{B(\mathbf{x},\lambda)}_{\text{Emission source term}} + \underbrace{\frac{\sigma_s(\mathbf{x},\lambda)}{4\pi}\int_{4\pi}\Phi(\mathbf{s}',\mathbf{s})\,I_\lambda(\mathbf{x},\mathbf{s}')\,d\mathbf{s}'}_{\text{In-scattering term}}$$

Spectrally integrated RTE

If the spectral details are not important, we can integrate RTE over a finite number of spectal bands (ignoring scattering for simplicity)

$$\mathbf{s} \cdot \nabla I_n(\mathbf{x}, \mathbf{s}) = B_n(\mathbf{x}) - \kappa_n(\mathbf{x}) I_n(\mathbf{x}, \mathbf{s}), \quad n = 1 \ldots N$$

$$B_n(\mathbf{x}) = \kappa_n(\mathbf{x}) I_{\mathrm{b},n}(\mathbf{x})$$

$$I_{b,n}(\mathbf{x}) = F_n \frac{\sigma [T(\mathbf{x})]^4}{\pi}$$

In typical fire simulation, $N = 1$

Radiation and the energy equation

Radiant heat flux vector

$$\dot{\mathbf{q}}_{\mathrm{r}}''(\mathbf{x}) = \int_{4\pi} \mathbf{s}'\, I(\mathbf{x},\mathbf{s}')\; \mathrm{d}\mathbf{s}'$$

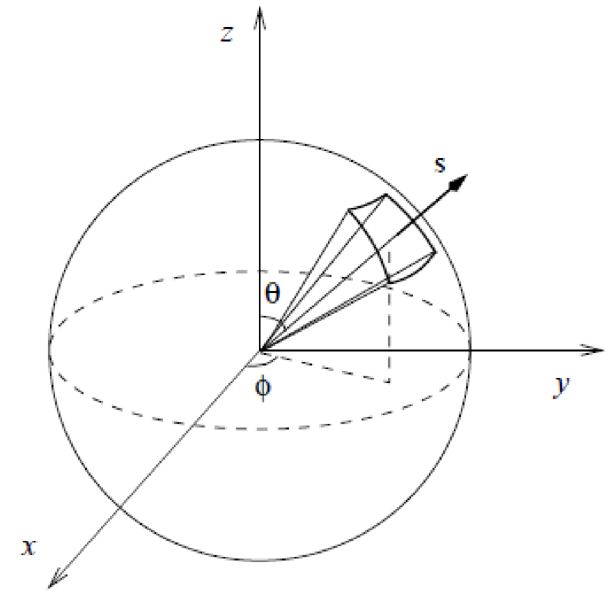
Radiative source term in energy equation

$$-\nabla\cdot\dot{\mathbf{q}}_{\mathrm{r}}''(\mathbf{x})(\mathrm{gas}) = \kappa(\mathbf{x})\,\left[U(\mathbf{x}) - 4\pi\, I_{\mathrm{b}}(\mathbf{x})\right] \quad ; \quad U(\mathbf{x}) = \int_{4\pi} I(\mathbf{x},\mathbf{s}')\,\mathrm{d}\mathbf{s}'$$

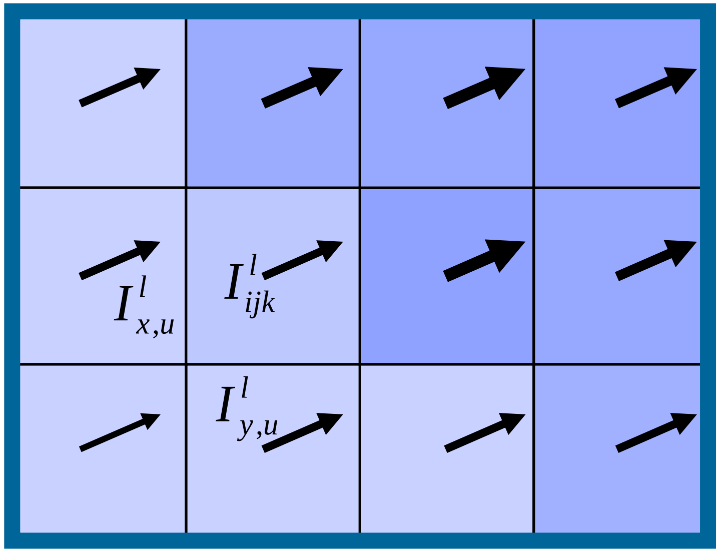
Boundary condition for intensity

$$I_{\mathrm{w}}(\mathbf{s}) = \frac{\varepsilon\,\sigma\,T_{\mathrm{w}}^4}{\pi} + \frac{1-\varepsilon}{\pi}\int_{\mathbf{s}'\cdot\mathbf{n}_{\mathrm{w}}<0} I_{\mathrm{w}}(\mathbf{s}')\,|\mathbf{s}'\cdot\mathbf{n}_{\mathrm{w}}|\;\mathrm{d}\mathbf{s}'$$

Finite Volume Method for Radiation 1



- Discretized solid angle
  - Elevation angle θ divided into N_θ parts (bands)
  - Each elevation band divided into $N_\phi(\theta)$ parts over azimuthal angle.
  - Symmetrical over co-ordinate axis planes.
- Explicit solution in CFD mesh.



FDS User's Guide:
NUMBER_RADIATION_ANGLES
TIME_STEP_INCREMENT
ANGLE_INCREMENT

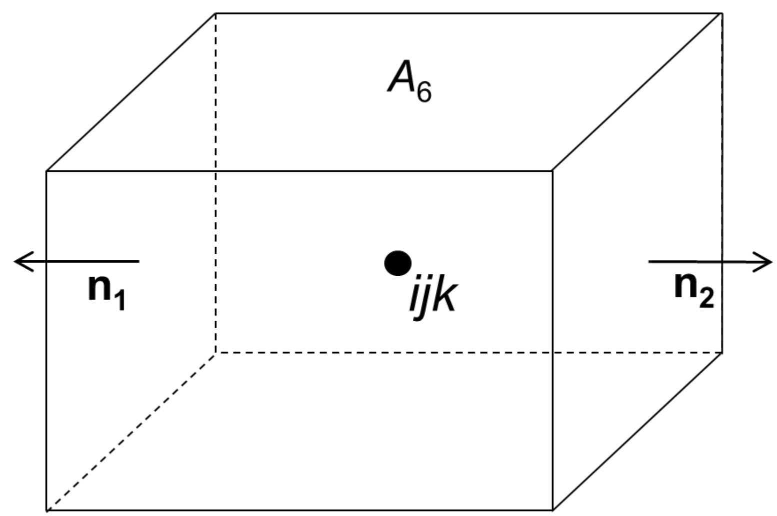
Finite Volume Method for Radiation 2

$$\int_{\delta\Omega^l}\int_{V_{ijk}} \mathbf{s}'\cdot\nabla I(\mathbf{x}',\mathbf{s}')\,\mathrm{d}\mathbf{x}'\,\mathrm{d}\mathbf{s}' = \int_{\delta\Omega^l}\int_{V_{ijk}} \kappa(\mathbf{x}')\ \left[I_\mathrm{b}(\mathbf{x}') - I(\mathbf{x}',\mathbf{s}')\right]\,\mathrm{d}\mathbf{x}'\,\mathrm{d}\mathbf{s}' \tag{6.14}$$

