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Benchmark Evaluation of Radiation Models in Simulations of Compartment Fires

Yu Jeong Kim [a], Arnaud Trouvé [a], Georgios Maragkos [b], Bart Merci [b]

[a] Department of Fire Protection Engineering, University of Maryland, College Park, MD, USA
[b] Department of Structural Engineering and Building Materials, Ghent University, Belgium

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Research Objectives

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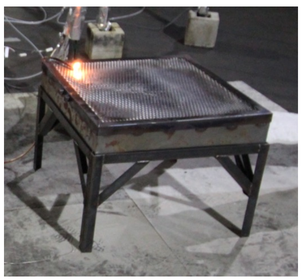
- General objective: to evaluate the performance of current modeling capabilities in the simulation of compartment fires using Fire Dynamics Simulator (FDS).

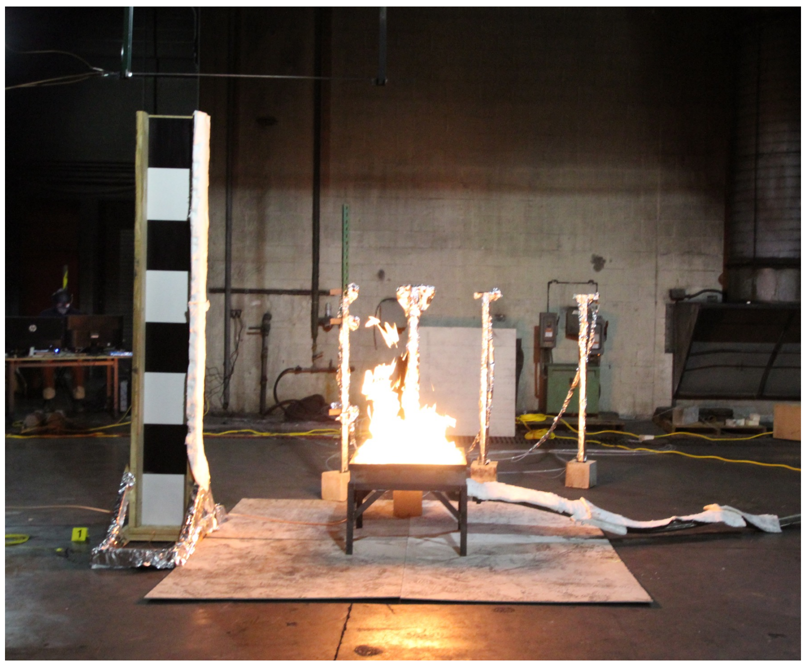
- Specific objectives: to identify best modeling options to simulate radiation heat transfer, flame extinction, soot production, and fuel production due to pyrolysis.
  - Pyrolysis model (production of fuel in burning furniture)
  - Combustion model (flame extinction due to under-ventilation)
  - Thermal radiation (gas and soot radiation)

- <u>Evaluation of the different thermal radiation modeling options in FDS.</u>

Experiments

- Compartment fire dynamics experiments (https://fireinvestigation.fsri.org/fire_dynamics/index.html)
- A series of experiments performed by UL's Fire Safety Research Institute in both free burn and compartment configurations with natural gas burners and upholstered furnishing.





A compartment of (3.66 × 3.66 × 2.44)-m3 size
A single door of (2 × 0.9)-m2 size

Simulations of Gas-burner Experiments

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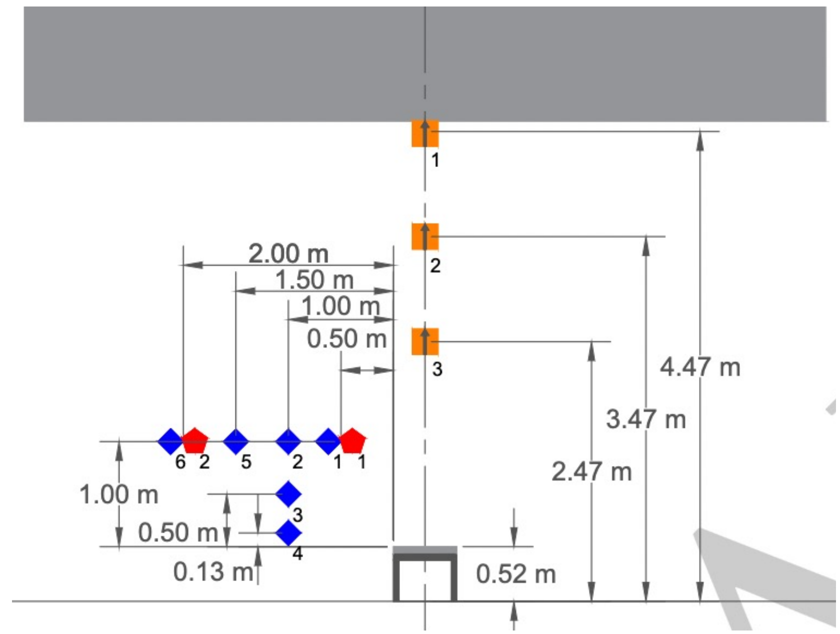
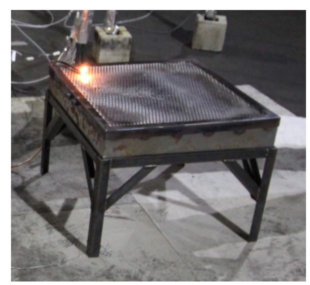
- Burner diameter (D) = **0.6 m**
- Radiative fraction (χ_r) = **0.23**
- **Fuel: Natural gas** (92.2% CH_4, 5.8% C_2H_6, 1.3% N_2, and 0.7% CO_2)
- Heat release rate, $\dot{Q}$ = 100, 500, 1000 kW

- Plume temperature and Z-velocity (Bi-Directional Probe, thermocouple: Inconel, diameter of 1.6 mm)
- Total and radiative heat fluxes (Heat flux gauges and radiometers, gauges temperature of 14 ℃ and gauge emissivity of 0.95)

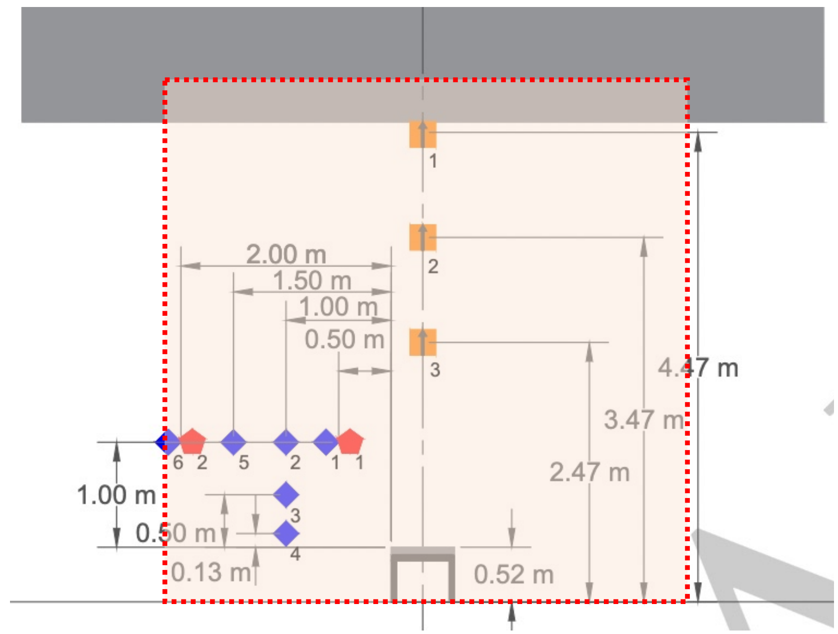


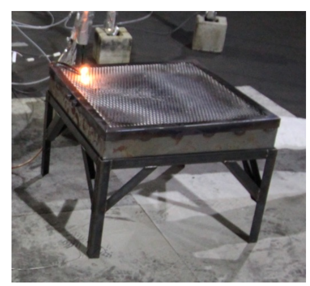


Radiometer
Heat Flux Gauge
Bi-Directional Probe (Arrow indicates positive flow direction)

Simulations of Gas-burner Experiments

- Fire Dynamics Simulator (FDS) developed by NIST (https://github.com/firemodels/fds)
- FDS version 6.7.7.
- Large eddy simulation (LES): Turbulence (Deardorff) and combustion (EDC)
- Computational domain = **5 m x 5 m x 5 m**
- OPEN BC at XMIN, XMAX, YMIN, YMAX, ZMAX
- **Fuel: Natural gas** (calculated heat of combustion of 47,800 kJ/kg)
- To identify best modeling options and practices in the baseline version of FDS
  - Grid resolution (0.1 m, 0.05 m, 0.025 m)
  - Angular resolution (NUMBER_RADIATION_ANGLES, N_{Ω}, from 104 up to 1200)
  - Radiation models (Default gray gas, WSGG, Wide band, optically thin)





Radiometer

Heat Flux Gauge

Bi-Directional Probe (Arrow indicates positive flow direction)

Spatial Resolution Criterion

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- Cross-section side length, D = 0.6 m
- Mean flame height (Heskestad plume): $L_f = 0.235\dot{Q}^{\frac{2}{5}} - 1.02D$
- Characteristic fire diameter:

$$D^* = \left(\frac{\dot{Q}}{\rho_\infty c_p T_\infty \sqrt{g}}\right)^{\frac{2}{5}}$$

- A-priori criterion of $D^*/\Delta \geq 15$
- Physical scale criterion of $D/\Delta \geq 10$, $L_f/\Delta_z \geq 10$

