Predicting radiative characteristics of hydrogen and hydrogen/methane jet fires using FireFOAM

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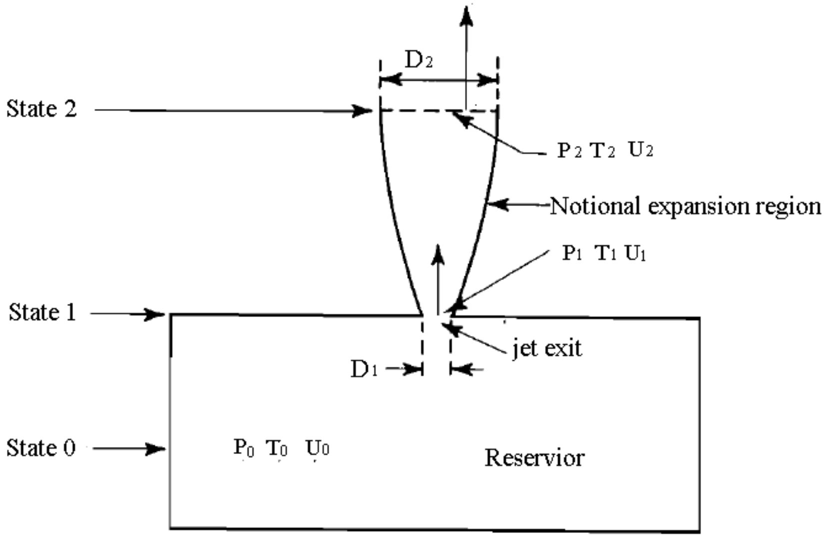
Outline

- Motivation and objectives
- Sub-models for combustion and radiative heat transfer
- Semi-empirical models for comparison
- Numerical set-up and results
- Concluding remarks

Motivation

★ Hydrogen safety in storage, transportation and utilization



Objectives

- To validate the FireFOAM code for large-scale hydrogen, hydrogen and methane jet fires

- To analyze the radative characteristic of large-scale H_2, H_2-CH_4 jet fires

- To analyse the effects of ground surface reflectance on the radiation characteristics

Sub-model for combustion

- The Eddy Dissipation Concept (EDC) extended to large eddy simulation (LES) by Chen et al.

  Chen, Z., Wen, J.X., Xu, B.P. and Dembele, S., "Large Eddy Simulation of Fire Dynamics with the Improved Eddy Dissipation Concept," 10th IAFSS Symposium, University of Maryland, USA, June 19-24, 2011.

- The recent extension of the EDC to multi-component fuels

The EDC for multi-component fuels based on infinitely fast chemistry

$$H_2 + 0.5O_2 \rightarrow H_2O$$

$$CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O$$

$$C_7H_{16} + 11O_2 \rightarrow 7CO_2 + 8H_2O$$

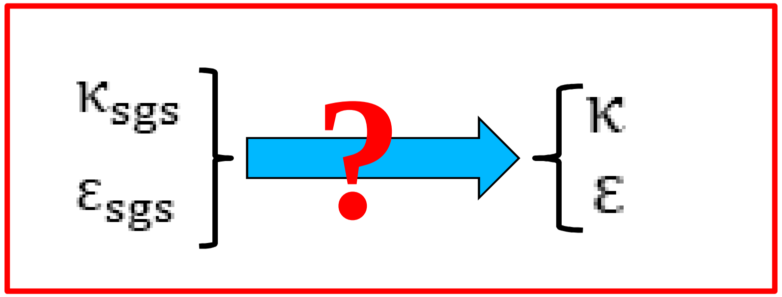
$$\vdots$$

$$\bar{\omega}_i = \bar{\rho}\dot{m}^* \frac{\gamma\chi}{1-\gamma\chi}\left(\tilde{Y}_i - Y_i^*\right)$$

The EDC for multi-component fuels based on infinitely fast chemistry

$$L^* = \frac{2}{3}\left(\frac{3C_{D2}^{\ 3}}{C_{D1}^{\ 2}}\right)^{1/4}\left(\frac{\upsilon^3}{\varepsilon}\right)^{1/4} \qquad \gamma = \left(\frac{L^*}{L'}\right)^{3-D}$$

$$u^* = \left(\frac{C_{D2}}{3C_{D1}^{\ 2}}\right)^{1/4}(\upsilon\varepsilon)^{1/4} \qquad \dot{m}^* = \frac{2u^*}{L^*} = \left(\frac{3}{C_{D2}}\right)^{1/2}\left(\frac{\varepsilon}{\upsilon}\right)^{1/2}$$


κ_{sgs}

ε_{sgs}

?