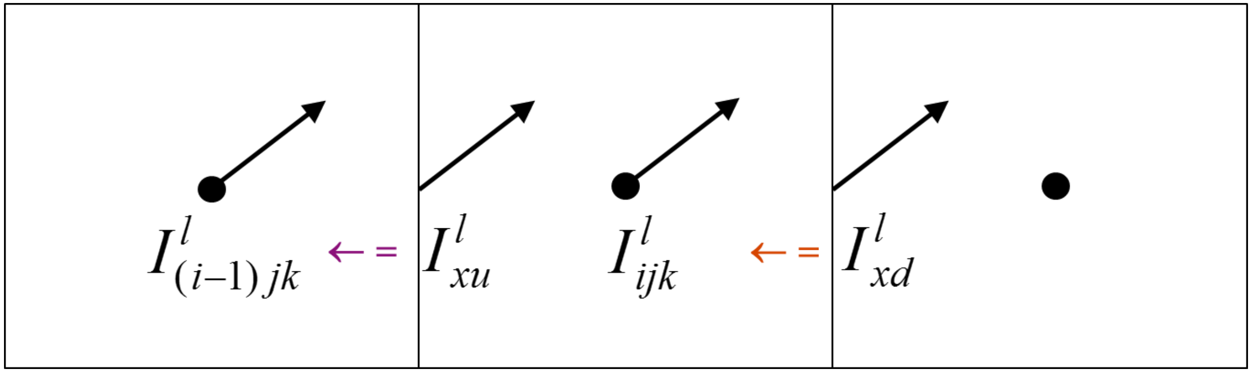
$$\int_{\delta\Omega^l}\int_{A_{ijk}} (\mathbf{s}'\cdot\mathbf{n}')\,I(\mathbf{x}',\mathbf{s}')\,\mathrm{d}\mathbf{n}'\,\mathrm{d}\mathbf{s}' = \int_{\delta\Omega^l}\int_{V_{ijk}} \kappa(\mathbf{x}')\ \left[I_\mathrm{b}(\mathbf{x}') - I(\mathbf{x}',\mathbf{s}')\right]\,\mathrm{d}\mathbf{x}'\,\mathrm{d}\mathbf{s}' \tag{6.15}$$

$$\sum_{m=1}^{6} A_m\, I_m^l \int_{\Omega^l} (\mathbf{s}'\cdot\mathbf{n}_m)\,\mathrm{d}\mathbf{s}' = \kappa_{ijk}\left[I_{\mathrm{b},ijk} - I_{ijk}^l\right] V_{ijk}\,\delta\Omega^l \tag{6.16}$$

Equation (6.16) is a discrete equation for intensity I_{ijk}^l . Solving (6.16) requires geometry data, κ_{ijk}, and face intensities I_m^l



Finite Volume Method for Radiation 3



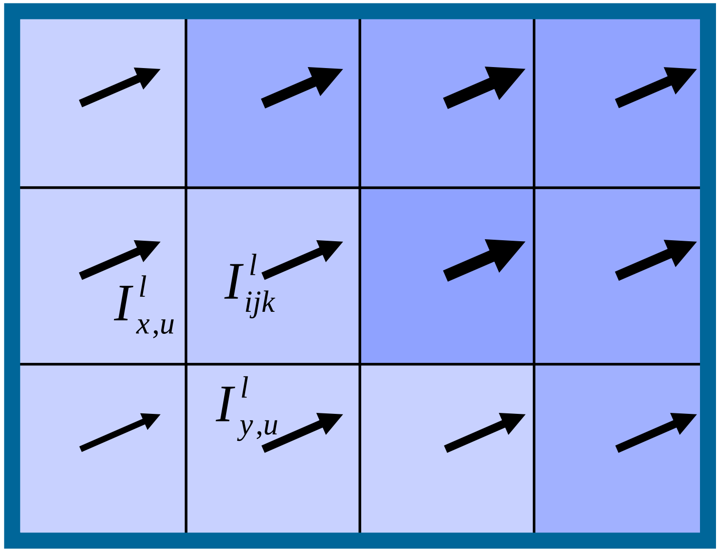
- In the FVM solver of FDS, the cell face intensities are approximated using step scheme (<u>first order upwind)</u> $\boxed{I^l_{xu} = I^l_{(i-1)jk}}$
- Define angular integrals $D^l_m = \int_{\Omega^l} (\mathbf{s}' \cdot \mathbf{n}_m)\, \mathrm{d}\mathbf{s}'$
- The discrete equation for I^l_{ijk} now becmes

$$
\begin{aligned}
&A_x I^l_{xu} D^l_{xu} + A_x I^l_{ijk} D^l_{xd} + \\
&A_y I^l_{yu} D^l_{yu} + A_y I^l_{ijk} D^l_{yd} + \\
&A_z I^l_{zu} D^l_{zu} + A_z I^l_{ijk} D^l_{zd} \\
&\qquad = \kappa_{ijk} I_{\mathrm{b},ijk} V_{ijk}\, \delta\Omega^l - \kappa_{ijk} I^l_{ijk} V_{ijk}\, \delta\Omega^l \qquad (6.20)
\end{aligned}
$$

Finite Volume Method for Radiation 4

- Combining I_{ijk}^{l} terms gives

$$a_{ijk}^{l} I_{ijk}^{l} = a_x^l I_{xu}^l + a_y^l I_{yu}^l + a_z^l I_{zu}^l + b_{ijk}^l$$

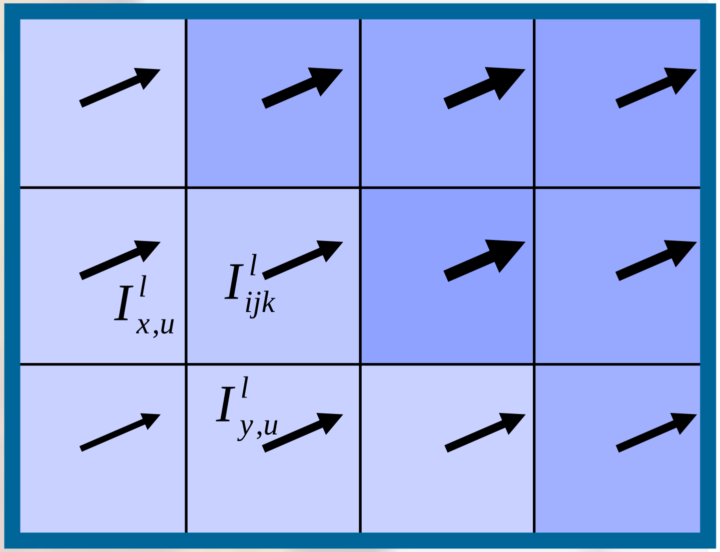


$$a_{ijk}^{l} = A_x |D_x^l| + A_y |D_y^l| + A_z |D_z^l| + \kappa_{ijk} V_{ijk} \delta\Omega^l$$

$$a_x^l = A_x |D_x^l|$$
$$a_y^l = A_y |D_y^l|$$
$$a_z^l = A_z |D_z^l|$$
$$b_{ijk}^l = \kappa_{ijk} I_{\mathrm{b},ijk} V_{ijk} \delta\Omega^l$$

Pair discussion:

How to choose which corner to start the ”sweep” from?

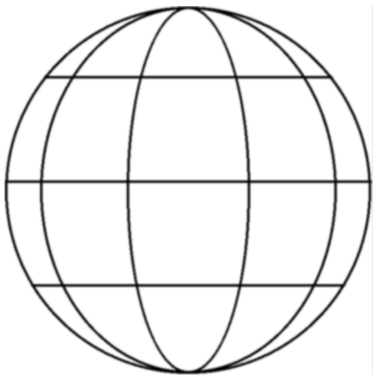


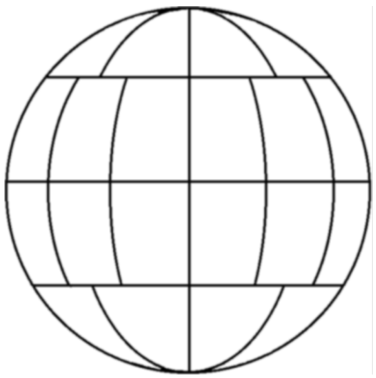
Assume you know integrals

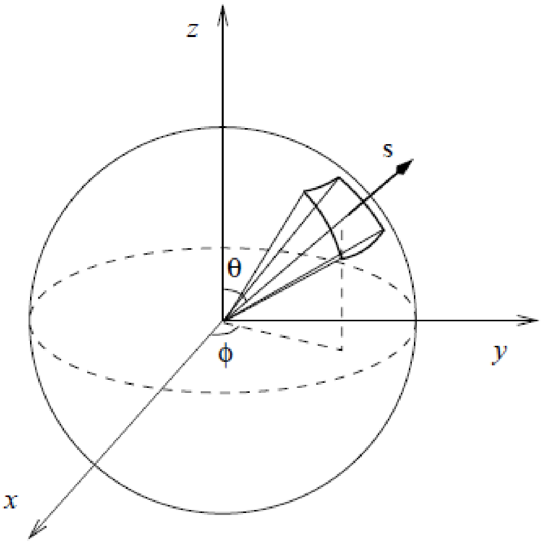
$$D^l_m = \int_{\Omega^l} (\mathbf{s}' \cdot \mathbf{n}_m)\, \mathrm{d}s'$$

Angular discretization schemes

- Classical Discrete Ordinates Method (DOM) schemes with $N_\phi \times N_\theta$ control angles.
  - Number of azimuthal (ϕ) bands
  - Number of polar (θ) bands
- More elaborate schemes naturally exist.
- FDS strategy: Equal control angles in all directions. Default number of control angles is 104.