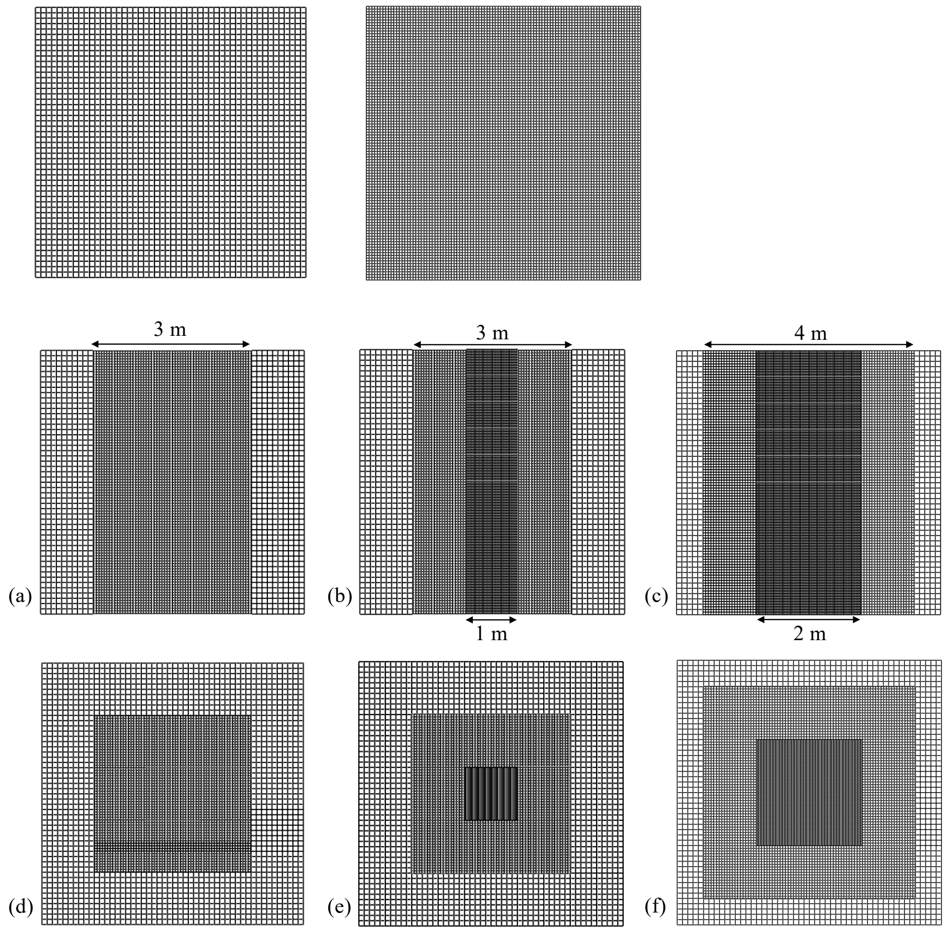
$\dot{Q}$ (kW)	D^* (m)	$D^*/0.1$ (-)	$D^*/0.05$ (-)	$D^*/0.025$ (-)
100	0.39	3.9	7.8	15.6
500	0.73	7.3	14.6	29.2
1000	0.97	9.7	19.4	38.8

D (m)	$D/0.1$ (-)	$D/0.05$ (-)	$D/0.025$ (-)
0.6	6	12	24

$\dot{Q}$ (kW)	L_f (m)	$L_f/0.1$ (-)	$L_f/0.05$ (-)	$L_f/0.025$ (-)
100	0.87	8.7	17.4	34.8
500	2.21	22.1	44.2	88.4
1000	3.11	31.1	62.2	124.4

- *$\Delta \leq 0.05$ m is required in general and finer grid sizes are required for smaller $\dot{Q}$.*

Spatial Resolution



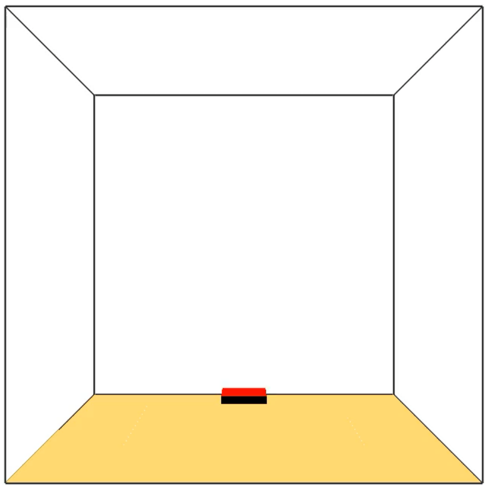
- Δ = 0.1 m, 0.05 m, or 0.025 m

Name	Grid structure	Grid size, Δ (m)	Total number of grid cells
10 cm	Uniform	0.1	125,000
5+10 cm	Hybrid	0.05 + 0.1	440,000
5 cm	Uniform	0.05	1,000,000
2.5+5 cm-1	Hybrid	0.025 + 0.05 + 0.1	720,000
2.5+5 cm-2	Hybrid	0.025 + 0.05 + 0.1	1,805,000