κ

ε

$$\varepsilon \approx \sqrt{\frac{2}{3}}C_{D1}\frac{k_{SGS}^{\ 3/2}}{\Delta} + \frac{2}{9}C_{D2}\upsilon\frac{k_{SGS}}{\Delta^2}$$

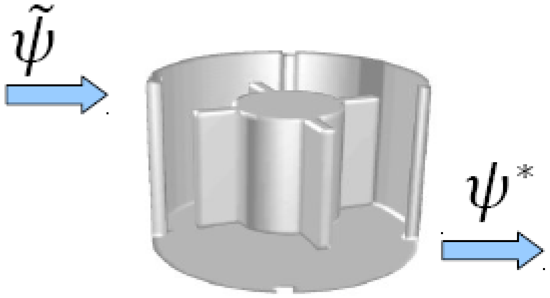
$$k = \left(\frac{3}{2C_{D1}^{\ 2}}\right)^{1/3}(\varepsilon L')^{2/3}$$

$$L' = \left(\frac{Q}{\rho_\infty c_p T_\infty \sqrt{g}}\right)^{2/5}$$

The EDC for multi-component fuels based on infinitely fast chemistry

$$\bar{\omega}_i = \bar{\rho}\dot{m}^* \frac{\gamma\chi}{1-\gamma\chi}\left(\tilde{Y}_i - Y_i^*\right)$$

Perfectly Stirred Reactor



Fuels:

$$Y_{f,i}^* = Y_{f,i}^{*old} - \left(\frac{Y_{f,i}^{*old}}{\sum_{j=1}^{N_F} \frac{Y_{f,j}^{*old}}{abs\left(\sum_{n=1}^{NT} \upsilon'_{f,jn} \cdot W_{f,j}\right)}} \right) \min\left(\sum_{j=1}^{N_F} \frac{Y_{f,j}^{*old}}{abs\left(\sum_{n=1}^{NR} \upsilon'_{f,jn} \cdot W_{f,j}\right)}, \frac{Y_{O2}^{*old}}{abs\left(\sum_{n=1}^{NR} \upsilon'_{O2,n} \cdot W_{O2}\right)} \right)$$

O_2:

$$Y_{O2}^* = Y_{O2}^{*old} - abs\left(\sum_{n=1}^{NR} \upsilon'_{O2,n} \cdot W_{O2}\right) \cdot \min\left(\sum_{j=1}^{N_F} \frac{Y_{f,j}^{*old}}{abs\left(\sum_{n=1}^{NR} \upsilon'_{f,jn} \cdot W_{f,j}\right)}, \frac{Y_{O2}^{*old}}{abs\left(\sum_{n=1}^{NR} \upsilon'_{O2,n} \cdot W_{O2}\right)} \right)$$

$$\chi \approx \begin{cases} \frac{Z}{Z_{st}}, & if\ 0 \le Z < Z_{st} \\ \frac{1-Z}{1-Z_{st}}, & if\ Z_{st} \le Z \le 1 \end{cases}$$

H_2O/CO_2

$$Y_{p,i}^* = Y_{p,i}^{*old} + abs\left(\sum_{n=1}^{NR} \upsilon'_{p,in} \cdot W_{p,i}\right) \cdot \min\left(\sum_{j=1}^{N_F} \frac{Y_{f,j}^{*old}}{abs\left(\sum_{n=1}^{NR} \upsilon'_{f,jn} \cdot W_{f,j}\right)}, \frac{Y_{O2}^{*old}}{abs\left(\sum_{n=1}^{NR} \upsilon'_{O2,n} \cdot W_{O2}\right)} \right)$$

