FDS for advanced

Theory, practical cases and rules of thumb

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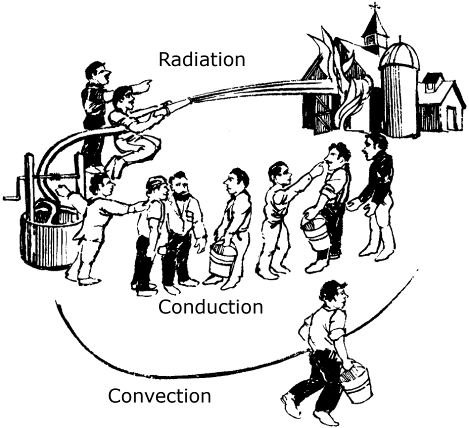
Presentation outline

1. Heat transfer modeling in FDS
2. Fire definition
3. Using FDS outputs
4. Examples
5. To go further

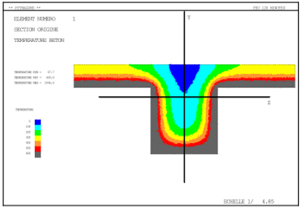
Heat transfer



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,

Heat conduction basics

- 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 :

$$\frac{\partial T}{\partial t} = \alpha \frac{\partial^2 T}{\partial x^2} \quad \text{where} \quad \alpha = \frac{\lambda}{\rho C_p} \quad \text{thermal diffusivity}$$

Heat convection basics

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

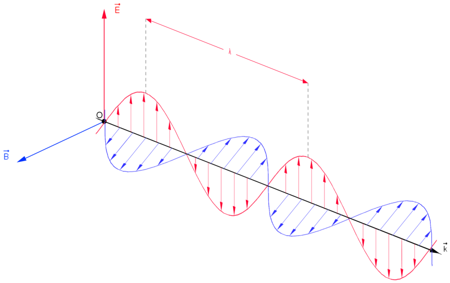
$$\varphi = h(T_{\text{fluid}} - T_{\text{solid}})$$

- The convection coefficient h is strongly linked to the flow characteristics
- FDS default formulation (planar surface) :

$$h = MAX\left[C|\Delta T|^{1/3}; \frac{k}{L}0.037Re^{4/5}Pr^{1/3}; \frac{k}{\delta n/2}\right]$$

Heat radiation basics

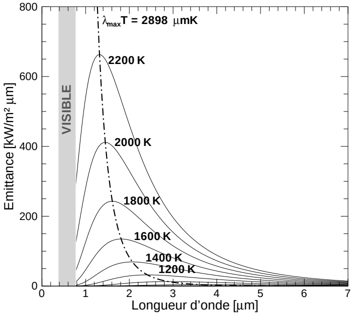
- Electromagnetic wave (Maxwell equations)
  - No material support is required
  - The two main characteristics are wavelength and intensity
- All solids are continuously exchanging radiation
- Radiation is the most important heat transfer mechanism in fires
- **Blackbody**
  - A body wich absorbs all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

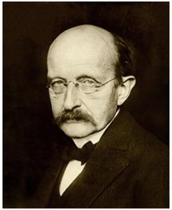


Blackbody radiant emittance

- **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 :