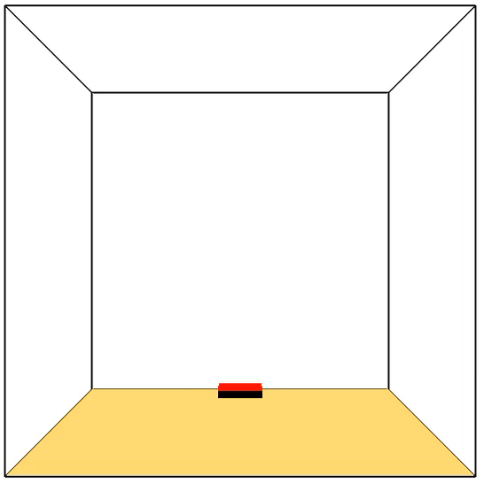
Spatial Resolution

- $\dot{Q}$ = *500 kW*

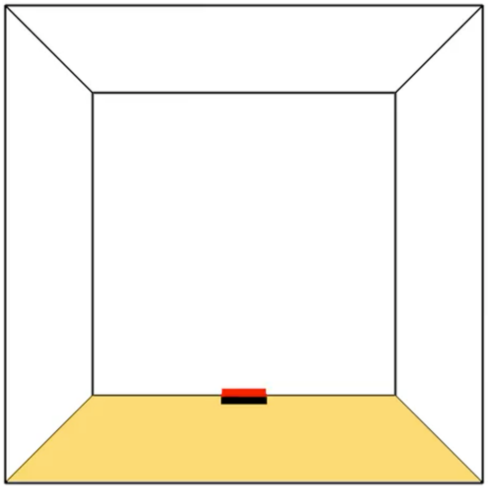
Δ = 0.1 m



Δ = 0.05 m



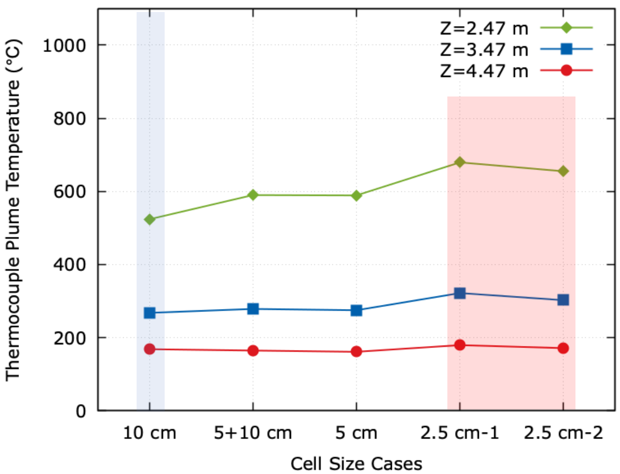
Δ = 0.025 m



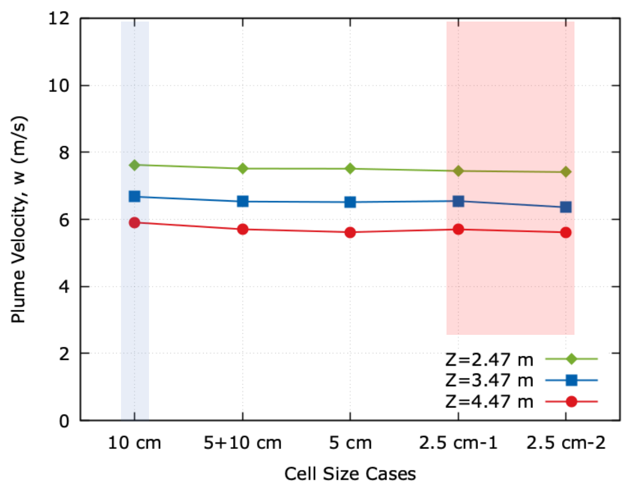
Spatial Resolution

- $\dot{Q}$ *= 500 kW*

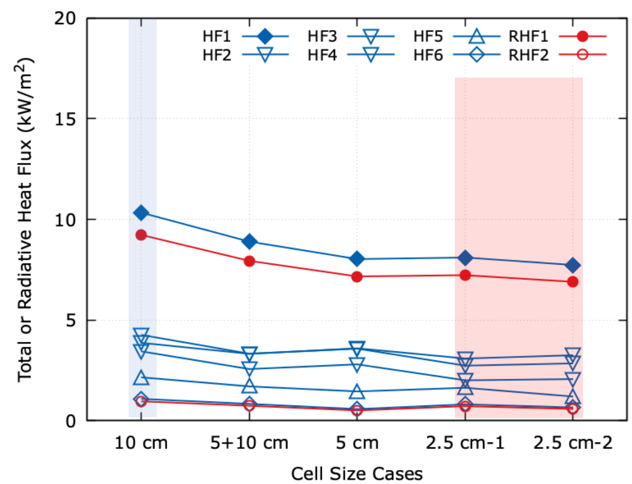
Plume temperature



Plume velocity



Total and radiative heat fluxes

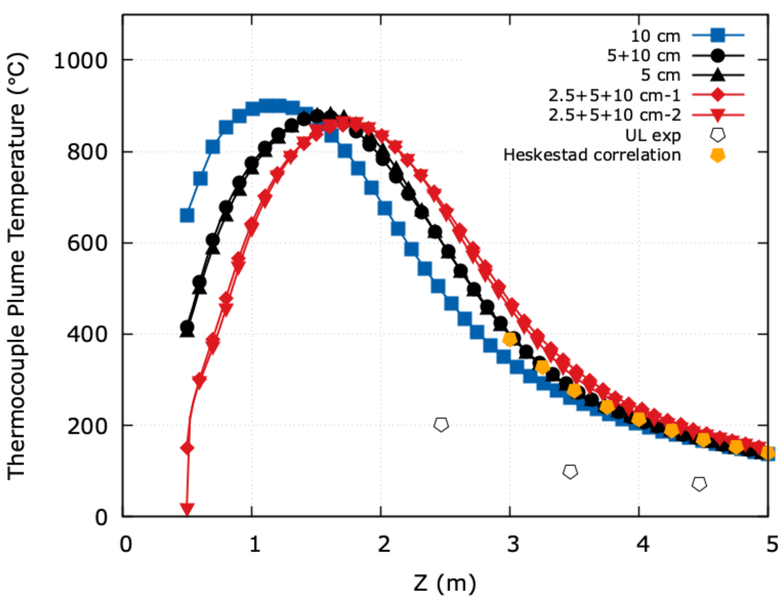


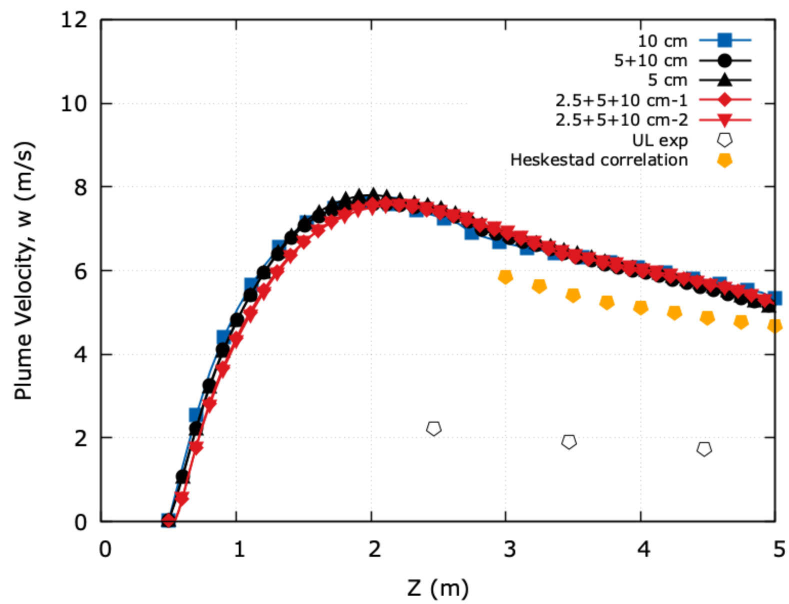
- Grid size of **0.05 m** shows convergence.

Spatial Resolution

- $\dot{Q}$ = *500 kW*

**Empirical correlations of plume region: temperature and velocity from G. Heskestad, Engineering relations for fire plumes, Fire Saf. J. 7 (1984) 25-32.*





- The predictions are in good agreement with empirical correlations, while it is significantly overpredicted of experimental data.

Radiation Modeling

- $\dot{Q}$ = 500 kW, Grid size (Δ) = 0.05 m, N_Ω = 104 (default) and N_Ω = 304 for selected models.
- The band specific Radiative Transport Equation (RTE) for a non-scattering gas:

$$\boldsymbol{s \cdot \nabla I_n(x,s) = E_n(x) - a_n(x)} \quad \boldsymbol{n = 1, \cdots, N}$$

$$E_n(x) = \kappa_n(x)\left(F_n \frac{\sigma T(x)^4}{\pi}\right) \qquad a_n(x) = \kappa_n(x) I_n(x,s)$$

$E_n(x)$: Emission source term.

$\kappa_n(x)$: Mean absorption coefficient for the band *n*.

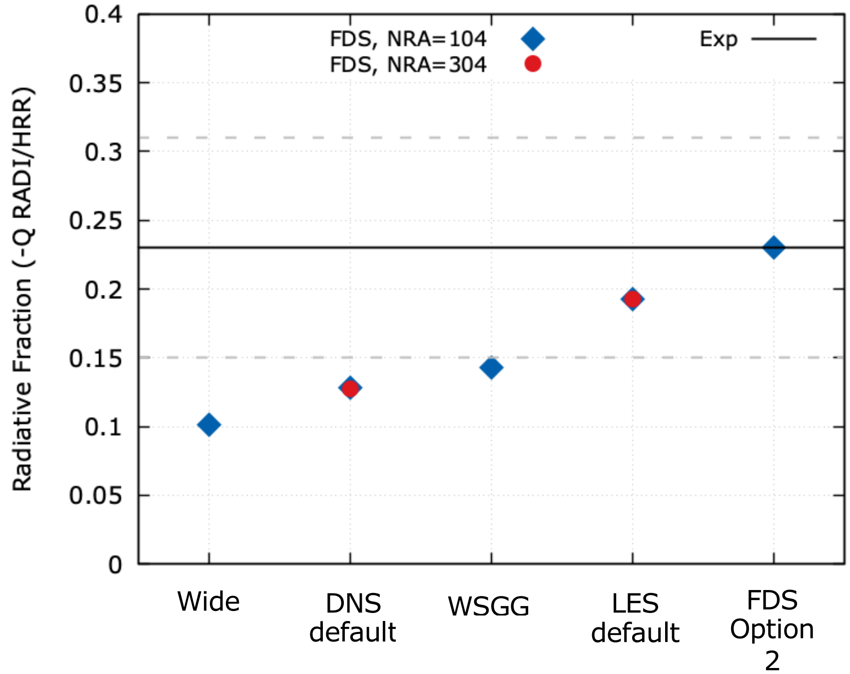
$I_n(x,s)$: The intensity integrated over the band *n*.

Wide band model	calculated $E_n(x)$ in both flame and plume regions
WSGG model	Prescribed χ_r , Prescribed $E_n(x)$ in flame region ($\chi_r \dot{q}''' > 10$) Calculated $E_n(x)$ in the plume region
DNS default, FDS option 4	calculated $E_n(x)$ in both flame and plume regions
LES default, FDS option 3	Prescribed χ_r , Prescribed $E_n(x)$ in flame region ($\chi_r \dot{q}''' > 10$) Calculated $E_n(x)$ in the plume region Correction of $E_n(x)$ in flame region ($\chi_r \dot{q}''' > 10$)
FDS option 2 (Optically Thin model)	Prescribed χ_r , Prescribed $E_n(x)$ $a_n(x) = 0$ Correction of $E_n(x)$ in flaming region ($\chi_r \dot{q}''' > 10$)

Radiation Modeling

- $\dot{Q}$ = *500 kW, Radiative Fraction,* χ_r

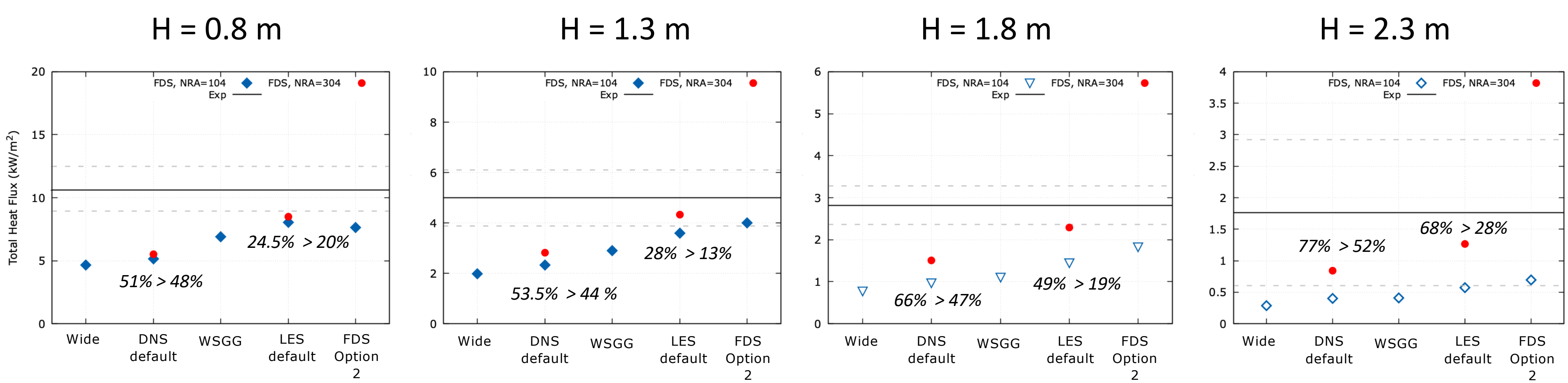
$$\chi_r = \frac{-\mathrm{Q\_RADI}}{\dot{Q}} \qquad \mathrm{Q\_RADI} = \dot{q}_{p,r} - \int \nabla \cdot \dot{\mathbf{q}}_r'' \mathrm{d}V$$



- LES default, FDS option 3 (Gray gas model, prescribed χ_r) shows the reasonable prediction.
- There is no effect of increased angular resolution on radiative fraction.