FVM vs. DOM

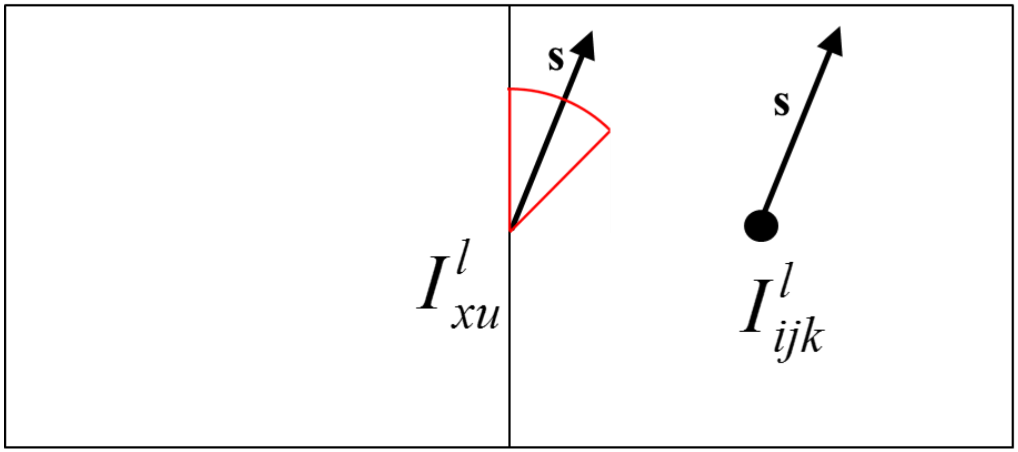
- The main difference between DOM and FVM is the treatment of angular integral

$$D_m^l = \int_{\Omega^l} (\mathbf{s}' \cdot \mathbf{n}_m)\, \mathrm{d}\mathbf{s}'$$

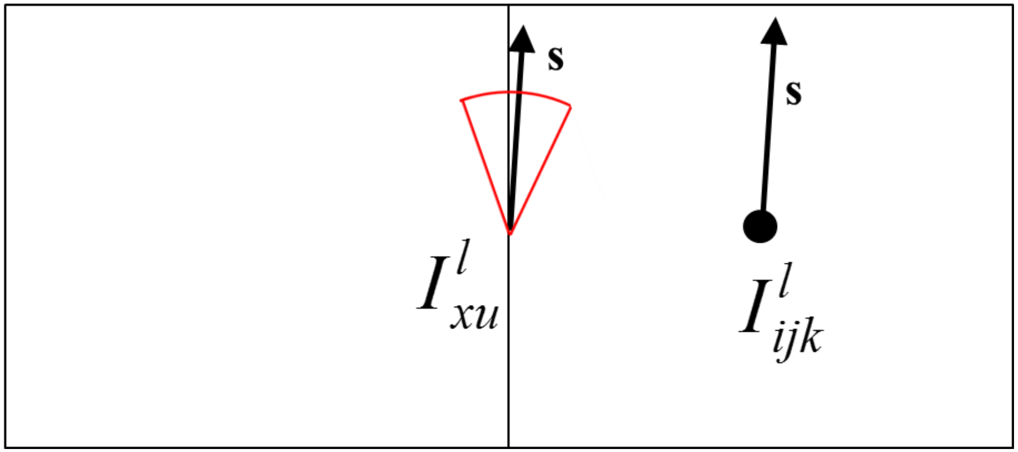
- In FVM, these integrals are calculated analytically and tabulated for the solver.
  - Exact, energy-conserving.
  - Difficult if control angles overlap with co-ordinate axes.
- In DOM, these integrals are *approximated* using *weighting sets* (Sn).

FVM angular discretization challenges

No overlap (overhang) $\Rightarrow$ D_m is easy to calculate

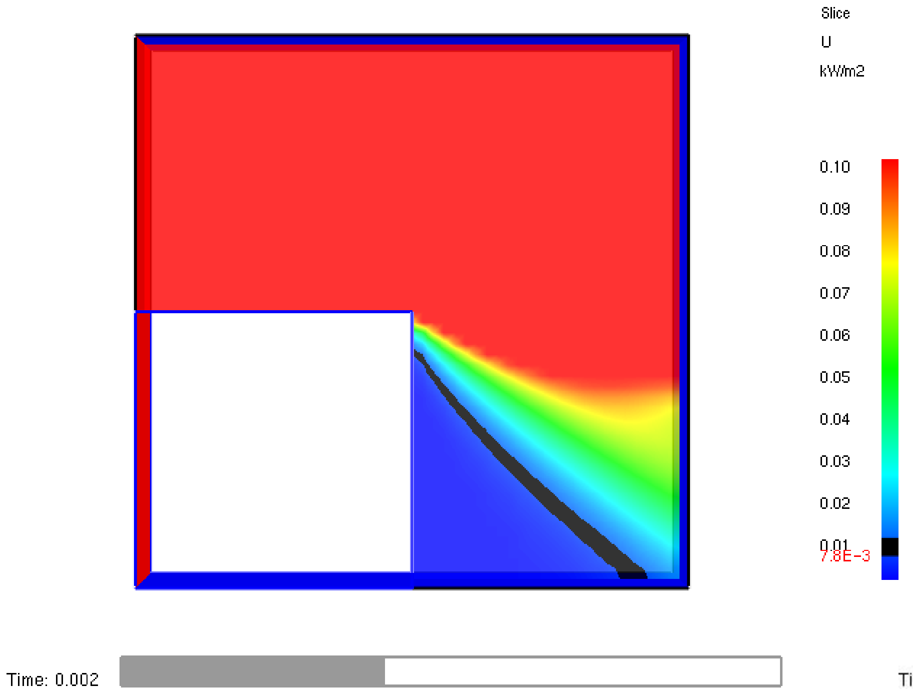


Control angle $\delta\Omega$ overlaps with cell boundary $\Rightarrow$ Only part of energy within $\delta\Omega$ contributes to the flux at ijk.
$\Rightarrow$ D_m is difficult to calculate.

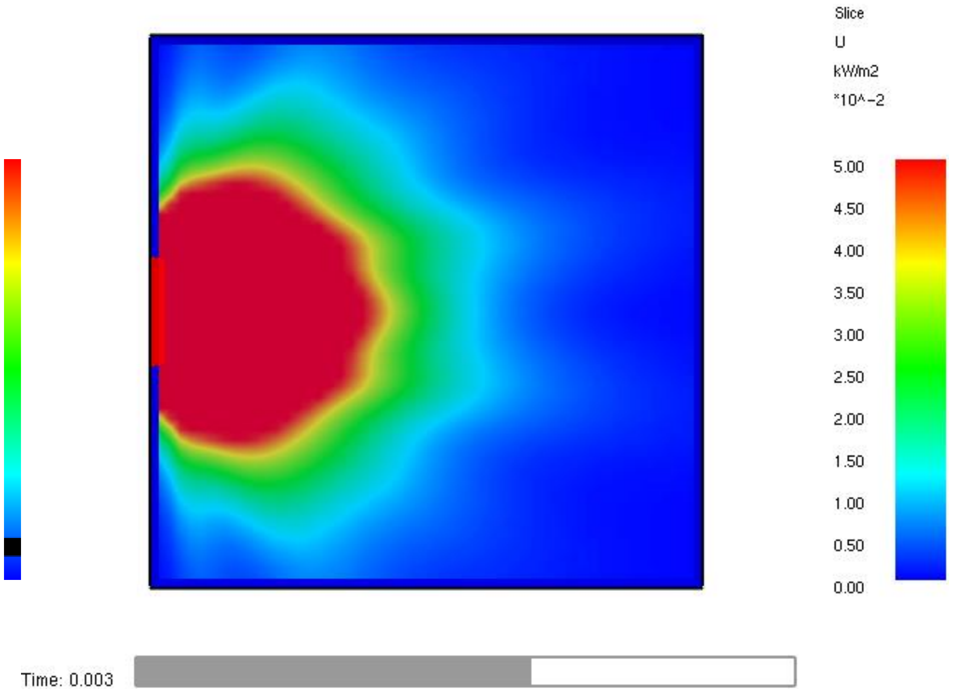


Challenges of numerical methods

Numerical diffusion



Ray effect



Exercise 1. Radiation box

Exercise 1: Radiation inside a box

8.2 Radiation inside a Box (`radiation_in_a_box`)

This verification case tests the computation of three-dimensional configuration factor Φ inside a cube box with one hot wall and five cold (0 K) walls. An overview of the test geometry is shown in Fig. 8.2. The