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

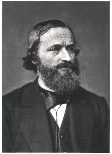
Radiative balance

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

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

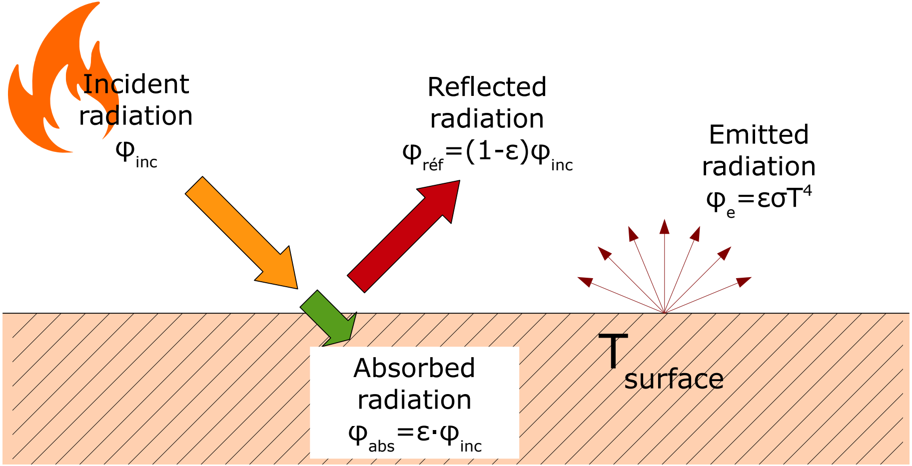
  - Common assumption : ε_λ does not change with wavelength (gray surfaces)

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



- Kirchhoff law : absorbed fraction of incoming radiation = emissivity

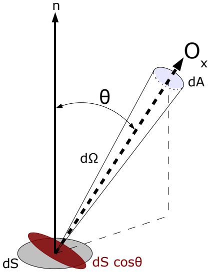
Radiative balance



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

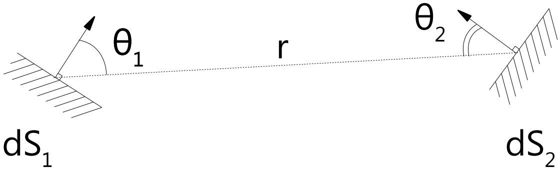
$$I_{O_x} = \frac{d\varphi_x}{d\Omega dS \cos\theta} \quad (1)$$



Radiative exchange between solids

- Radiative flux emitted by an elementary surface dS_1 with radiant intensity I_1 to another elementary surface dS_2 :

$$d\varphi = I_1 d\Omega dS_1 \cos\theta_1 = I_1 \frac{dS_1 \cos\theta_1 dS_2 \cos\theta_2}{r^2} \tag{2}$$



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

Radiant intensity and emittance

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

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

- 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

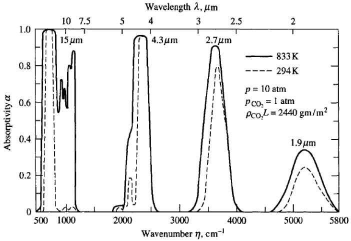
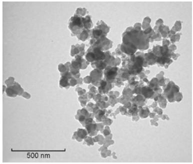
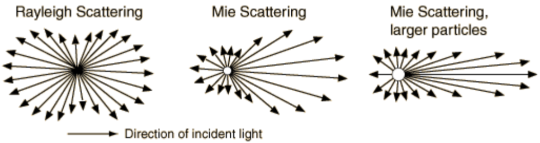


FIGURE 1-15
Spectral absorptivity of an isothermal mixture of nitrogen and carbon dioxide, from Edwards [16].





Radiative transfer equation (RTE)

- Radiant intensity variation I_λ along the path s :

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

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

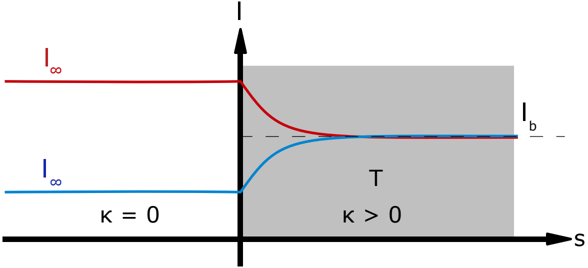
Radiative transfer equation : a simple example

- 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

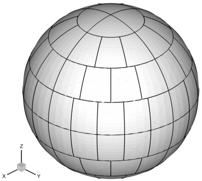
$$\mathbf{s} \cdot \nabla I(\mathbf{x},\mathbf{s}) = \kappa(\mathbf{x}) \left[\frac{\sigma T(\mathbf{x})^4}{\pi} - I(\mathbf{x},\mathbf{s}) \right] \tag{12}$$