Radiation Modeling

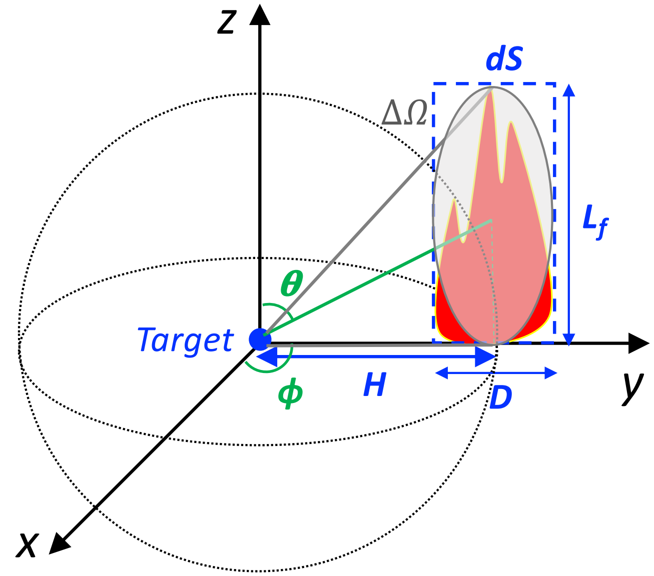
- Total heat flux gauges
- H = distance from the burner center



- Increased number radiation angles (NRA) improves the prediction of total heat fluxes.
- LES default (FDS option 3) shows the better prediction. Simulated heat fluxes are within 13%-28% of measurements with increased angular resolution (24.5%-68% with default angular resolution).

Angular Resolution

- Grid size = 0.1 m
- LES default, FDS option 3 (Gray gas model, prescribed χ_r)
- Solid angles from 104 (default 100) to 1200 are used.
- The estimation of required total number of angles:
  - Solid angle, $\Delta\Omega$
  - Flame surface (dS) ~ D (m) x L_f (m)
  - Distance between the burner center and a gauge ~ H (m)
  - NUMBER_RADIATION_ANGLES (NRA): N_Ω



$\dot{Q}$ (kW)	N_Ω *for radiometer 1 (H = 0.8 m)*	N_Ω *for radiometer 2 (H = 2.3 m)*
100	154	1273
500	61	501
1000	43	356

Total number of angles:

$$N_\Omega = \sum_{i=1}^{N_\theta} N_\phi(\theta_i) \qquad \Delta\Omega_{FDS} = \frac{4\pi}{N_\Omega} \qquad \Delta\Omega \sim \frac{dS}{H^2}$$

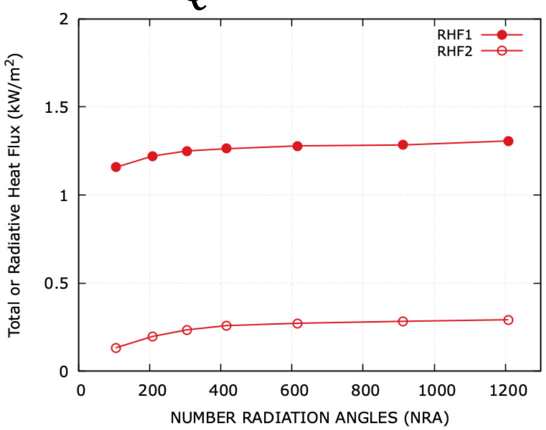
$$\boldsymbol{\Delta\Omega \geq 10\Delta\Omega_{FDS}}$$

Required NUMBER_RADIATION_ANGLES:

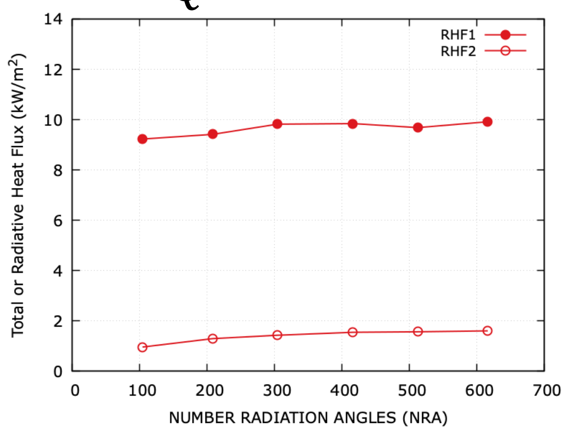
$$\boxed{\boldsymbol{N_\Omega \geq 40\pi H^2/dS}}$$

Angular Resolution

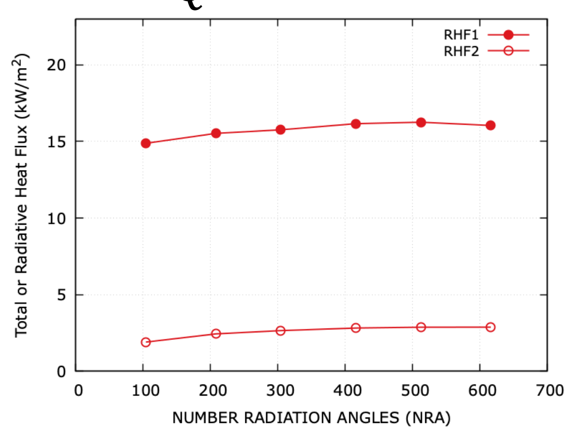
$\dot{Q}$ = *100 kW*



$\dot{Q}$ = *500 kW*



$\dot{Q}$ = *1000 kW*



- The estimation of required N_Ω

$\dot{Q}$ (kW)	N_Ω *for radiometer 1 (H = 0.8 m)*	N_Ω *for radiometer 2 (H = 2.3 m)*
100	154	1273
500	61	501
1000	43	356

- FDS converged N_Ω (~ 10 % variation)

$\dot{Q}$ (kW)	N_Ω *for radiometer 1 (H = 0.8 m)*	N_Ω *for radiometer 2 (H = 2.3 m)*
100	104	416
500	104	304
1000	104	304

Angular Resolution

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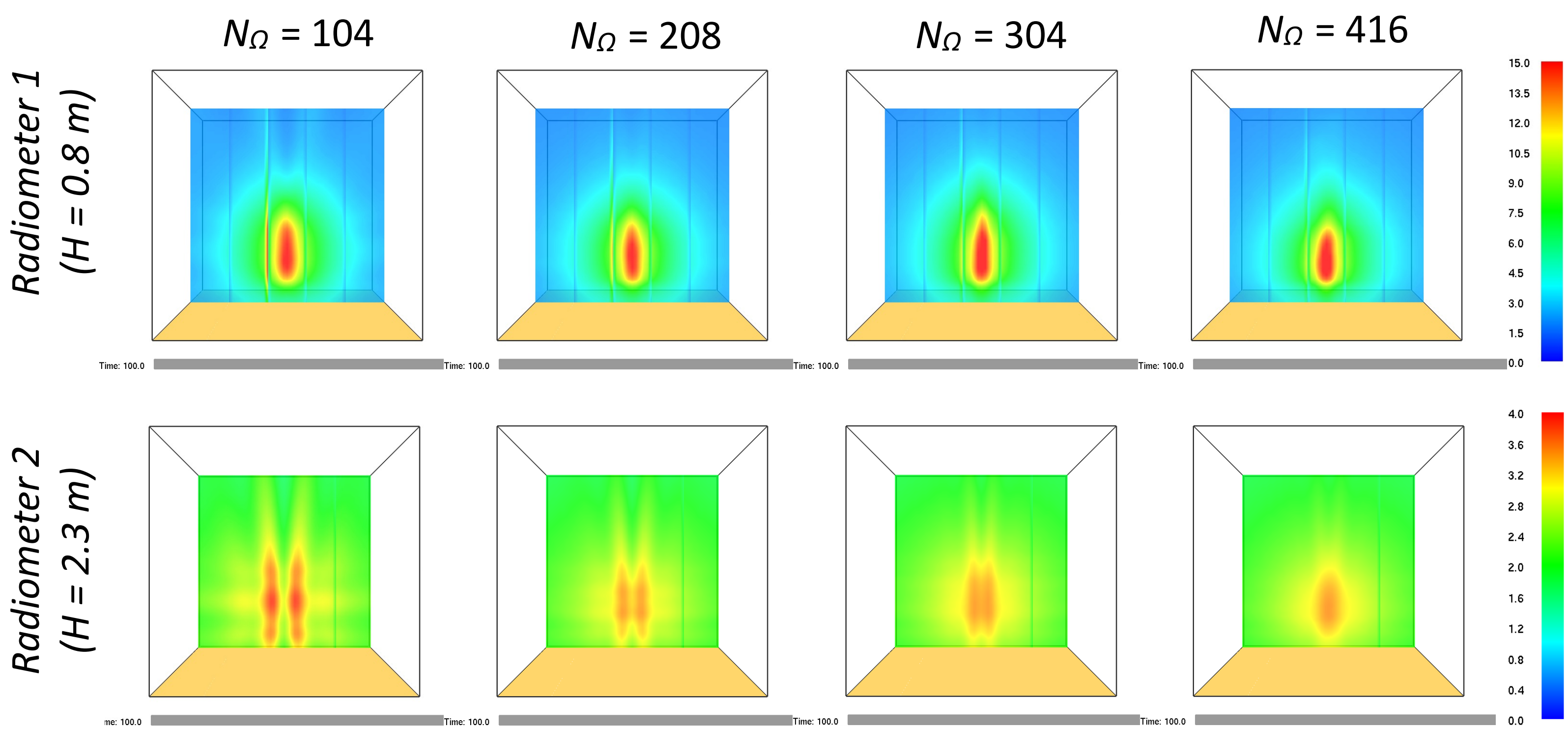
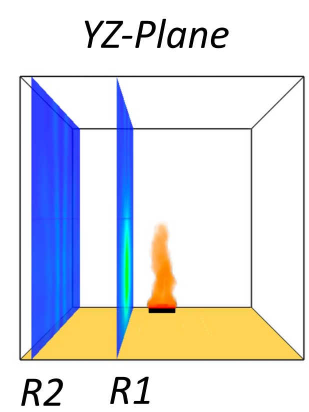
- $\dot{Q}$ = *500 kW,* FDS converged N_Ω = 104 for radiometer 1, N_Ω = 304 for radiometer 2.
- Integrated Intensities, $U(x) = \int_{4\pi} I(x,\Omega)d\Omega$, as a function of N_Ω