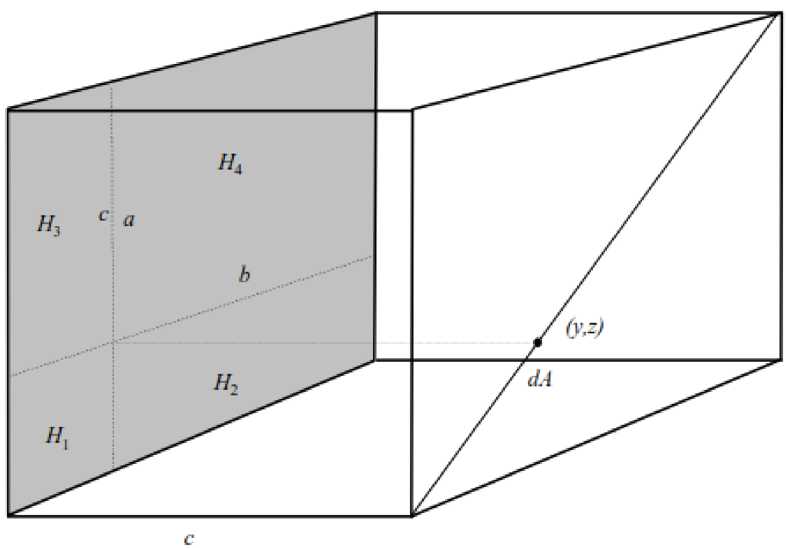


Figure 8.2: Radiation in a box geometry.

Exercise 1: Verification results

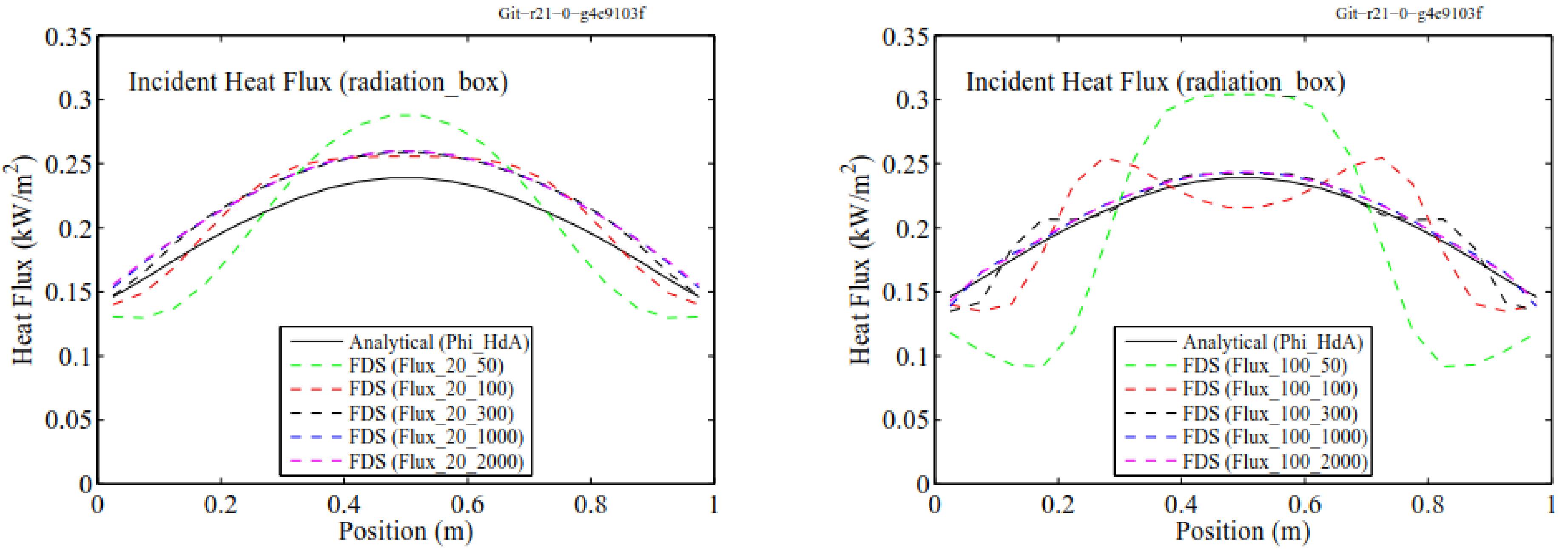
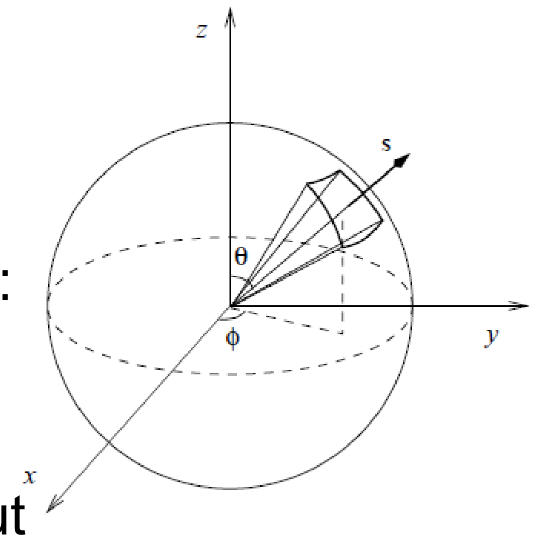


Figure 8.3: Incident heat flux.

Exercise 1:A Solver parameters



1. Run the radiation_box__50__100.fds
2. What is the purpose of the following input lines:
```
&RADI NUMBER_RADIATION_ANGLES=100
      TIME_STEP_INCREMENT = 1
      ANGLE_INCREMENT = 1 /
```
3. Look at the 'Radiation Model Information' in .out file. How many radiation control angles are used and how are they distributed? Roughly how many degrees do the control angles span in θ- and φ-directions?
4. Using the results of the FDS Verification guide, discuss the effect of the angular and spatial resolutions on the heat flux distribution of the opposite wall.

Exercise 1:B Angular discretization

Investigate if the predicted heat fluxes are invariant to the choice of primary axis direction X, Y or Z.

Steps:

1. Modify the radiation_box__50__100.fds by changing the emitting hot surface to the YMIN or ZMIN boundary.
2. Name the cases as `radiation_box__50__100_y` and `radiation_box__50__100_z`.
3. Plot the heat fluxes on the diagonal in all three cases (X,Y,Z) and compare against the exact values using plot_box.py (edit the scipt to choose what to plot.)
4. Discuss the findings with your pair.

Part 3. Radiation properties

Radiation Transport Equation (RTE)

$$\mathbf{s}\cdot\nabla I_\lambda(\mathbf{x},\mathbf{s}) = \underbrace{-\kappa(\mathbf{x},\lambda)\, I_\lambda(\mathbf{x},\mathbf{s})}_{\text{Energy loss by absorption}} - \underbrace{\sigma_s(\mathbf{x},\lambda)\, I_\lambda(\mathbf{x},\mathbf{s})}_{\text{Energy loss by scattering}} +$$

$$\underbrace{B(\mathbf{x},\lambda)}_{\text{Emission source term}} + \underbrace{\frac{\sigma_s(\mathbf{x},\lambda)}{4\pi}\int_{4\pi}\Phi(\mathbf{s}',\mathbf{s})\, I_\lambda(\mathbf{x},\mathbf{s}')\, d\mathbf{s}'}_{\text{In-scattering term}}$$