  - 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

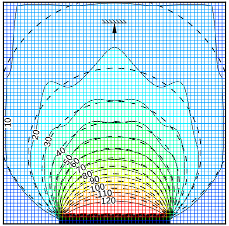
- Angular discretisation



- 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

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

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

$$\tau_k = \frac{m_k}{E} = \frac{\nu_k M_k}{\Delta H_{O_2} \nu_{O_2} M_{O_2}} \qquad (\mathrm{g/MJ}) \qquad = \frac{\dot{m}_k}{\mathrm{HRR}} \tag{20}$$

- Soot and fuel

$$\tau_{\mathrm{soot}} = \frac{m_{\mathrm{soot}}}{E} = \frac{\nu_{\mathrm{soot}} M_{\mathrm{soot}}}{\Delta H_c M_{\mathrm{fuel}}} = \frac{y_{\mathrm{soot}}}{\Delta H_c} \qquad (\mathrm{g/MJ}) \tag{21}$$

Infinitely fast chemistry : mixture fraction concept

- Combustion equation

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

- 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 :

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

with $s = \frac{\nu_{O_2} M_{O_2}}{\nu_F M_F}$ the stoichiometric coefficient

Infinitely fast chemistry : mixture fraction concept

- Mixture fraction

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

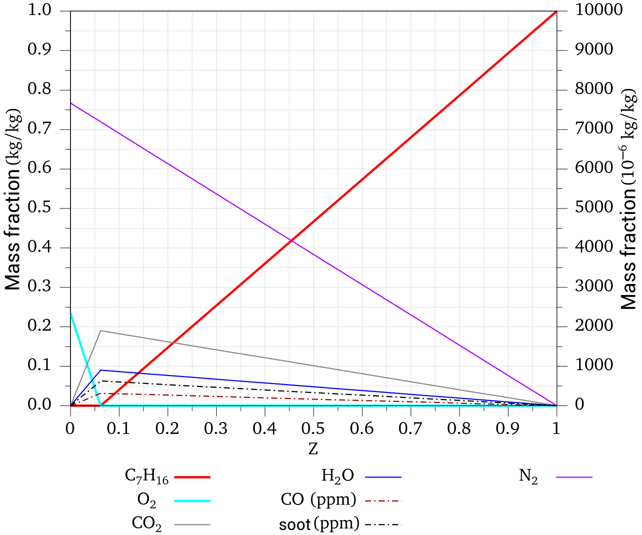
- Infinitely fast chemistry means fuel and air vanish at

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

- 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



Finite rate chemistry : lumped species approach

- Example : methane complete combustion

$$\underbrace{CH_4}_{Fuel} + 2\underbrace{(O_2 + 3{,}76N_2)}_{Air} \rightarrow \underbrace{CO_2 + 2H_2O + 7{,}52N_2}_{Products} \quad (27)$$

$$\begin{pmatrix} 0.77 & 0.00 & 0.73 \\ 0.23 & 0.00 & 0.00 \\ 0.00 & 1.00 & 0.00 \\ 0.00 & 0.00 & 0.15 \\ 0.00 & 0.00 & 0.12 \end{pmatrix} \begin{pmatrix} Z_{Air} \\ Z_{Fuel} \\ Z_{Products} \end{pmatrix} = \begin{pmatrix} Y_{N_2} \\ Y_{O_2} \\ Y_{CH_4} \\ Y_{CO_2} \\ Y_{H_2O} \end{pmatrix} \quad (28)$$

- Solve 2 transport equations : for Z_{Fuel} and for $Z_{Products}$
- $Z_{Air} = 1 - Z_{Fuel} - Z_{Products}$