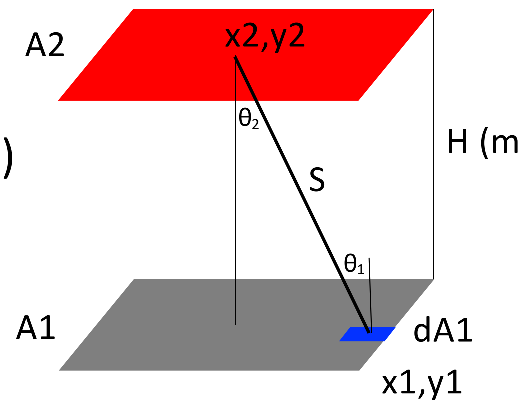




- Integrated intensity indicates that radiometer 2 needs N_Ω = 416 rather than 304.

Verification Examples

- *FDS version 6.7.9*
- ***plate_view_factor_cart.fds***
- 3D cartesian, Parallel plates, **grid size of 0.05 m**
- Radiation source: Square (2 m x 2 m) and rectangle plates (2 m x 1 m)
- Surface temperature is at 1000 ℃ and an emissivity of 1.0.
- Heat flux at the surface: 148.98 kW/m^2
- **NUMBER_RADIATION_ANGLES (NRA) from 30 to 1600**



- Changing the distance, H (m), from the hot plate.
- Computed view factor (F_{d1-2}), radiative heat flux, integrated intensity using MATLAB
- Comparison between MATLAB solutions and FDS predictions

$$F_{d1-2} = \int_{A2} \frac{\cos\theta_1 \cos\theta_2}{\pi S^2} dA_2$$

- *Objective: to validate acceptable number radiation angles with the present of ray effects.*

Integrated Intensity, U: FDS vs. MATLAB

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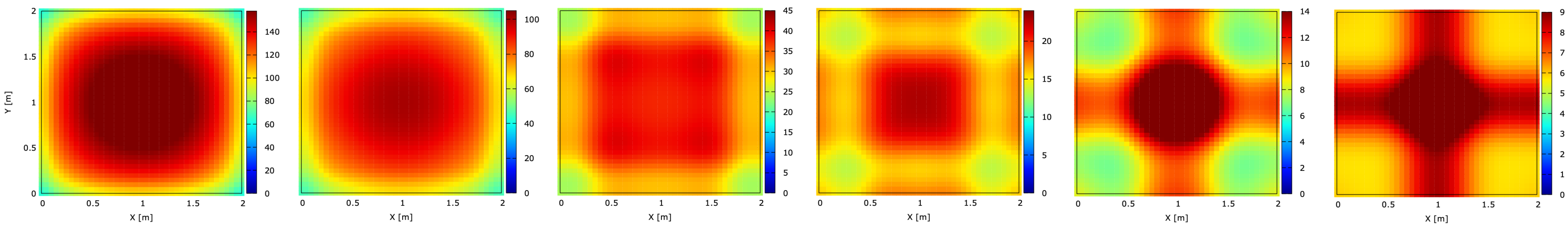
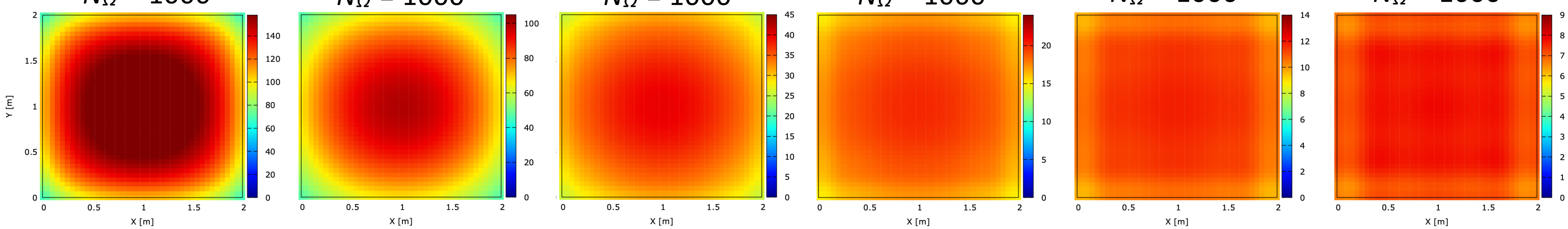
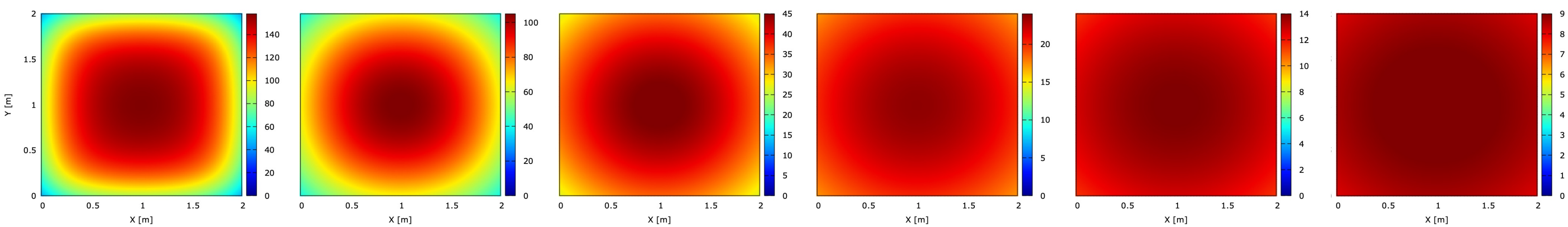
$H = 0.5\ m$	$H = 1.0\ m$	$H = 2.0\ m$	$H = 3.0\ m$	$H = 4.0\ m$	$H = 5.0\ m$
N_Ω = 104	N_Ω = 104	N_Ω = 104	N_Ω = 104	N_Ω = 104	N_Ω = 104



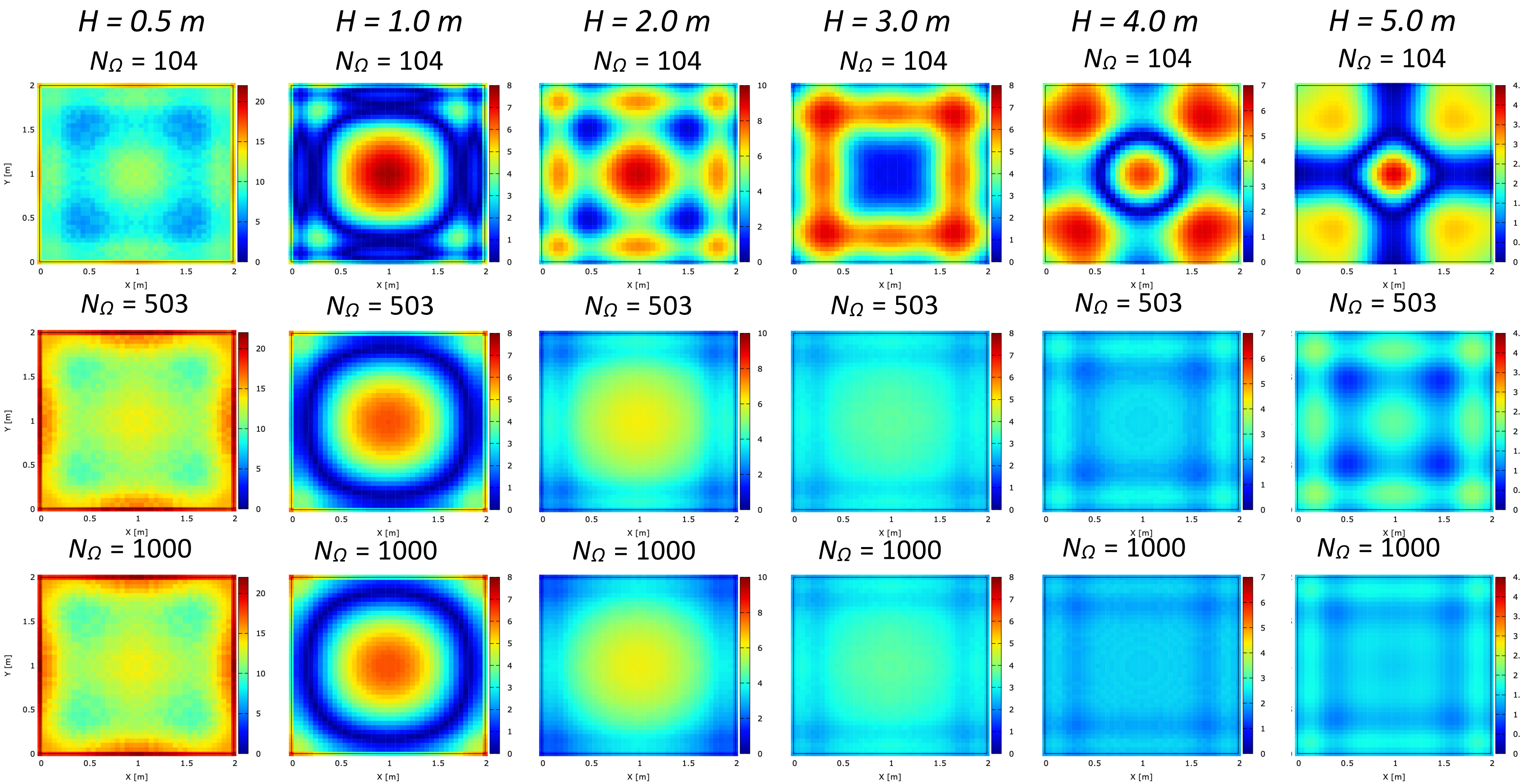
N_Ω = 1000	N_Ω = 1000	N_Ω = 1000	N_Ω = 1000	N_Ω = 1000	N_Ω = 1000