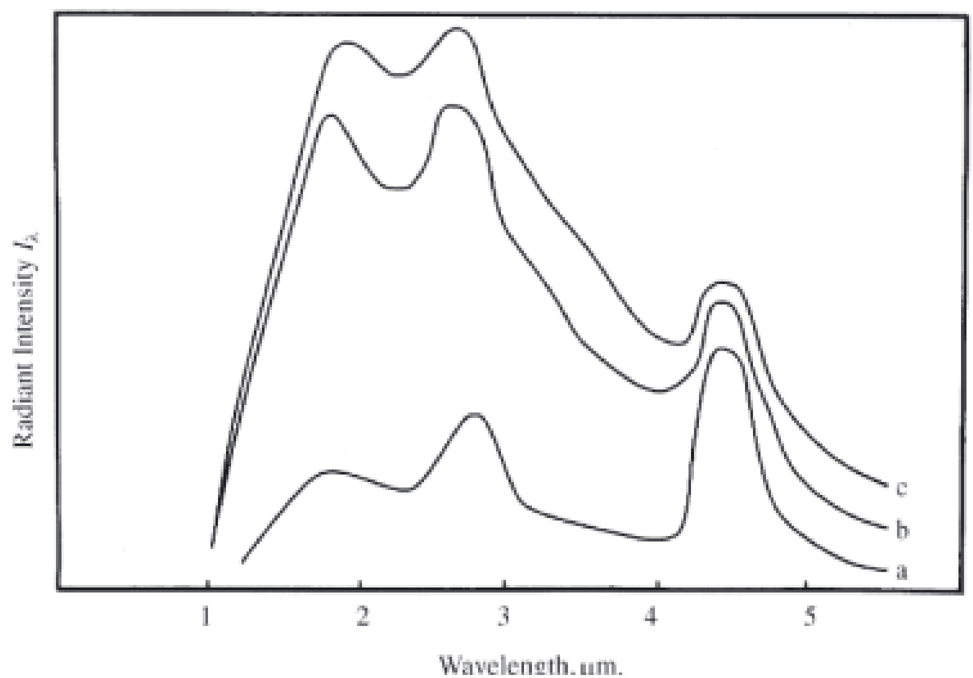
Integrated over a wavelength band n (usually N=1)

$$\mathbf{s}\cdot\nabla I_n(\mathbf{x},\mathbf{s}) = B_n(\mathbf{x}) - \kappa_n(\mathbf{x})\, I_n(\mathbf{x},\mathbf{s}), \quad n = 1\ldots N$$

$$B_n(\mathbf{x}) = \kappa_n(\mathbf{x})\, I_{b,n}(\mathbf{x})$$

Flame radiation

- Flame radiation is emitted by soot and multi-atomic gases (H_2O, CO_2, CO, HCl, HCN, NO_3,…).
- O_2 and N_2 do not emit or absorb radiation.
- Soot radiation spectrum is continuous and very close to black body radiation.
- Gas radiation spectra are very discontinuous.

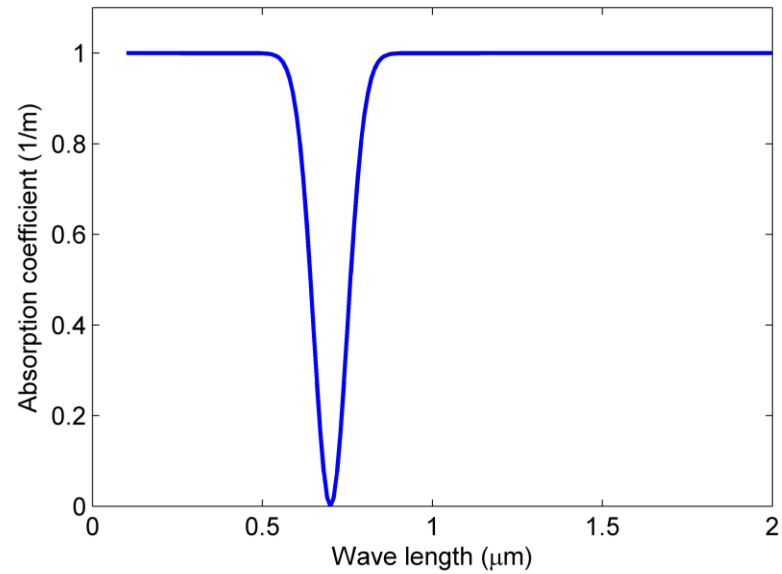


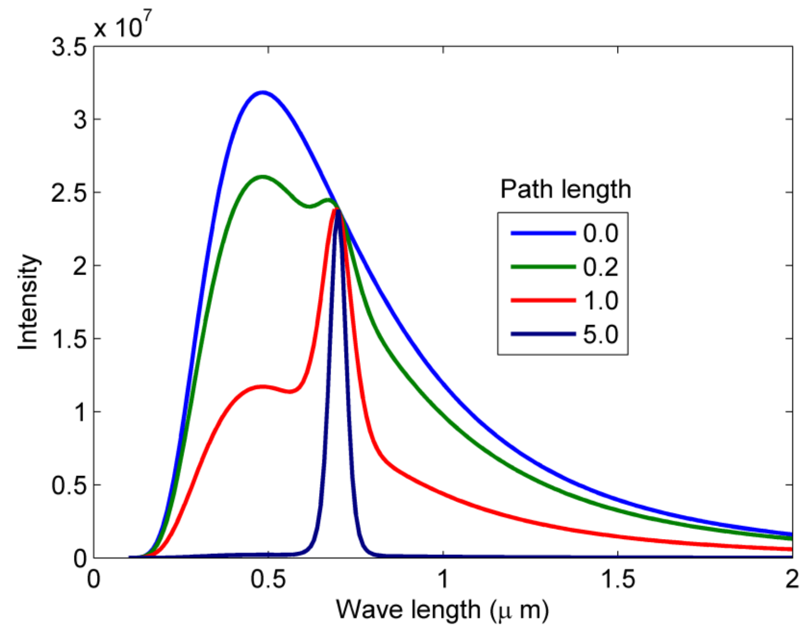
Wood flame radiation for different flame thicknesses (Drysdale / Hägglund & Peterson 1976)

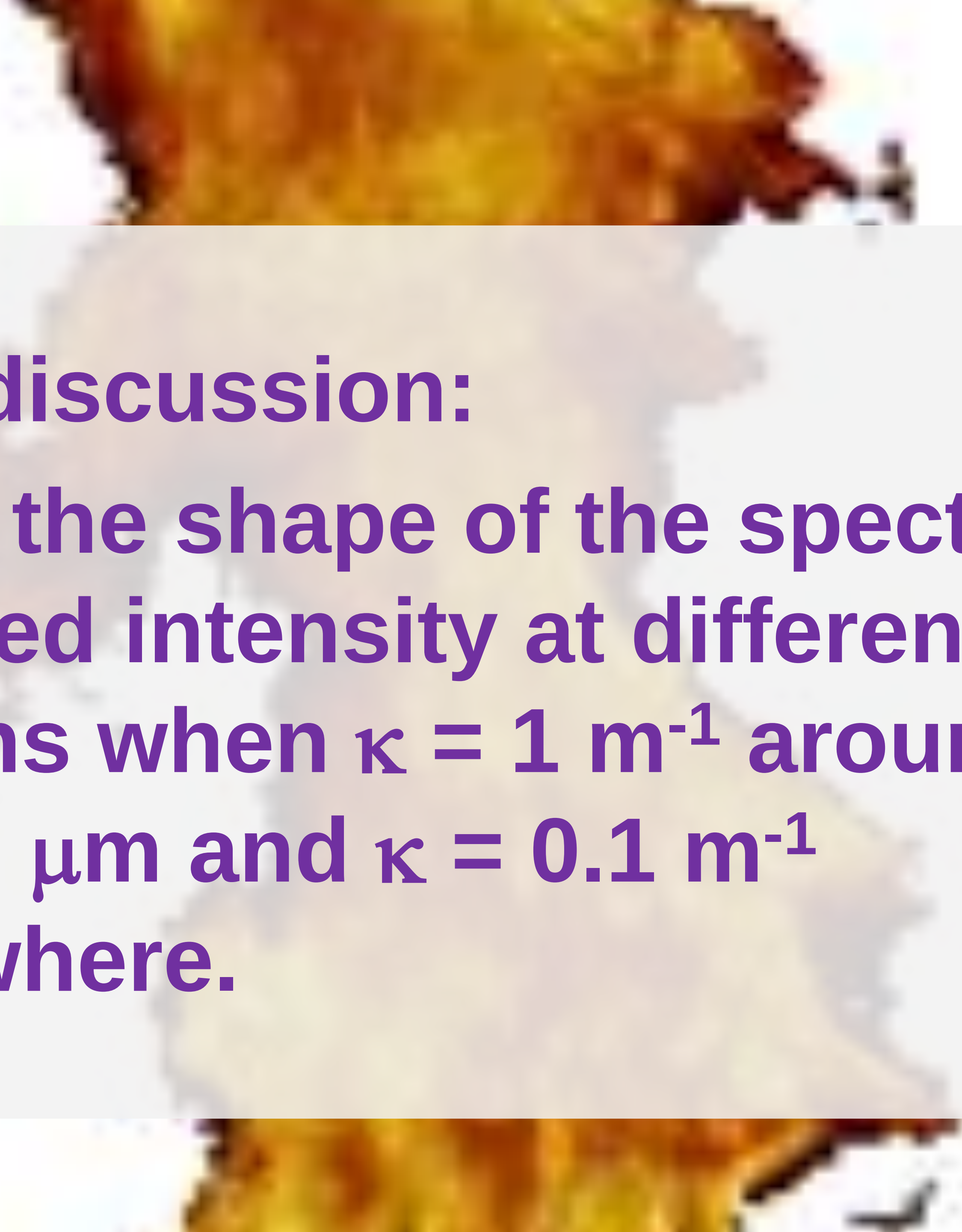
Absorption by discontinuous spectrum

- Assume a black body radiation entering gas with spectral absorption coefficient that is constant, except for λ=0.7 μm, where it goes to zero.
- Intensity changes now differently at different wavelengths, according to equation

