FDS for advanced

Sylvain DESANGHERE

Lombardi Group

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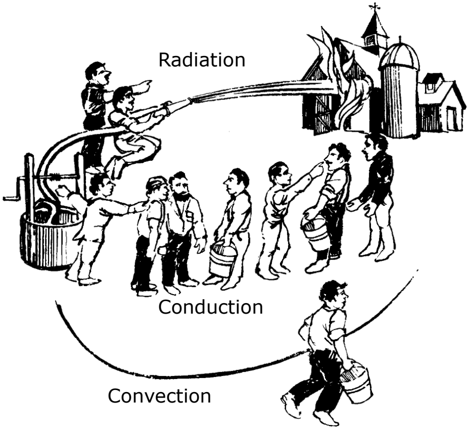
Presentation outline

1. Heat transfer modeling in FDS
2. Fire definition
3. Using FDS outputs

Heat transfer

Heat transfer



Adapted from : A Heat Transfer Textbook, 4th edition John H. Lienhard IV, Professor, University of Houston, John H. Lienhard V, Professor, Massachusetts Institute of Technology, Copyright (c) 2000-2011, John H. Lienhard IV and John H. Lienhard V. All rights reserved.

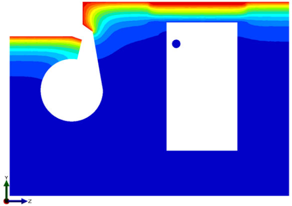
Heat conduction basics

- Very weak within the gases
- First propagation mechanism of heat within solids
- Fourier's law :

$$j = -\lambda \nabla T$$

- Heat equation :

$$\nabla \cdot (\lambda \nabla T) + \dot{q} = \rho C_p \frac{\partial T}{\partial t}$$



- One dimensional form, without heat source and with homogeneous λ :

$$\frac{\partial T}{\partial t} = \alpha \frac{\partial^2 T}{\partial x^2}$$

where

$$\alpha = \frac{\lambda}{\rho C_p}$$ thermal diffusivity

Heat convection basics

- Fluid movement is required
- **Natural convection** : governed by density differences
- **Forced convection** : governed by the forced flow
- Convective flux :

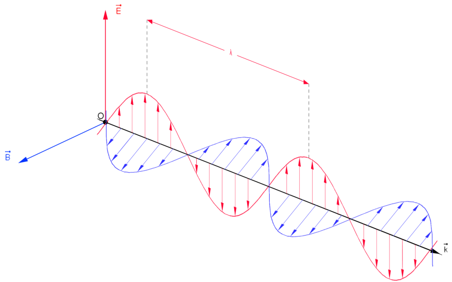
$$\varphi = h(T_{\text{fluid}} - T_{\text{solid}})$$

- The convection coefficient *h* is strongly linked to the flow characteristics
- FDS formulation :

$$h = MAX\left[C|\Delta T|^{1/3}; \frac{k}{L} 0.037 Re^{4/5} Pr^{1/3}\right]$$

Heat radiation basics

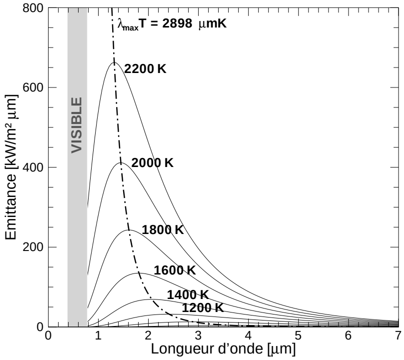
- Electromagnetic wave (Maxwell equations)
  - No material support is required
  - The two main characteristics are wavelength and intensity
- All solids are continuously exchanging radiation
- Radiation is the most important heat transfer mechanism in fires
- **Blackbody**
  - A body wich absorbs all incoming radiation
  - Diffuse radiation : no preferred direction



Blackbody radiant emittance

- **Radiant emittance** : total energy per unit time per unit surface, radiated by an elementary surface
- Blackbody radiant emittance → Planck's function :

$$e_{\lambda,b} = \frac{2hc_0^2\lambda^{-5}}{exp(\frac{hc_0}{\lambda kT}) - 1}$$



- Stefan law :

$$e_b = \int e_{\lambda,b} d\lambda = \sigma T^4$$

Radiative balance

- Emissivity of a material
  - Ratio between radiation emitted by the material and the radiation emitted by a blackbody at the same temperature