- MATLAB solutions:



Absolute Error from MATLAB Solutions

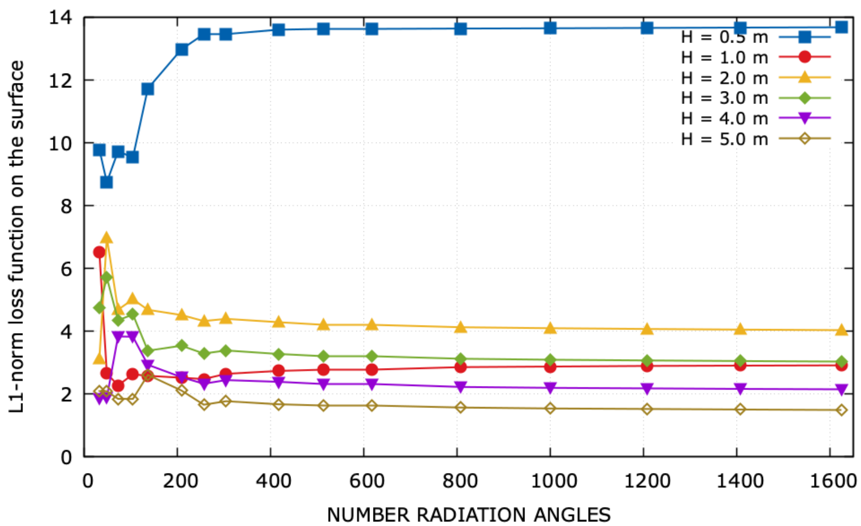


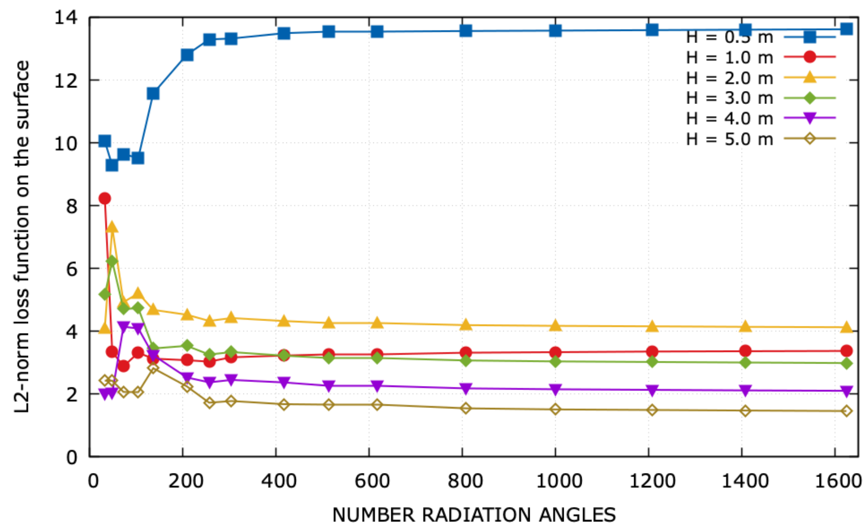
Integrated Intensity, U: FDS vs. MATLAB

- L1: the absolute difference between the FDS prediction and the MATLAB solutions.
- L2: the squared difference between the FDS prediction and the MATLAB solutions.

$$\mathrm{L1} = \frac{1}{NX}\frac{1}{NY}\sum_{i=1}^{NX*NY}\left|U_{FDS,i} - U_{MATLAB,i}\right|$$

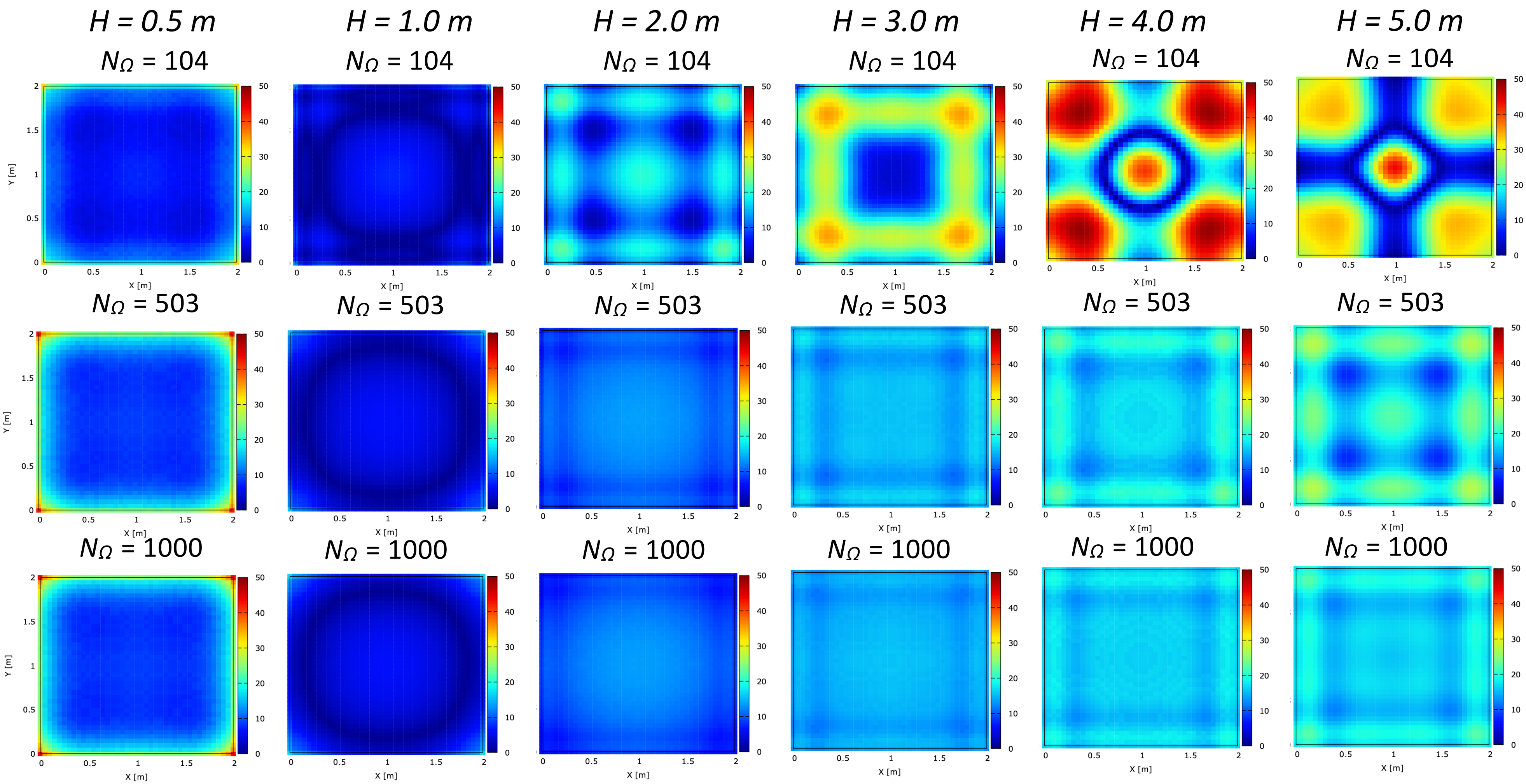
$$\mathrm{L2} = \sqrt{\frac{1}{NX}\frac{1}{NY}\sum_{i=1}^{NX*NY}\left(U_{FDS,i} - U_{MATLAB,i}\right)^2} \qquad [kW/m^2]$$





- 2-D analysis of the error indicates that NRA ≥ 250 shows convergence.