$$I_\lambda(L) = I_{\lambda,0} \exp\left(-\kappa_\lambda L\right)$$





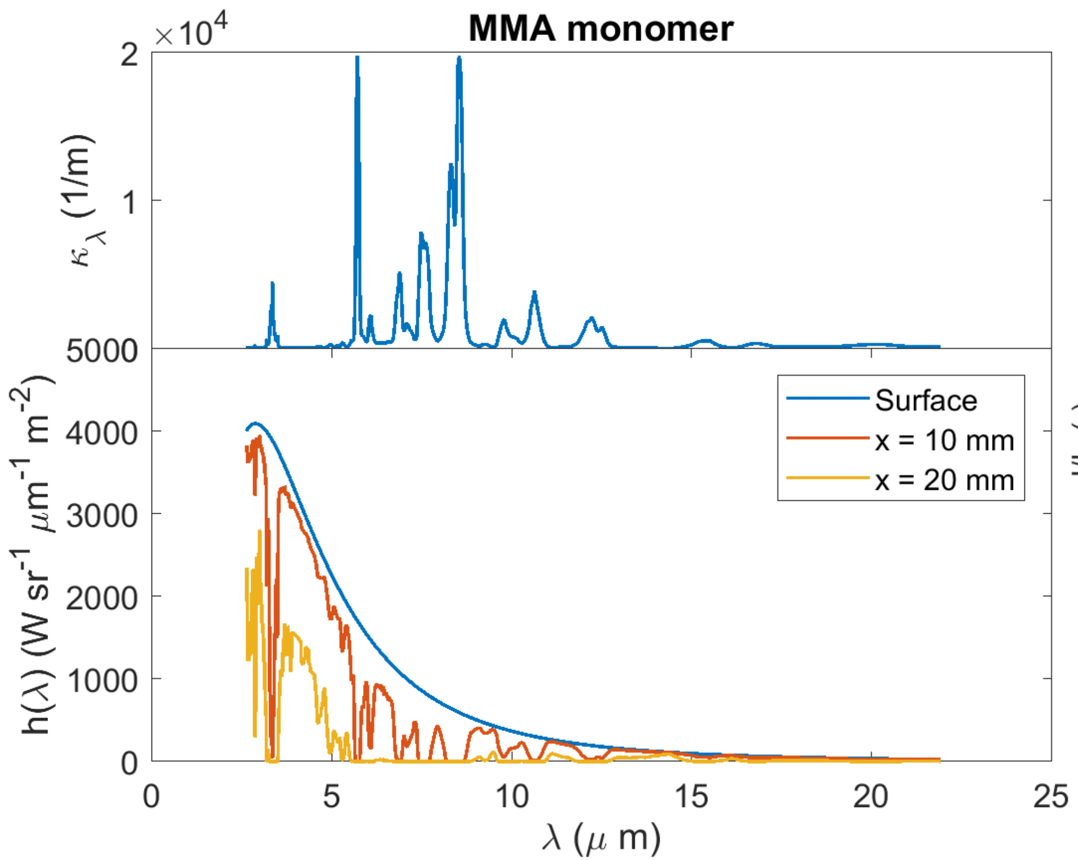


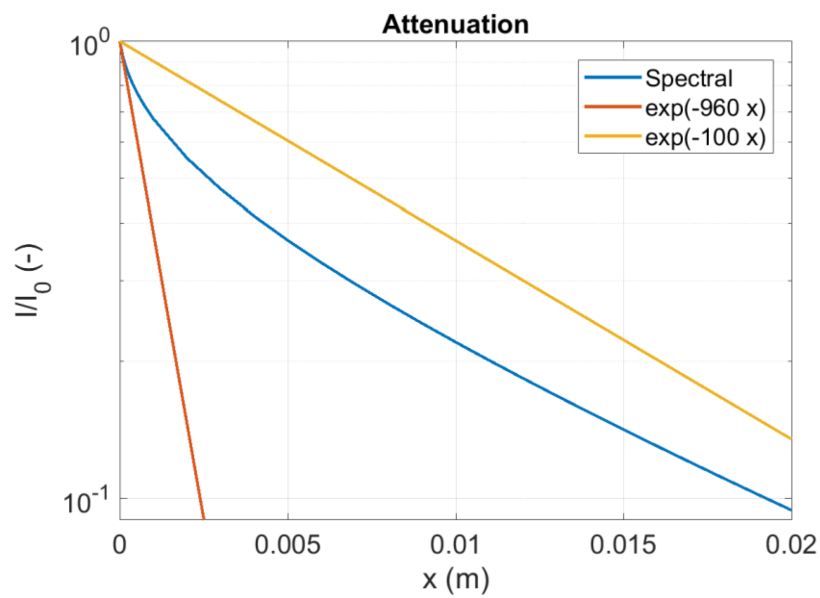
Pair discussion:

Draft the shape of the spectral emitted intensity at different depths when κ = 1 m^{-1} around λ=0.7 μm and κ = 0.1 m^{-1} elsewhere.

Example 1: Absorption by MMA

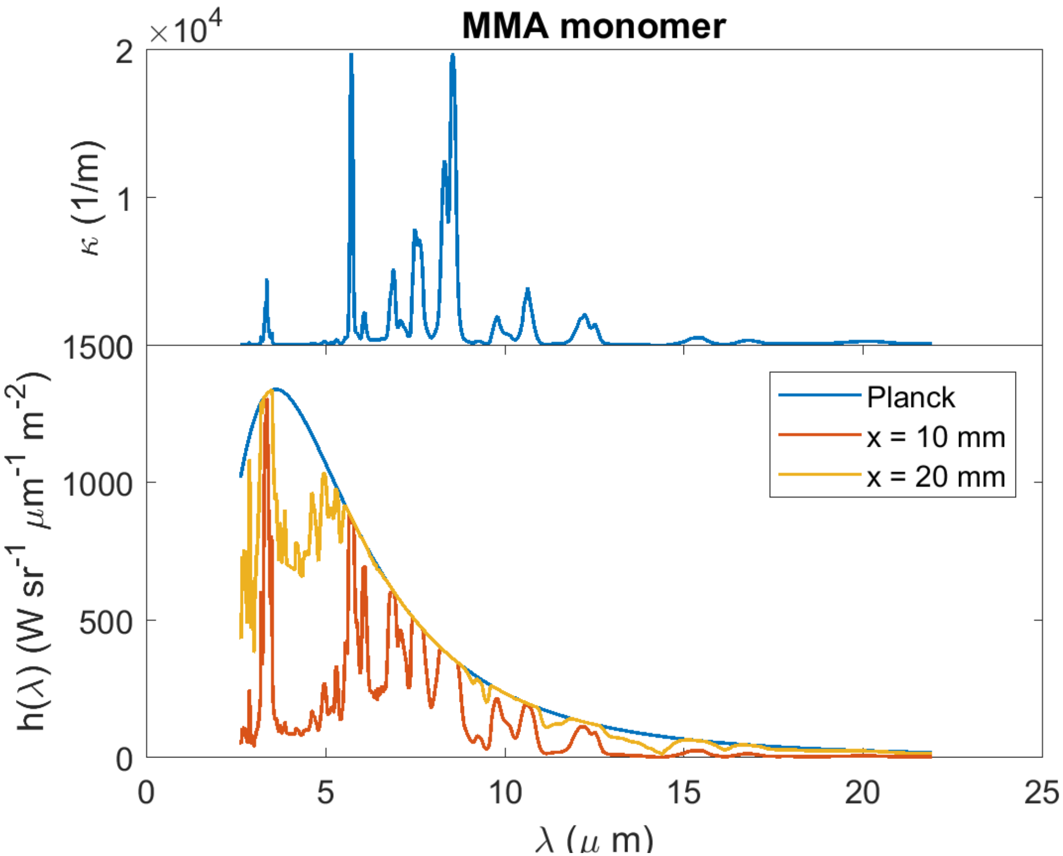
- Blackbody radiation from 1000 K source is absorbed by a cold (0 K) layer of MMA monomer solution.
- Different wavelengths are removed at different distances.