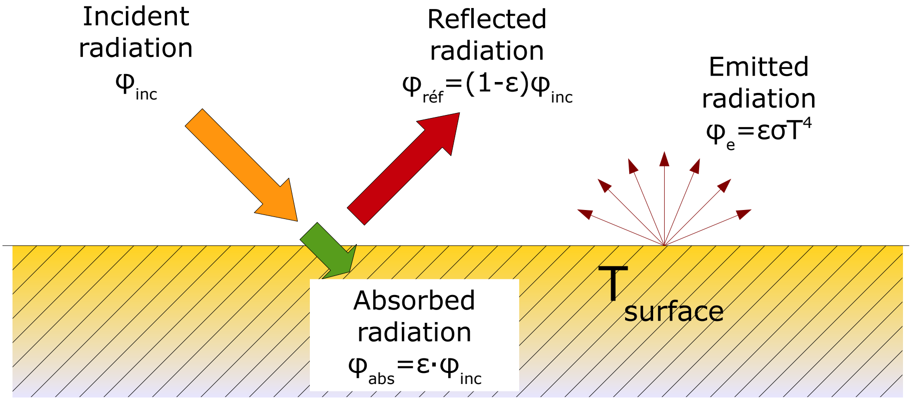
$$\varepsilon_\lambda = \frac{e_\lambda}{e_{\lambda,b}} \in [0;1]$$

  - Common assumption : ε_λ does not change with wavelength (gray surfaces)

$$e = \varepsilon \sigma T^4$$

- Kirchoff law : absorbed fraction of incoming radiation = emissivity

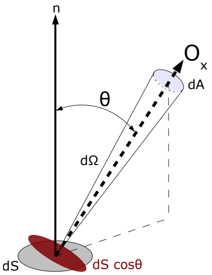
Radiative balance



Radiant intensity

- **Radiant intensity** I_{O_x} emitted by an elementary surface dS in a direction O$_x$ = radiant flux emitted in a solid angle Ω around O$_x$ direction, divided by the projection of the source on the direction

$$I_{O_x} = \frac{\mathrm{d}\varphi_x}{\mathrm{d}\Omega \mathrm{d}S \cos\theta} \tag{1}$$

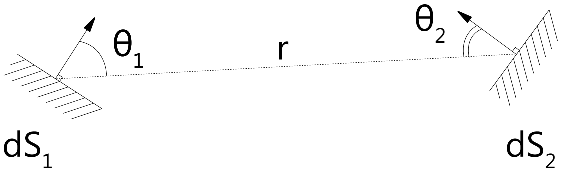


Radiative exchange between solids

- Radiative flux emitted by an elementary surface $\mathrm{d}S_1$ with radiant intensity I_1 to another elementary surface $\mathrm{d}S_2$:

$$\mathrm{d}\varphi = I_1 \mathrm{d}\Omega \mathrm{d}S_1 \cos\theta_1 = I_1 \frac{\mathrm{d}S_1 \cos\theta_1 \mathrm{d}S_2 \cos\theta_2}{r^2} \tag{2}$$

View factors catalog http://www.thermalradiation.net/indexCat.html



Radiant intensity and emittance

- *Diffuse* radiation = radiant intensity is independent of direction O_x and :

$$\begin{aligned}\frac{1}{dS}\int \varphi_x &= \int_{2\pi} L_{O_x} \cos\theta\Omega \\ &= L\int_0^{2\pi}\int_0^{\pi/2} \sin\theta\cos\theta\theta\phi \\ &= \pi I \qquad (3)\end{aligned}$$

- Link between radiant intensity and emittance $I = e/\pi$
- Blackbody : $I_b = \sigma T^4/\pi$
- In FDS, output INTEGRATED INTENSITY is :

$$U = \int I dS \qquad \text{At } 20\ ^\circ\text{C :} \qquad U = 4\pi I_b = 4\sigma T^4 \qquad (4)$$