Relative Error from MATLAB Solutions



Integrated Intensity, U: FDS vs. MATLAB

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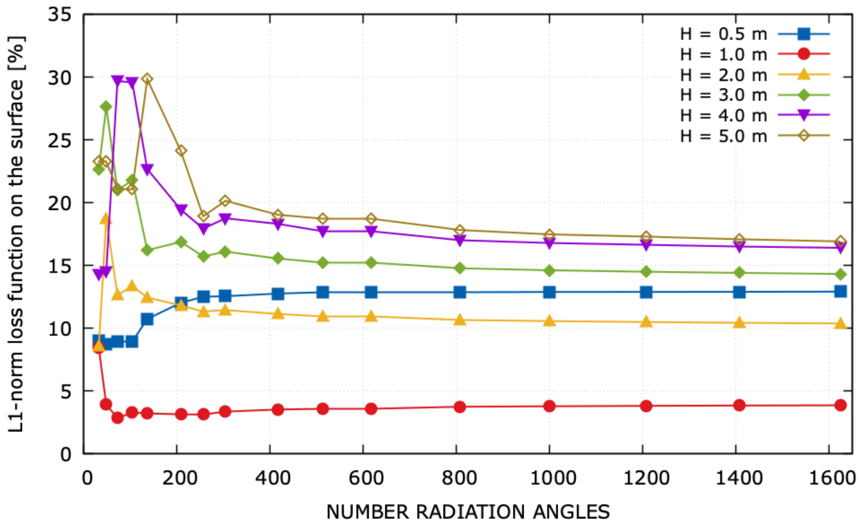
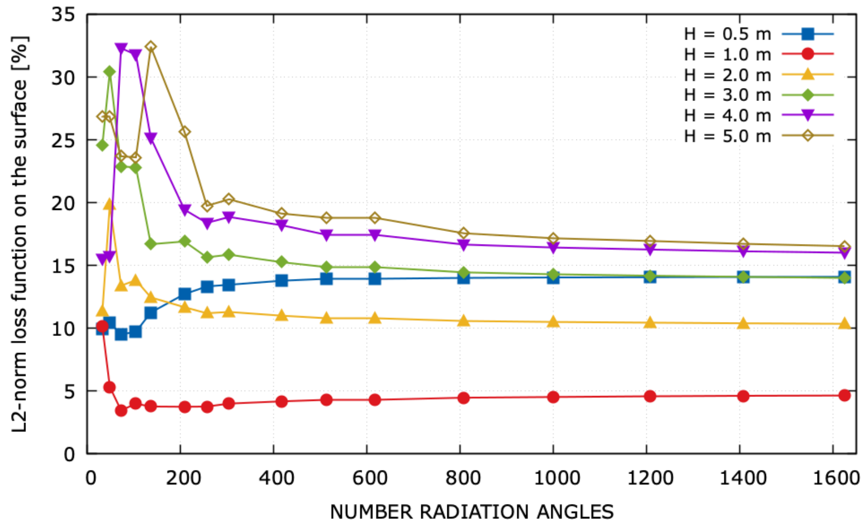
$$\mathrm{L1} = \frac{1}{NX}\frac{1}{NY}\sum_{i=1}^{NX*NY}\frac{\left|U_{FDS,i} - U_{MATLAB,i}\right|}{U_{MATLAB,i}}$$

$$\mathrm{L2} = \sqrt{\frac{1}{NX}\frac{1}{NY}\sum_{i=1}^{NX*NY}\left(\frac{U_{FDS,i} - U_{MATLAB,i}}{U_{MATLAB,i}}\right)^2} \quad [\%]$$



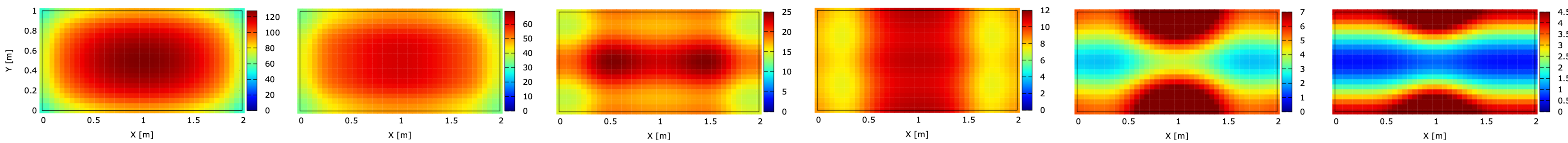


- FDS does not converge to the exact solution.

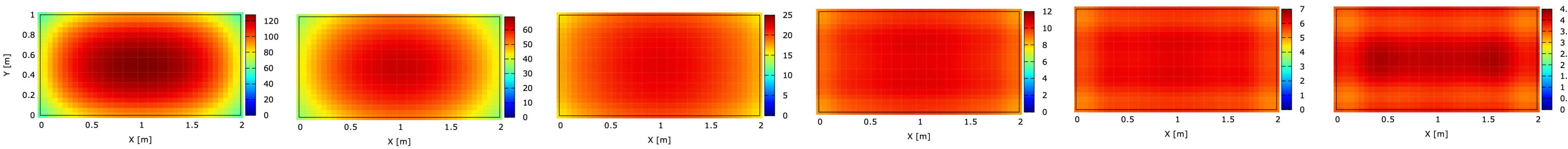
Integrated Intensity: FDS vs. MATLAB

H = 0.5 m | *H = 1.0 m* | *H = 2.0 m* | *H = 3.0 m* | *H = 4.0 m* | *H = 5.0 m*

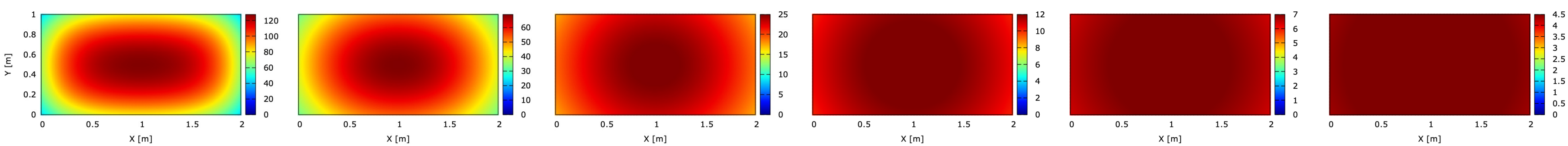
N_Ω = 104 | N_Ω = 104 | N_Ω = 104 | N_Ω = 104 | N_Ω = 104 | N_Ω = 104



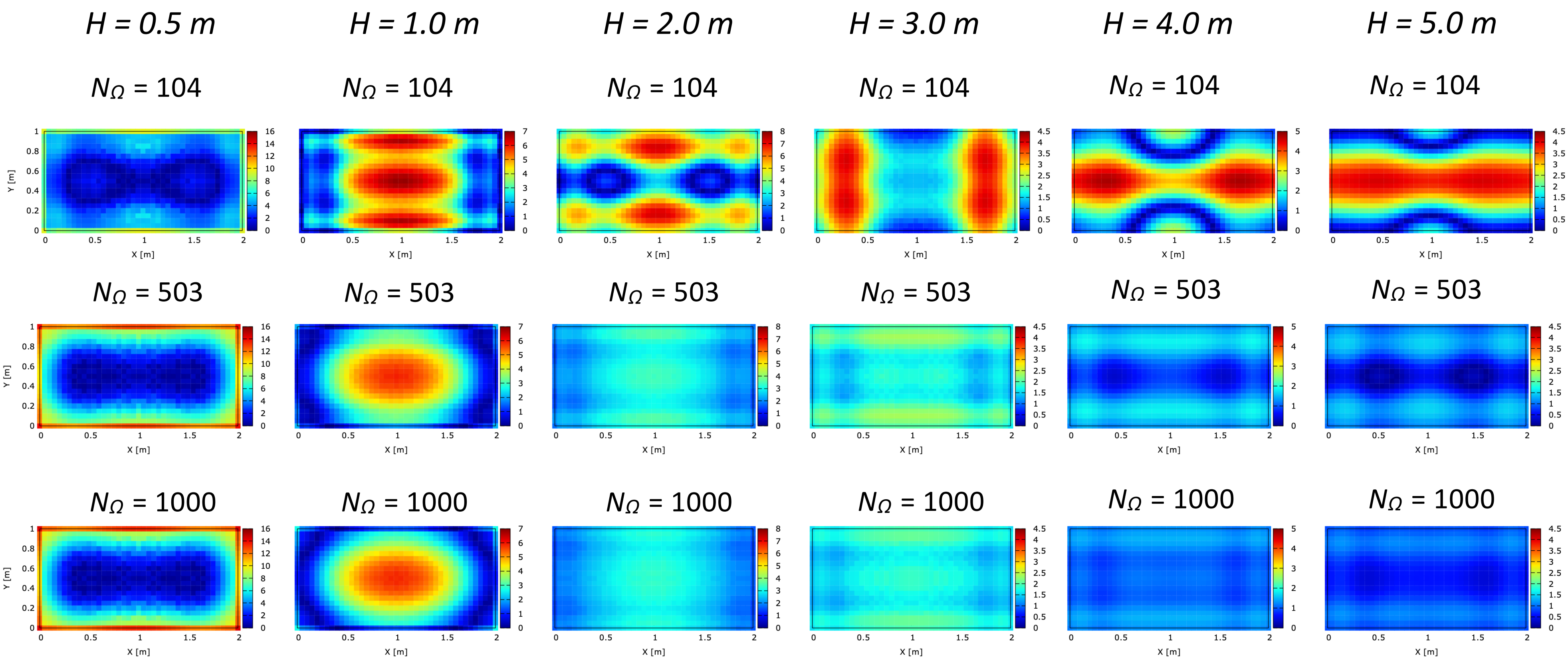
N_Ω = 1000 | N_Ω = 1000 | N_Ω = 1000 | N_Ω = 1000 | N_Ω = 1000 | N_Ω = 1000



- MATLAB solutions:



Absolute Error from MATLAB Solutions



Integrated Intensity, U, using FDS vs. MATLAB

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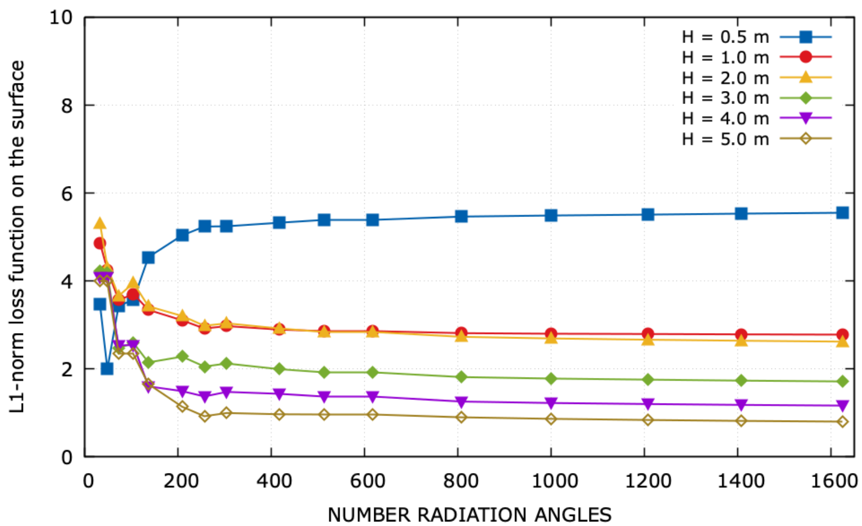
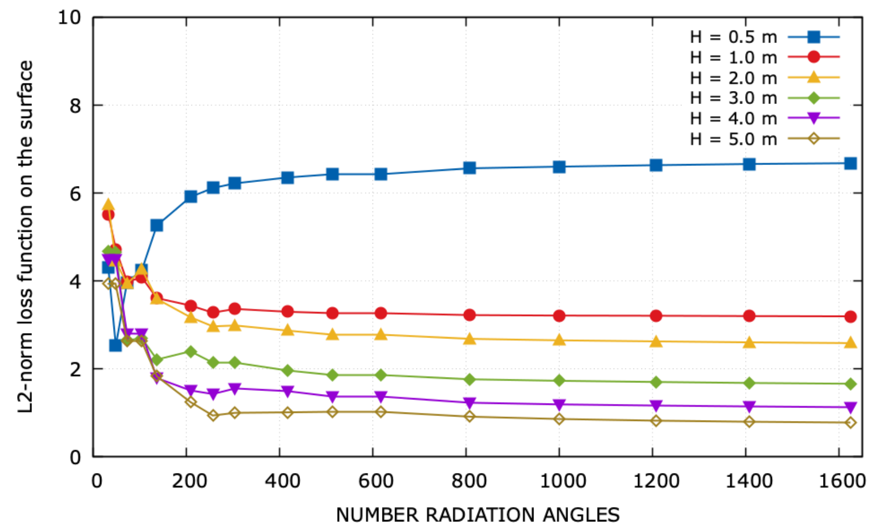
- L2: the squared difference between the FDS prediction and the MATLAB solutions.

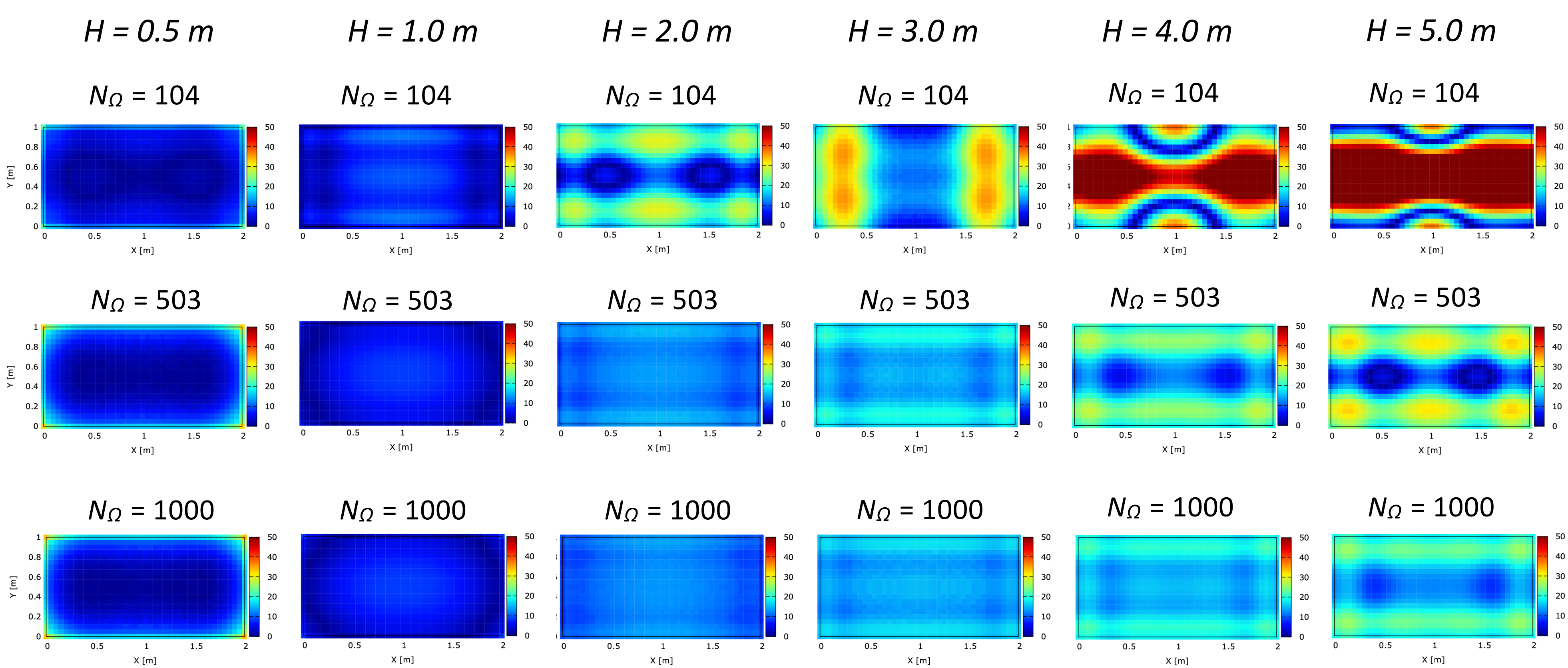
$$\mathrm{L1} = \frac{1}{NX}\frac{1}{NY}\sum_{i=1}^{NX*NY}\left|U_{FDS,i} - U_{MATLAB,i}\right| \qquad \mathrm{L2} = \sqrt{\frac{1}{NX}\frac{1}{NY}\sum_{i=1}^{NX*NY}\left(U_{FDS,i} - U_{MATLAB,i}\right)^2} \quad [kW/m^2]$$





- 2-D analysis of the error indicates that NRA ≥ 250 shows convergence.

Relative Error from MATLAB Solutions



Integrated Intensity, U: FDS vs. MATLAB

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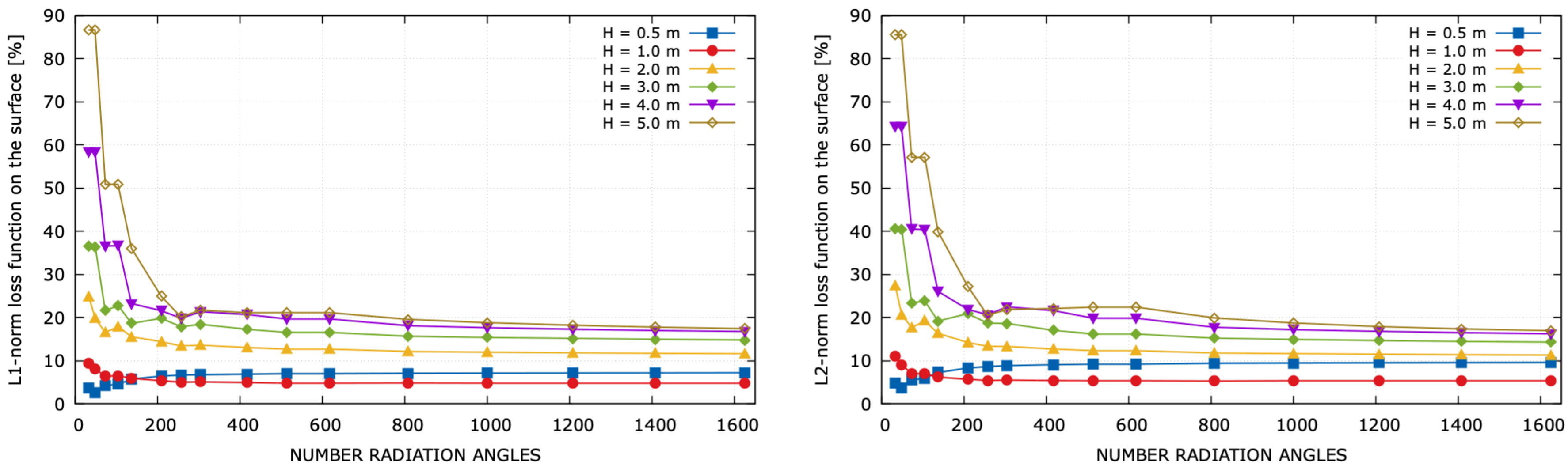
- L1: the absolute difference between the FDS prediction and the MATLAB solutions.
- L2: the squared difference between the FDS prediction and the MATLAB solutions.

$$\mathrm{L1} = \frac{1}{NX}\frac{1}{NY}\sum_{i=1}^{NX*NY}\frac{\left|U_{FDS,i} - U_{MATLAB,i}\right|}{U_{MATLAB,i}} \qquad \mathrm{L2} = \sqrt{\frac{1}{NX}\frac{1}{NY}\sum_{i=1}^{NX*NY}\left(\frac{U_{FDS,i} - U_{MATLAB,i}}{U_{MATLAB,i}}\right)^2} \qquad [\%]$$



- Relative error of H = 0.5 m and 1.0 m ~ 10%, while others are larger than 10%

Conclusions

Evaluation of the different thermal radiation modeling options in FDS.

- Five different radiation modeling options were evaluated. LES default model (FDS option 3) gave the best predictions.
- NUMBER_RADIATION_ANGLES (NRA) need to be adapted according to objectives of simulation project.
- Simulated heat fluxes are within 13%-28% of measurements with increased angular resolution (24.5%-68% with default angular resolution).
- For integrated intensity, FDS does not converge to exact solution and there is a residual modeling error at high values of NRA.

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Thank you

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