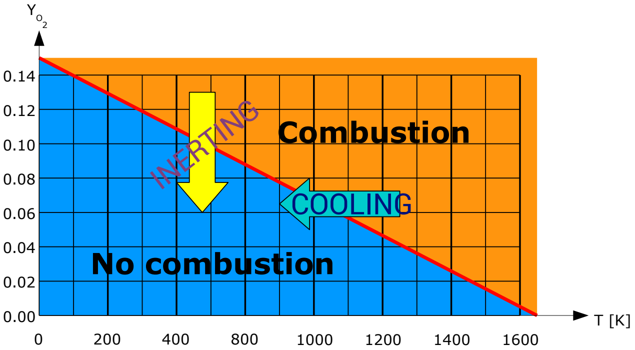
Simple extinction model

- 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 $\Delta H_f / r_{O_2}$:

$$Y_{O_2,\mathrm{lim}} = \frac{1.2(1\ 700 - T_0)}{13\ 100} \tag{29}$$

Simple extinction model

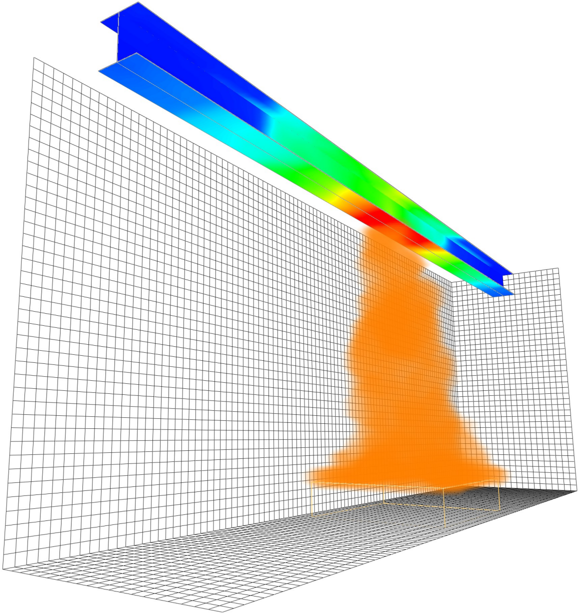
$$Y_{O_2,\lim} = \frac{1.2(1\,700 - T_0)}{13\,100}$$



Frequently used fire definition

- Wood
  &REAC FUEL = 'WOOD',C = 3.4, H = 6.2, O = 2.5, CO_YIELD = 0.02, SOOT_YIELD = 0.035, HEAT_OF_COMBUSTION = 15000 /
- Polyurethane
  &REAC FUEL = 'PUR',C = 6.3, H = 7.1, O = 2.1, N = 1, CO_YIELD = 0.04, SOOT_YIELD = 0.10, HEAT_OF_COMBUSTION = 18724 /
- Plastic/wood
  &REAC FUEL = 'MIXED',C = 5.0, H = 7.43, O = 1.65, CO_YIELD = 0.025, SOOT_YIELD = 0.05, HEAT_OF_COMBUSTION = 24954 /
- Heptane
  &REAC FUEL = 'HEPTANE',C = 7, H = 16, CO_YIELD = 0.005, SOOT_YIELD = 0.01, HEAT_OF_COMBUSTION = 45625 /
- Adjust RADIATIVE_FRACTION from 0.2 to 0.4 (default value is 0.35)

Using FDS outputs for fire resistance study



Radiative balance at solid surface

- Radiative flux emitted

$$\varphi_{\mathrm{e}}^{\mathrm{rad}} = \varepsilon\sigma T^4 \tag{30}$$

- Received radiative flux

$$\varphi_{\mathrm{r}}^{\mathrm{rad}} = \varepsilon\varphi_{\mathrm{incident}}^{\mathrm{rad}} \tag{31}$$

- Net radiative flux

$$\varphi_{\mathrm{net}}^{\mathrm{rad}} = \varphi_{\mathrm{r}}^{\mathrm{rad}} - \varphi_{\mathrm{e}}^{\mathrm{rad}} = \varepsilon(\varphi_{\mathrm{incident}}^{\mathrm{rad}} - \sigma T^4) \tag{32}$$