Interaction between radiation and gases

- Ambient air : no effect, transparent
- Smoke : participating media
  - **Absorption** → Radiant energy is partially accumulated by electrically asymmetric molecules (CO_2,H_2O, CH_4, etc.) and soot
  - **Diffusion** → Radiant energy is partially deviated by particles

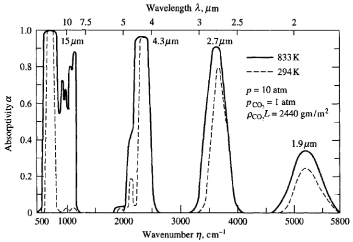
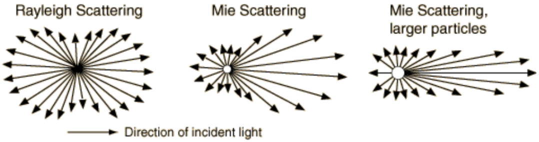


FIGURE 1-15
Spectral absorptivity of an isothermal mixture of nitrogen and carbon dioxide, from Edwards [16].



Radiative transfer equation (RTE)

- Radiant intensity variation I_λ along the path s :

$$\frac{\mathrm{d}I_\lambda}{\mathrm{d}s} = \underbrace{-\kappa I_\lambda}_{\text{absorption}} + \underbrace{\kappa I_{\lambda,b}}_{\text{emission}} \underbrace{-\sigma I_\lambda + \frac{\sigma}{4\Pi}\int_{4\Pi} \Phi I_\lambda \mathrm{d}\Omega}_{\text{diffusion}}$$

- Radiant attenuation governed by the absorption coefficient κ
  - Inhomogeneous
  - Linked the the gases compostion (mainly soot density)

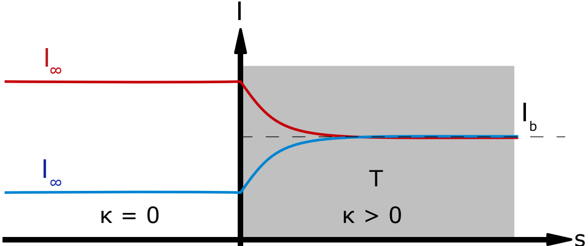
Radiative transfer equation : a simple example

- Monodimensional case, homogeneous media

$$\frac{dI}{ds} = \kappa(I_b - I) = \kappa(\frac{\sigma T^4}{\Pi} - I) \quad \text{where} \quad I(0) = I_\infty$$

- Solution

$$I(s) = (I_\infty - I_b)\exp(-\kappa \cdot s) + I_b$$



Radiative transfer equation in FDS

- Spectral decomposition

$$I(\mathbf{x},\mathbf{s}) = \int_0^\infty I_\lambda(\mathbf{x},\mathbf{s})\mathrm{d}\lambda \tag{5}$$

- RTE

$$\begin{aligned}\frac{\mathrm{d}I_\lambda(\mathbf{x},\mathbf{s})}{\mathrm{d}\mathbf{s}} &= \mathbf{s}\cdot\nabla I_\lambda(\mathbf{x},\mathbf{s})\\ &= -[\kappa(\mathbf{x},\lambda)+\sigma(\mathbf{x},\lambda)]I_\lambda(\mathbf{x},\mathbf{s})+B(\mathbf{x},\lambda)\\ &+ \frac{\sigma(\mathbf{x},\lambda)}{4\pi}\int_{4\pi}\Phi(\mathbf{s},\mathbf{s}')I_\lambda(\mathbf{x},\mathbf{s}')\Omega\end{aligned} \tag{6}$$

- Simplification : non diffusive media

$$\mathbf{s}\cdot\nabla I_\lambda(\mathbf{x},\mathbf{s}) = \kappa(\mathbf{x},\lambda)[I_b(\mathbf{x}) - I_\lambda(\mathbf{x},\mathbf{s})] \tag{7}$$

Radiative transfer equation in FDS

- Spectral bands decomposition

$$\mathbf{s}\cdot\nabla I_n(\mathbf{x},\mathbf{s}) = \kappa_n(\mathbf{x})\left[I_{b,n}(\mathbf{x}) - I_n(\mathbf{x},\mathbf{s})\right] \quad \text{with} \quad n = 1,\ldots,N \tag{8}$$