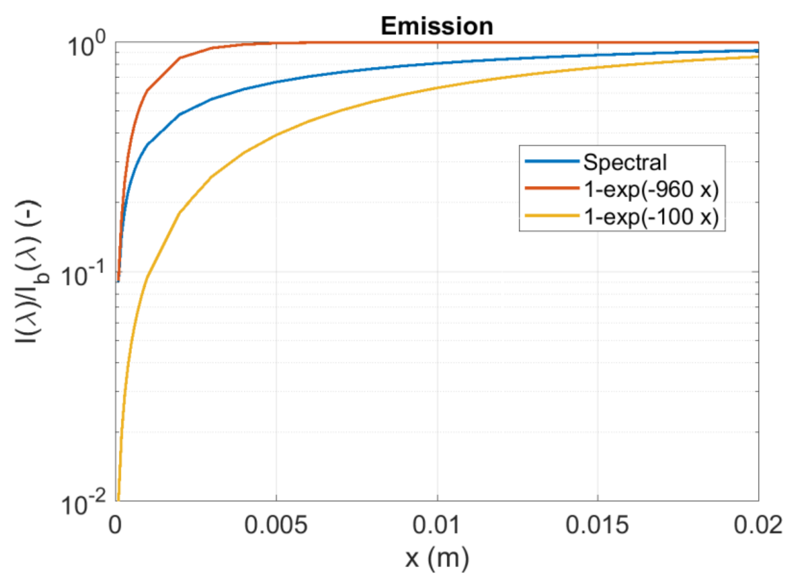




Example 2: Emission by MMA

- A layer of hot (800 K) MMA solution emits radiation.
- Different wavelengths approach Planck function at different distances.
- There is no average coefficient that would yield a correct profile.





RADCAL – Narrow Band Model

- RADCAL solves the single beam calculation for a large number of wavelength bands and integrates the result over spectrum.
- Outputs: Planck κ_P and effective κ_e mean absorption coefficients.

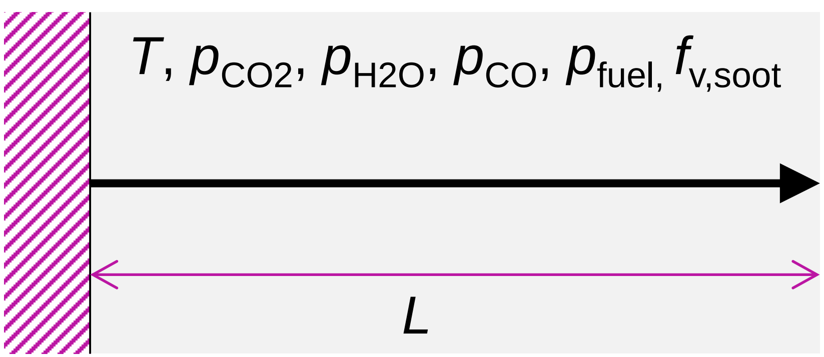
NIST Technical Note 1402

RADCAL: A Narrow-Band Model for Radiation Calculations in a Combustion Environment

William L. Grosshandler

Fire Science Division
Building and Fire Research Laboratory
National Institute of Standards and Technology
Gaithersburg, MD 20899

April 1993



$$\kappa_P = \frac{\int_0^\infty I_{b,\lambda} \kappa_\lambda \, d\lambda}{\int_0^\infty I_{b,\lambda} \, d\lambda}$$

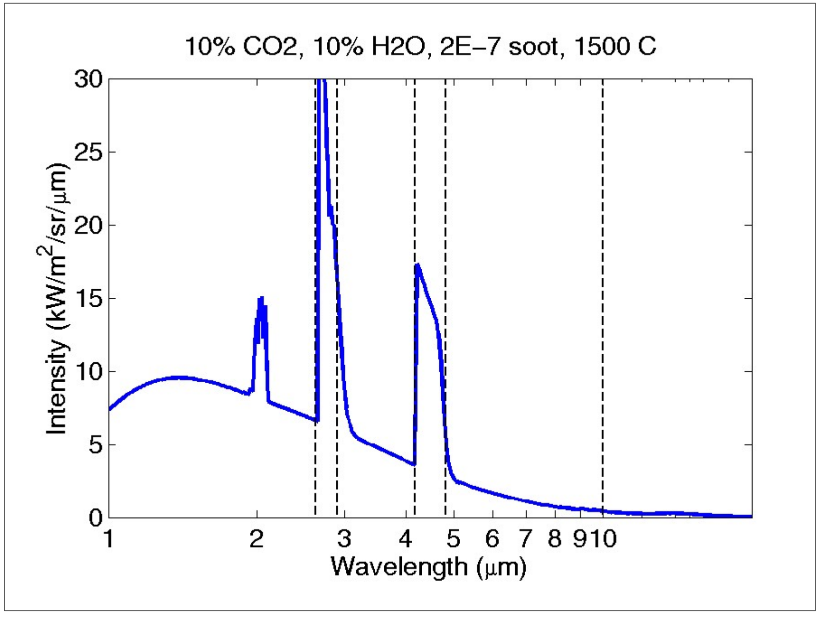
$$I_\lambda(L) = I_{\lambda,w} e^{-a_e L} \int_0^{\tau(L)} I_{b,\lambda} \exp\left[-(\tau(L) - \tau(L'))\right] d\tau(L')$$

$$I(L) = \frac{\sigma}{\pi}\left[e^{-\kappa_e L} T_{rad}^4 + \left(1 - e^{-\kappa_e L}\right) T^4\right]$$

Optical properties of gases

- Original RADCAL included CO_2, H_2O, CO and CH_4 –bands + soot.
- Other fuels were added to FDS by Vivien Lecoustre.
- Non-gray model is called wide band model

```
METHANE,        CARBON DIOXIDE,
ETHYLENE,       CARBON MONOXIDE,
ETHANE,         WATER VAPOR,
PROPANE,        SOOT
N-HEPTANE,
METHANOL,
TOLUENE,
PROPYLENE,
MMA
```



FDS User's Guide:
RADCAL_ID
FUEL_RADCAL_ID
WIDE_BAND_MODEL

Soot absorption coefficient

RADCAL calculates the soot absorption coefficient as a product of volume fraction f_v and specific absorption coefficient κ'_λ.

$$\kappa_\lambda(\mathbf{x}) = f_v(\mathbf{x})\ \kappa'_\lambda = f_v(\mathbf{x})\ \frac{7}{\lambda}$$

W. H. Dalzell and A. F. Sarofim **Optical Constants of Soot and Their Application to Heat-Flux Calculations.** *J. Heat Transfer* 91(1), 100-104 (1969) doi:10.1115/1.3580063

Gas property calculation procedure

```
INIT RADIATION *
    LOOP over T (K), concentrations (J), and species (NS)
        Call RADCAL(AP0,AMEAN)
        RADCAL_SPECIES2KAPPA(NS,J,K) = MIN(AMEAN,AP0)
    End Loop

SOLVE RADIATION
    For each location (I,J,K)
        KAPPA_GAS(I,J,K)=KAPPA_GAS(I,J,K)+GET_KAPPA(ZZ_GET,TYY)
    End for

FUNCTION GET_KAPPA(Z_IN,TYY,IBND)
    DO N = 1, N_RADCAL_ARRAY_SIZE
        GET_KAPPA = GET_KAPPA + RADCAL_SPECIES2KAPPA(N,Z_IN,TYY)
    ENDDO
```


**) Real code is a bit more compled (interpolations, bands)*

Source term of RTE

- The emission power density from gas mixture

$$B(\mathbf{x}) = \int_{V_{ijk}} \kappa(\mathbf{x}) I_b(\mathbf{x}) d\mathbf{x} \approx \int_{V_{ijk}} \kappa(\mathbf{x}) d\mathbf{x} \times \frac{\sigma}{\pi} \int_{V_{ijk}} T(\mathbf{x})^4 d\mathbf{x} \approx \bar{\kappa}_{ijk} \frac{\sigma}{\pi} \bar{T}_{ijk}^4$$