Thermal balance at solid surface

- Convective balance

$$\varphi^{\mathrm{conv}}_{\mathrm{net}} = h(T_g - T) \tag{33}$$

- Thermal balance

$$\varphi_{\mathrm{net}} = \varphi^{\mathrm{rad}}_{\mathrm{net}} + \varphi^{\mathrm{conv}}_{\mathrm{net}} = \varepsilon(\varphi^{\mathrm{rad}}_{\mathrm{incident}} - \sigma T^4) + h(T_g - T) \tag{34}$$

- Written as

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

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

Extracting (a) from FDS calculation ?

FDS usual outputs at solid surface

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

$$\varphi_{\text{net}} = \varepsilon\sigma\left(T_{\text{AST}}^4 - T^4\right) + h(T_{\text{AST}} - T) \quad (36)$$

- 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

$$\varepsilon\varphi_{\text{incident}}^{\text{rad}} + h \cdot T_g = \varepsilon\sigma T_{\text{AST}}^4 + hT_{\text{AST}} \quad (37)$$

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

FDS outputs away from solid surface

- Obstruction not needed
- RADIATIVE HEAT FLUX GAS : $\varphi_{\text{net}}^{\text{rad}} = \varepsilon(\varphi_{\text{incident}}^{\text{rad}} - \sigma T^4)$

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&DEVC ID='hf', QUANTITY='RADIATIVE HEAT FLUX GAS', XYZ=..., ORIENTATION=-1,0,0/
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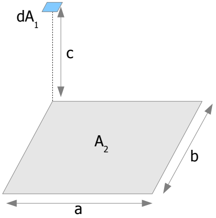
- THERMOCOUPLE

$$\rho c \frac{\mathrm{d}T}{\mathrm{d}t} = \varepsilon(U/4 - \sigma T^4) + h(T_g - T) = 0 \tag{38}$$

Examples

?

Radiant panel test case

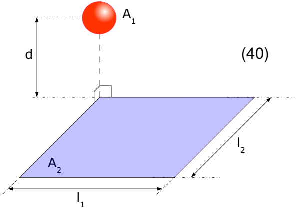


- **Radiative exchange between solids**
- Rectangle to differential planar target

$$F_{d1-2} = \frac{1}{2\pi}\left(\frac{A}{\sqrt{1+A^2}}\,\text{atan}\left[\frac{B}{\sqrt{1+A^2}}\right] + \frac{B}{\sqrt{1+B^2}}\,\text{atan}\left[\frac{A}{\sqrt{1+B^2}}\right]\right) \quad \text{with} \quad A = \frac{a}{c} \text{ and } B = \frac{b}{c} \tag{39}$$

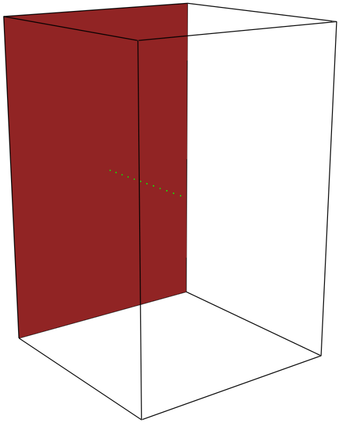
- Rectangle to spherical target

$$F_{1-2} = \frac{1}{4\pi}\,\text{atan}\sqrt{\frac{1}{D_1^2 + D_2^2 + D_1^2 \cdot D_2^2}} \quad \text{with} \quad D_1 = \frac{d}{l_1} \text{ and } D_2 = \frac{d}{l_2} \tag{40}$$