- Total radiative intensity

$$I(\mathbf{x},\mathbf{s}) = \sum_{n=1}^{N} I_n(\mathbf{x},\mathbf{s}) \tag{9}$$

- Radiative flux vector divergence and integrated intensity

$$-\nabla\cdot\mathbf{q_r} = \sum_{n=1}^{N}\kappa_n(\mathbf{x})\left[U_n(\mathbf{x}) - 4\pi L_{b,n}(\mathbf{x})\right] \tag{10}$$

$$U_n(\mathbf{x}) = \int_{4\pi} I_n(\mathbf{x},\mathbf{s})\Omega \tag{11}$$

Absorption coefficients κ_n depend on temperature and gas composition (**RadCal**)

Radiative transfer equation in FDS

- In standard use of FDS : gray gas
    - Radiation is driven by soot
    - Continuous spectrum for soot
    - $\Rightarrow$ one band model

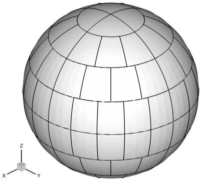
$$\mathbf{s} \cdot \nabla I(\mathbf{x},\mathbf{s}) = \kappa(\mathbf{x}) \left[\frac{\sigma T(\mathbf{x})^4}{\pi} - I(\mathbf{x},\mathbf{s}) \right] \tag{12}$$

- Then, use the solution to evaluate

$$-\nabla \cdot \mathbf{q_r} = \kappa(\mathbf{x}) \left[\int_{4\pi} I(\mathbf{x},\mathbf{s}) \Omega - 4\sigma T(\mathbf{x})^4 \right] \tag{13}$$

Radiative transfer equation in FDS

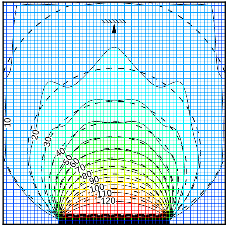
- Angular discretisation



- Special topics
  - Combustion zone

$$\kappa I_b = \max\left(\chi_r \frac{\dot{q}'''}{4\pi}, \kappa \frac{\sigma T(\mathbf{x})^4}{\pi}\right) \tag{14}$$

  - Strongly linked to gas composition (κ), radiation in T^4, fluctuations, etc.
  - There are some preferential directions



Fire definition

Combustion modeling

- Global chemical equation

$$
\begin{aligned}
C_xH_yO_zN_vX_w &+ \nu_{O_2}\left(O_2 + 3.76N_2\right) \rightarrow \\
& \nu_{CO_2}CO_2 \\
&+ \nu_{H_20}H_2O \\
&+ \nu_{CO}CO \\
&+ \nu_{soot}Soot \\
&+ \nu_{H_2}H_2 \\
&+ \nu_{N_2}N_2 \\
&+ \nu_{X}X
\end{aligned}
\tag{15}
$$

Heat of combustion

- Total energy obtained by combustion

$$E = m_{O_2} \cdot \Delta H_{O_2} \tag{16}$$

- $\Delta H_{O_2} \simeq 13{,}1$ MJ/kg
- Ideal combustion of $C_xH_yO_z$

$$C_xH_yO_z + (x + \frac{y}{4} - \frac{z}{2})O_2 \rightarrow xCO_2 + \frac{y}{2}H_2O \tag{17}$$

$$\Delta H_c = \frac{32(x + y/4 - z/2)}{12x + y + 16z}\Delta H_{O_2} \tag{18}$$

Conversion factors

- Link between consumption and production of species

$$m_k = \frac{\nu_k}{\nu_{O_2}} \frac{M_k}{M_{O_2}} m_{O_2} = \frac{\nu_k}{\nu_{O_2}} \frac{M_k}{M_{O_2}} \frac{E}{\Delta H_{O_2}} \tag{19}$$

- Conversion factor

$$\tau_k = \frac{m_k}{E} = \frac{\nu_k M_k}{\Delta H_{O_2} \nu_{O_2} M_{O_2}} \tag{20}$$