- Three error types:
  1) κ-T correlations (Radiation-Turbulence Interaction)
  2) T-distriution with a cell $\langle T^4 \rangle \neq \langle T \rangle^4$
  3) κ and T errors, e.g. $(0.85\,T)^4 \approx 0.52\,T^4$
- Usually we want to ensure a radiative fraction $\chi_r\, q'''$ ⇒ Modelled

$$I_{\mathrm{b,f}}(\mathbf{x}) = C\,\frac{\sigma\,T(\mathbf{x})^4}{\pi} \quad ; \quad C = \frac{\sum_{\dot{q}'''_{ijk}>0} \left(\chi_{\mathrm{r}}\, \dot{q}'''_{ijk} + \kappa_{ijk}\, U_{ijk} \right)\, \mathrm{d}V}{\sum_{\dot{q}'''_{ijk}>0} \left(4\, \kappa_{ijk}\, \sigma\, T^4_{ijk} \right)\, \mathrm{d}V}$$

FDS User's Guide: `RADIATIVE_FRACTION`

Exercise 2: Gas emission

Exercise 2: Hottel's charts

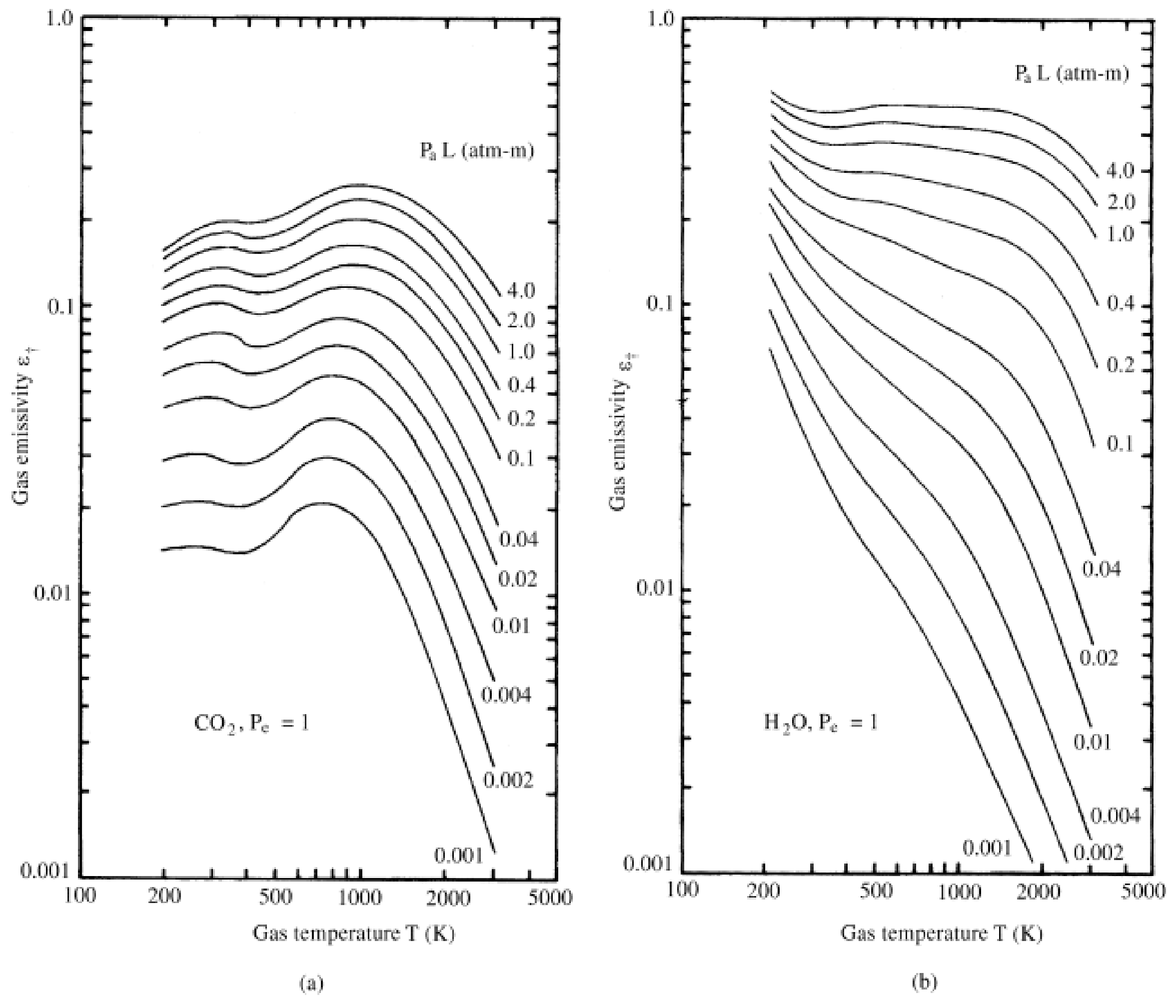


Figure 2.32 (a) Emissivity of carbon dioxide at 1 atmosphere total pressure and near zero partial pressure. (b) Emissivity of water vapour at 1 atmosphere total pressure and near zero partial pressure. From Edwards (1985). Reproduced by permission of the Society of Fire Protection Engineers

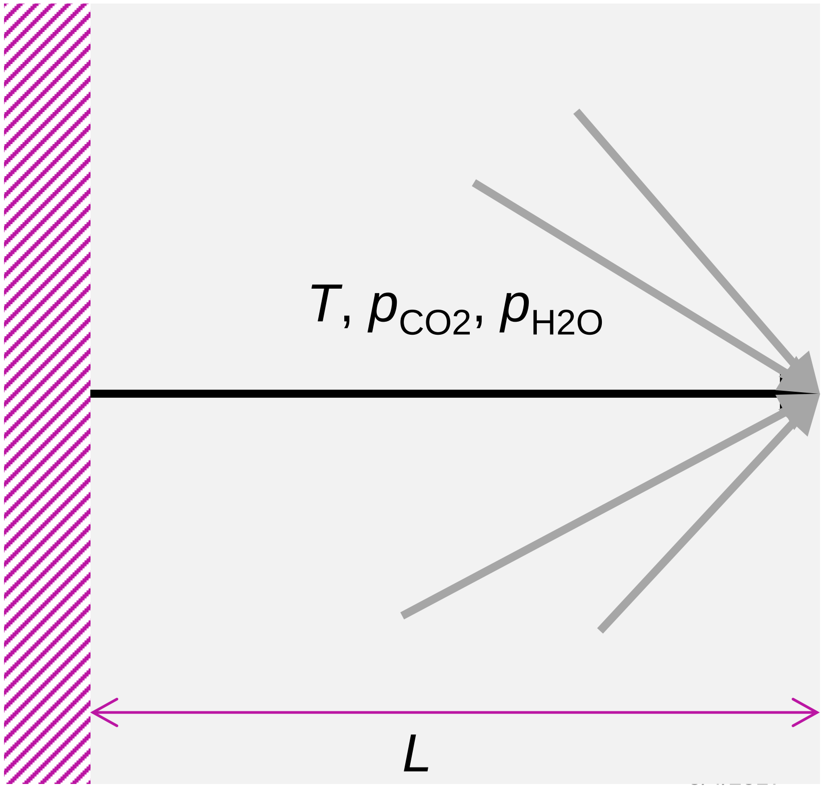
Drysdale, D. Introduction to Fire Dynamics, 3rd ed.

Exercise 2: Emissivity calculation

- Classical beam emissivity would come from $I(L) = \underbrace{\left(1 - e^{-kL}\right)}_{\varepsilon} \frac{\sigma T^4}{\pi}$

- Here, we assume that the Hottel's 'gray body' behaves as a layer, and the emissivity becomes

$$\varepsilon = \frac{\mathbf{q}_{incident}(L)}{\sigma T^4}$$



Exercise 2: Reproduce Hottel's curve

1. Study the input file **hottel_array.fds**
2. Pick one of H_2O or CO_2 curves in Hottel's charts, and specify the corresponding gas concentration into the FDS model.
   - Hottel's curves use product $p_{gas}L$
   - In the model, L = 1 m and P_{tot} = 1 atm $\Rightarrow$ $p_{gas}L$ = volume fraction. So, you just need to specify volume fraction. But FDS initialization only works for mass fraction. You calculate them as

$$Y_{CO2} = \frac{X_{CO2}\,44}{X_{CO2}\,44 + (1\ - X_{CO2}\,)28.8} \qquad Y_{H2O} = \frac{X_{H2O}\,18}{X_{H2O}\,18 + (1\ - X_{H2O}\,)28.8}$$

   - CO_2 mass fraction can be specified using `Y_CO2_INFTY` at `MISC` line.
   - H_2O mass fraction must be set on `&INIT` lines
3. Run the model and plot the emissivity at different temperatures using **plot_hottel.py**.
4. Discuss with your neighbor how the code works.