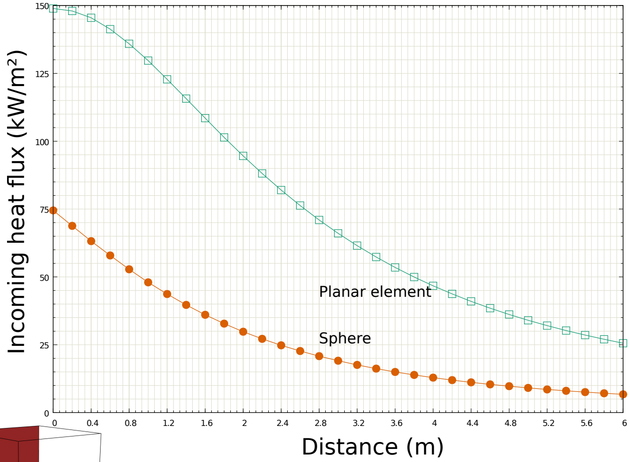


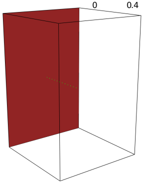
Test case : radiant panel

$$\Phi_s = \sigma T^4 = 5.67 \times 10^{-8} \times 1273.15^4 = 148{,}9\ \mathrm{kW} \cdot \mathrm{m}^{-2} \qquad (41)$$

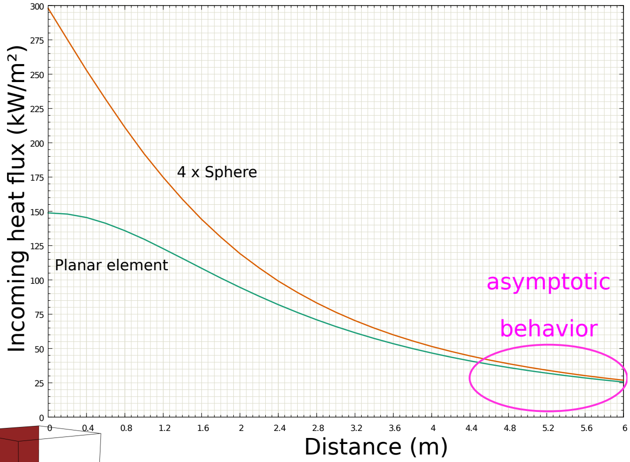


Test case : analytical solutions

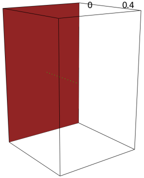




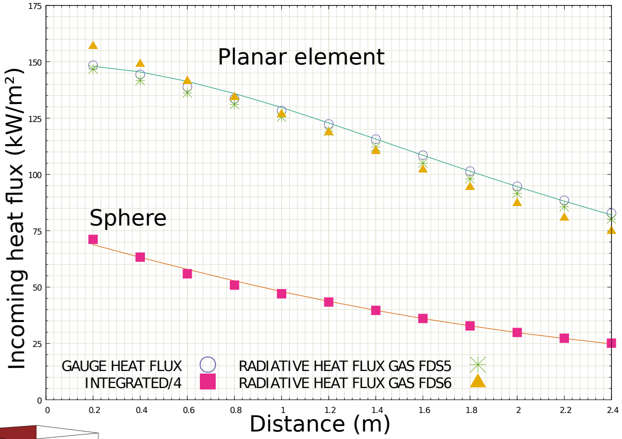
Test case

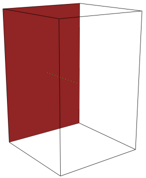


Incoming heat flux (kW/m²)
Distance (m)
4 x Sphere
Planar element
asymptotic
behavior