The EDC for multi-component fuels based on infinitely fast chemistry

Assume number of reaction equals to number of fuel and there is only one fuel involved in each reaction.

$$\overline{\omega}_i = \overline{\rho}\dot{m}^* \frac{\gamma\chi}{1-\gamma\chi}\omega_{fi}^*$$

For Fuel:

$$\omega_{fi}^* = \left(\frac{Y_{f,i}}{\sum_{j=1}^{N_F} \frac{Y_{f,j}\cdot\upsilon'_{O2,j}\cdot W_{O2}}{\upsilon'_{f,j}\cdot W_{f,j}}} \right)\cdot\min\left(\sum_{j=1}^{N_F}\frac{Y_{f,j}\cdot\upsilon'_{O2,j}\cdot W_{O2}}{\upsilon'_{f,j}\cdot W_{f,j}}, Y_{O2}\right)$$

For Oxygen:

$$\omega_{O2}^* = \sum_{i=1}^{N_F}\left(\omega_{fi}^*\frac{\upsilon'_{O2,i}\cdot W_{O2}}{\upsilon'_{f,i}\cdot W_{f,i}}\right)$$

For H2O:

$$\omega_{H2O}^* = \sum_{i=1}^{N_F}\left(\omega_{fi}^*\frac{\upsilon'_{H2O,i}\cdot W_{H2O}}{\upsilon'_{f,i}\cdot W_{f,i}}\right)$$

For CO2:

$$\omega_{CO2}^* = \sum_{i=1}^{N_F}\left(\omega_{fi}^*\frac{\upsilon'_{CO2,i}\cdot W_{CO_2}}{\upsilon'_{f,i}\cdot W_{f,i}}\right)$$

Sub-model for radiative heat transfer

Finite volume discrete ordinates model (fvDOM)

$$\hat{s}\cdot\nabla I_n(x,\hat{s}) = \kappa_n(x) I_{b,n}(x) - \beta_n(x) I_n(x,\hat{s}) + \frac{\sigma_n(x)}{4\pi}\int_{4\pi} I_n(x,\hat{s}')\Phi_n(x,\hat{s},\hat{s}')\,d\Omega'$$