- Soot and fuel

$$\tau_{\mathrm{soot}} = \frac{m_{\mathrm{soot}}}{E} = \frac{\nu_{\mathrm{soot}} M_{\mathrm{soot}}}{\Delta H_c M_{\mathrm{fuel}}} = \frac{y_{\mathrm{soot}}}{\Delta H_c} \tag{21}$$

Mixture fraction

- Combustion equation

$$\nu_{\mathrm{F}}\mathrm{F} + \nu_{\mathrm{O_2}}\mathrm{O_2} \rightarrow \sum_i \nu_i \mathrm{P}_i$$

- Transport equation

$$\frac{\partial \rho Y_k}{\partial t} + \nabla \cdot (\rho \mathbf{u} Y_k) = \nabla \cdot (\rho D_k \nabla Y_k) + \dot{\omega}_k \tag{22}$$

- Production and consumption are linked by :

$$\dot{\omega}_{\mathrm{O_2}} = s\dot{\omega}_{\mathrm{F}} \qquad \text{et} \qquad \dot{\omega}_{\mathrm{P}} = -(1+s)\dot{\omega}_{\mathrm{F}} \tag{23}$$

with $s = \dfrac{\nu_{\mathrm{O_2}} M_{\mathrm{O_2}}}{\nu_{\mathrm{F}} M_{\mathrm{F}}}$

Mixture fraction

- Mixture fraction

$$Z = \frac{sY_F - (Y_{O_2} - Y_{O_2}^{\infty})}{sY_F^I + Y_{O_2}^{\infty}} \tag{24}$$

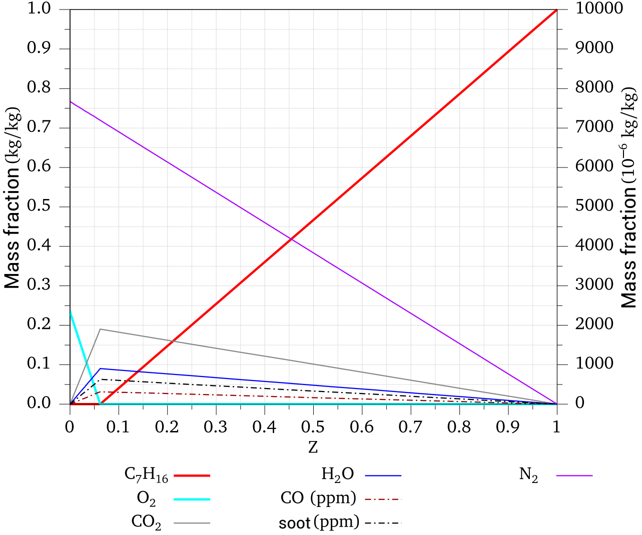
- Infinitely fast chemistry means

$$Z_{st} = \frac{Y_{O_2}^{\infty}}{sY_F^I + Y_{O_2}^{\infty}} \tag{25}$$

- Transport equation for mixture fraction

$$\frac{\partial \rho Z}{\partial t} + \nabla \cdot (\rho \mathbf{u} Z) = \nabla \cdot (\rho D \nabla Z) \tag{26}$$

Example : heptane



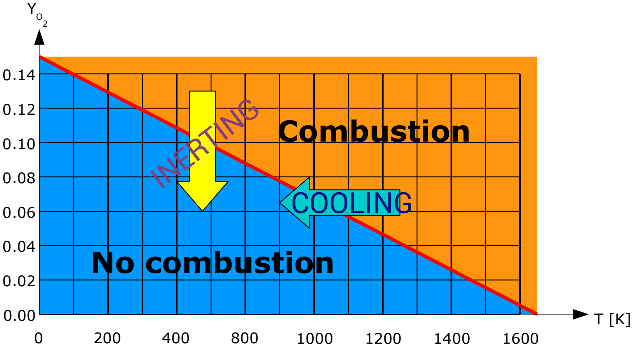
Simple extinction model

- Oxygen combustion : $Q = m \cdot Y_{O_2} \frac{\Delta H_f}{r_{O_2}}$
- Adiabatic flame temperature : $T_f = T_0 + \frac{Q}{m \cdot \overline{C_p}}$
- Hence : $Y_{O_2} = \frac{\overline{C_p}(T_f - T_0)}{\Delta H_f / r_{O_2}}$
- With typical values of $\overline{C_p}$, T_f et $\Delta H_f / r_{O_2}$:

$$Y_{O_2,\text{lim}} = \frac{1.2(1\,700 - T_0)}{13\,100} \tag{27}$$

Simple extinction model

$$Y_{O_2,\mathrm{lim}} = \frac{1.2(1\,700 - T_0)}{13\,100}$$



Using FDS outputs

Radiative balance at solid surface

- Radiative flux emitted

$$\varphi_{\mathrm{e}}^{\mathrm{rad}} = \varepsilon\sigma T^4 \tag{28}$$

- Received radiative flux

$$\varphi_{\mathrm{r}}^{\mathrm{rad}} = \varepsilon\varphi_{\mathrm{incident}}^{\mathrm{rad}} \tag{29}$$

- Net radiative flux

$$\varphi_{\mathrm{net}}^{\mathrm{rad}} = \varphi_{\mathrm{r}}^{\mathrm{rad}} - \varphi_{\mathrm{e}}^{\mathrm{rad}} = \varepsilon(\varphi_{\mathrm{incident}}^{\mathrm{rad}} - \sigma T^4) \tag{30}$$

Thermal balance at solid surface

- Convective balance

$$\varphi_{\text{net}}^{\text{conv}} = h(T_g - T) \tag{31}$$

- Thermal balance

$$\varphi_{\text{net}} = \varphi_{\text{net}}^{\text{rad}} + \varphi_{\text{net}}^{\text{conv}} = \varepsilon(\varphi_{\text{incident}}^{\text{rad}} - \sigma T^4) + h(T_g - T) \tag{32}$$

- Written as

$$\boxed{\varphi_{\text{net}} = \underbrace{\left(\varepsilon\varphi_{\text{incident}}^{\text{rad}} + hT_g\right)}_{(a)} - \underbrace{\left(\varepsilon\sigma T^4 + hT\right)}_{(b)}} \tag{33}$$

  - (a) is the thermal environment calculated by FDS
  - (b) is the thermal response of the surface

Extracting (a) from FDS calculation ?

FDS usual outputs

- CONVECTIVE_HEAT_FLUX : $\varphi_{\text{net}}^{\text{conv}} = h(T_g - T)$
- RADIATIVE_HEAT_FLUX : $\varphi_{\text{net}}^{\text{rad}} = \varepsilon(\varphi_{\text{incident}}^{\text{rad}} - \sigma T^4)$
- NET_HEAT_FLUX : $\varphi_{\text{net}} = \varphi_{\text{net}}^{\text{conv}} + \varphi_{\text{net}}^{\text{rad}}$
- INCIDENT_HEAT_FLUX : $\frac{\varphi_{\text{net}}^{\text{rad}}}{\varepsilon} + \sigma T^4 + h(T_g - T)$
- GAUGE_HEAT_FLUX : $\varphi_{\text{net}}^{0} = \varphi_{\text{incident}}^{\text{rad}} - \sigma T_\infty^4 + h(T_g - T_\infty)$
- RADIOMETER : $\varphi^{\text{RD}} = \frac{\varphi_{\text{net}}^{\text{rad}}}{\varepsilon} + \sigma(T^4 - T_\infty^4)$
- None of them is really adapted to transfer information to FEM model

Adiabatic Surface Temperature

- Root of

$$\varphi_{\text{net}} = \varepsilon\sigma\left(T_{\text{AST}}^4 - T^4\right) + h(T_{\text{AST}} - T) \tag{34}$$

- Temperature of an adiabatic surface ($\varphi_{\text{net}} = 0$)
- Temperature seen by the surface (used exactly as the ISO curve for input in FEM heat conduction calculation)
- (a) quantity can be calculated as

$$\varepsilon\varphi_{\text{incident}}^{\text{rad}} + h \cdot T_g = \varepsilon\sigma T_{\text{AST}}^4 + hT_{\text{AST}} \tag{35}$$

- T_{AST} is the best way of transfering heat fluxes on surfaces normal to the main axis