Test case : FDS results

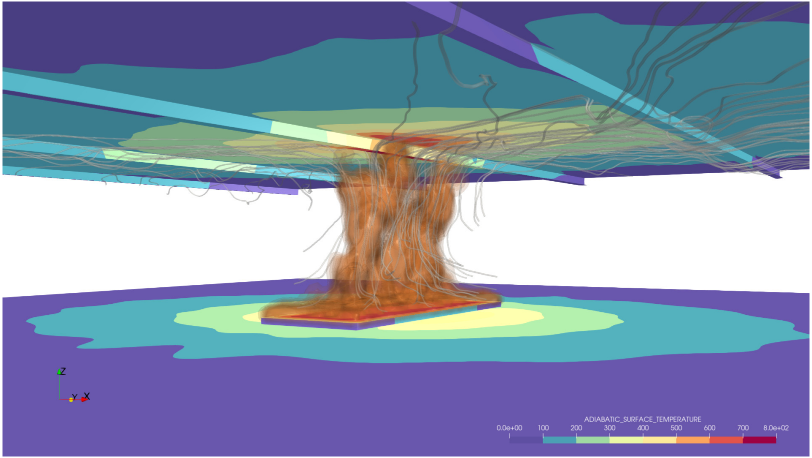




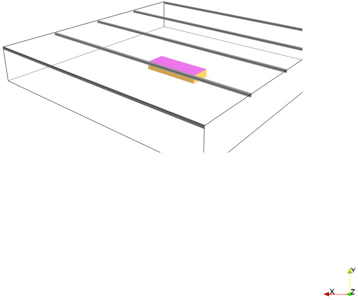
Test case : conclusion

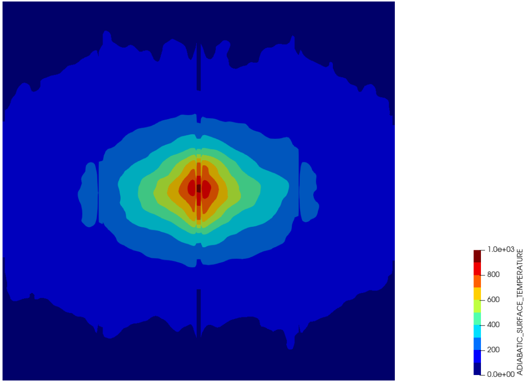
- INTEGRATED INTENSITY / 4 is relevant for spherical target
- RADIATIVE HEAT FLUX GAS is relevant for planar target
- INTEGRATED INTENSITY is a conservative approach to evaluate heat flux, espacially close to the fire
- Use ADIABATIC SURFACE TEMPERATURE as much as possible !

Heat fluxes to structure in a car park

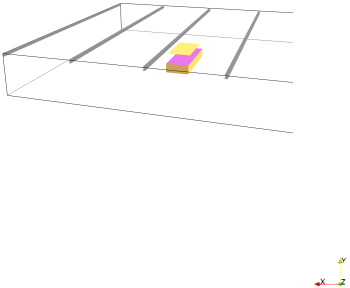


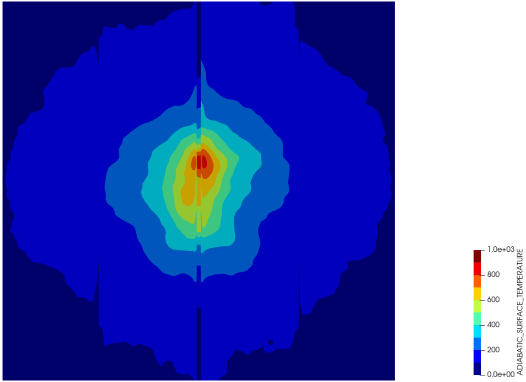
Case 01 (reaction 2)



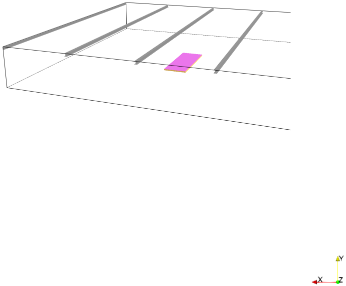


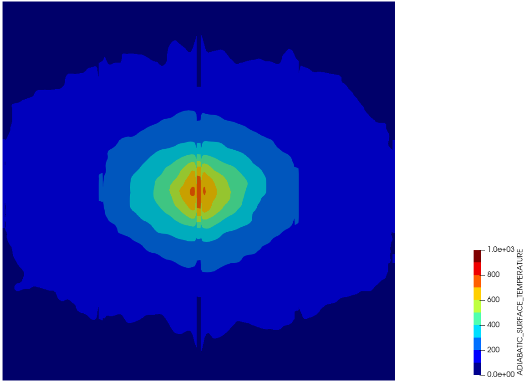
Case 02 (reaction 2)