Gas Absorption coefficients: **Weighted Sum of grey gas model (WSGGM)**

optical thickness $a_p \times S$ $\ll 1$ optically thin

$\gg 1$ optically thick

Schefer's :	~0.8
Studer 's	~ 1.2
Ekoto 's	~2.1

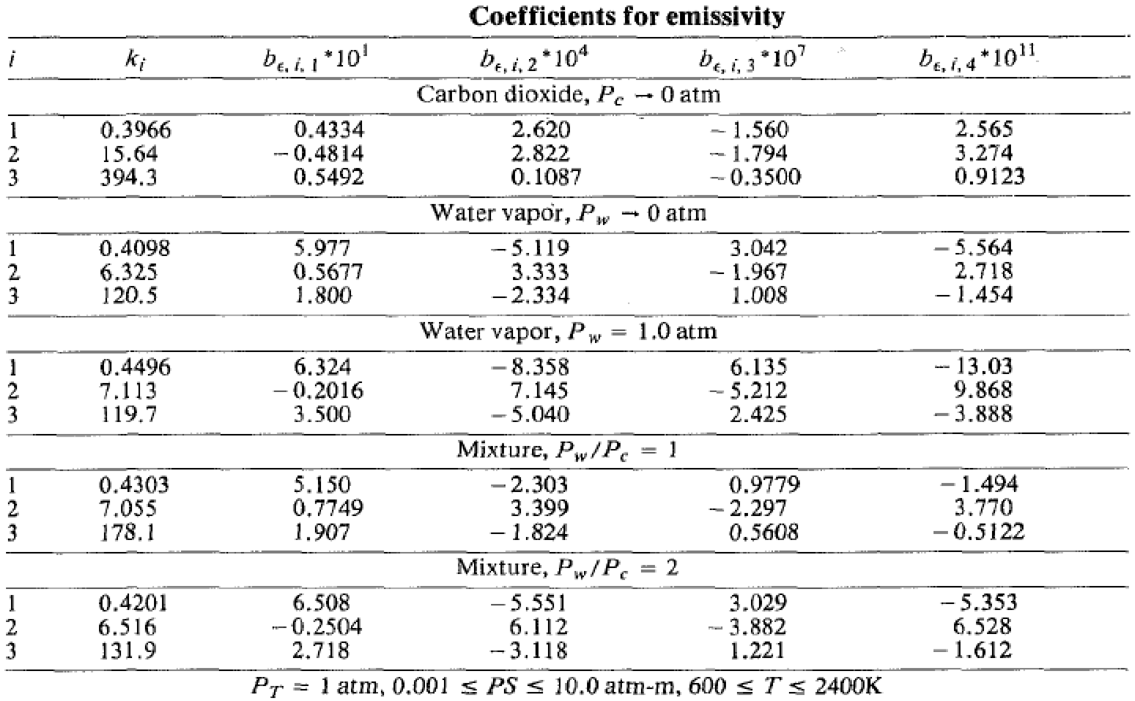
Sub-model for radiative heat transfer

Weighted Sum of grey gas model (WSGGM)

$$\epsilon = \sum_{i=0}^{I} a_{\epsilon,i}(T)(1 - e^{-\kappa_i ps})$$

$$a_{\epsilon,i} = \sum_{j=1}^{J} b_{\epsilon,i,j} T^{j-1}$$

$$a = -\frac{\ln(1-\epsilon)}{s}$$



Coefficients for emissivity

i	k_i	$b_{\epsilon,i,1} * 10^1$	$b_{\epsilon,i,2} * 10^4$	$b_{\epsilon,i,3} * 10^7$	$b_{\epsilon,i,4} * 10^{11}$
			Carbon dioxide, $P_c \to 0$ atm		
1	0.3966	0.4334	2.620	−1.560	2.565
2	15.64	−0.4814	2.822	−1.794	3.274
3	394.3	0.5492	0.1087	−0.3500	0.9123
			Water vapor, $P_w \to 0$ atm		
1	0.4098	5.977	−5.119	3.042	−5.564
2	6.325	0.5677	3.333	−1.967	2.718
3	120.5	1.800	−2.334	1.008	−1.454
			Water vapor, $P_w = 1.0$ atm		
1	0.4496	6.324	−8.358	6.135	−13.03
2	7.113	−0.2016	7.145	−5.212	9.868
3	119.7	3.500	−5.040	2.425	−3.888
			Mixture, $P_w/P_c = 1$		
1	0.4303	5.150	−2.303	0.9779	−1.494
2	7.055	0.7749	3.399	−2.297	3.770
3	178.1	1.907	−1.824	0.5608	−0.5122
			Mixture, $P_w/P_c = 2$		
1	0.4201	6.508	−5.551	3.029	−5.353
2	6.516	−0.2504	6.112	−3.882	6.528
3	131.9	2.718	−3.118	1.221	−1.612

$P_T = 1$ atm, $0.001 \le PS \le 10.0$ atm-m, $600 \le T \le 2400$K

Semi-empirical models for comparison

Flame length

$$L_{vis} = \frac{L^{*} d_{sd} \sqrt{\rho_{sd} / \rho_{\infty}}}{f_s}$$

buoyancy dominated regime ($Fr_f < 5$)

$$L^{*} = \frac{13.5 \mathrm{Fr}_f^{2/5}}{\left(1 + 0.07 Fr_f^2\right)^{1/5}}$$

$$Fr_f = \frac{u_{sd} f_s^{\;3/2}}{\left(\rho_{sd} / \rho_{\infty}\right)^{1/4} \left[\left(\left(T_{ad} - T_{\infty}\right)/T_{\infty}\right) g d_{sd}\right]^{1/2}}$$

momentum-dominated regime

$$L^{*} = 23$$

Radiant fraction

Studer et al (for CH4/H2)