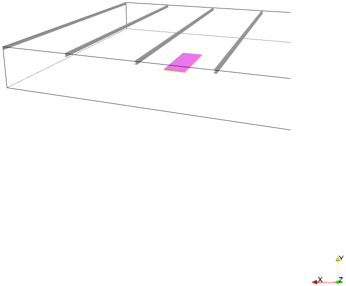


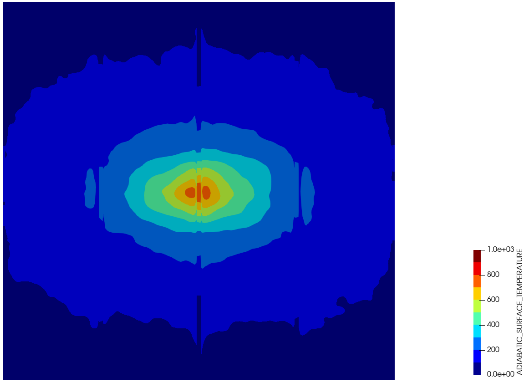
Case 03 (reaction 2)



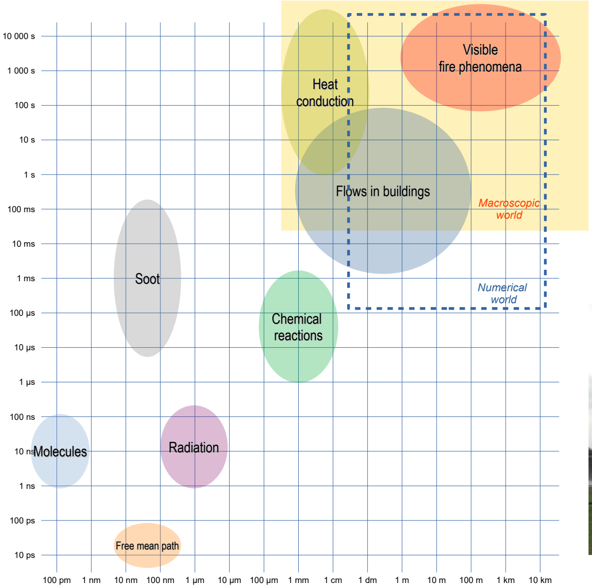


Case 04 (reaction 2)





A huge diversity of scales



To go further

NIST Special Publication 1019
Sixth Edition

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User's Guide

Kevin McGrattan
Simo Hostikka
Randall McDermott
Jason Floyd
Marcos Vanella

http://dx.doi.org/10.6028/NIST.SP.1019

VTT Technical Research Centre of Finland

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National Institute of Standards and Technology
U.S. Department of Commerce

NIST Special Publication 1018-1
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http://dx.doi.org/10.6028/NIST.SP.1018

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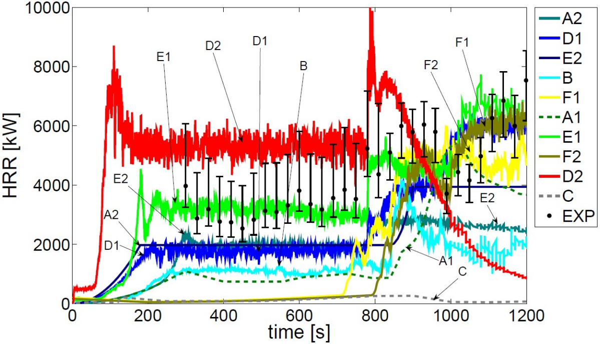
The "user effect" on CFD when predicting HRR



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