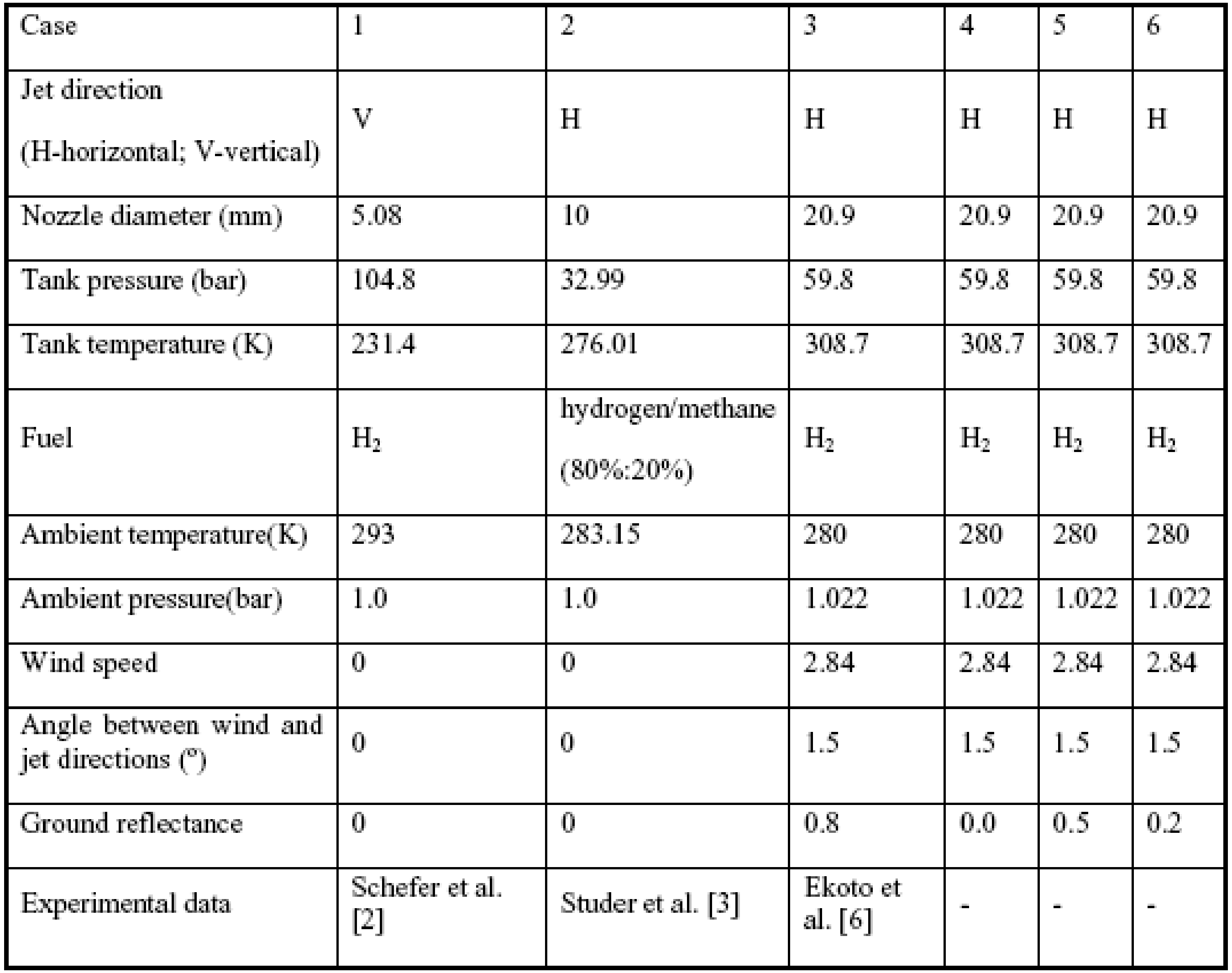
$$R_r = 0.08 \log_{10}\left(\tau_f a_p T_{ad}^4\right) - 1.14$$

Ekoto et al (for H2)

$$R_r = 0.08916 \log_{10}\left(\tau_f a_p T_{ad}^4\right) - 1.2172$$

$$\tau_f = \frac{\rho_f W_f^2 L_{vis} f_s}{3 \rho_{sd} d_{sd}^2 u_{sd}}$$

Numerical setup



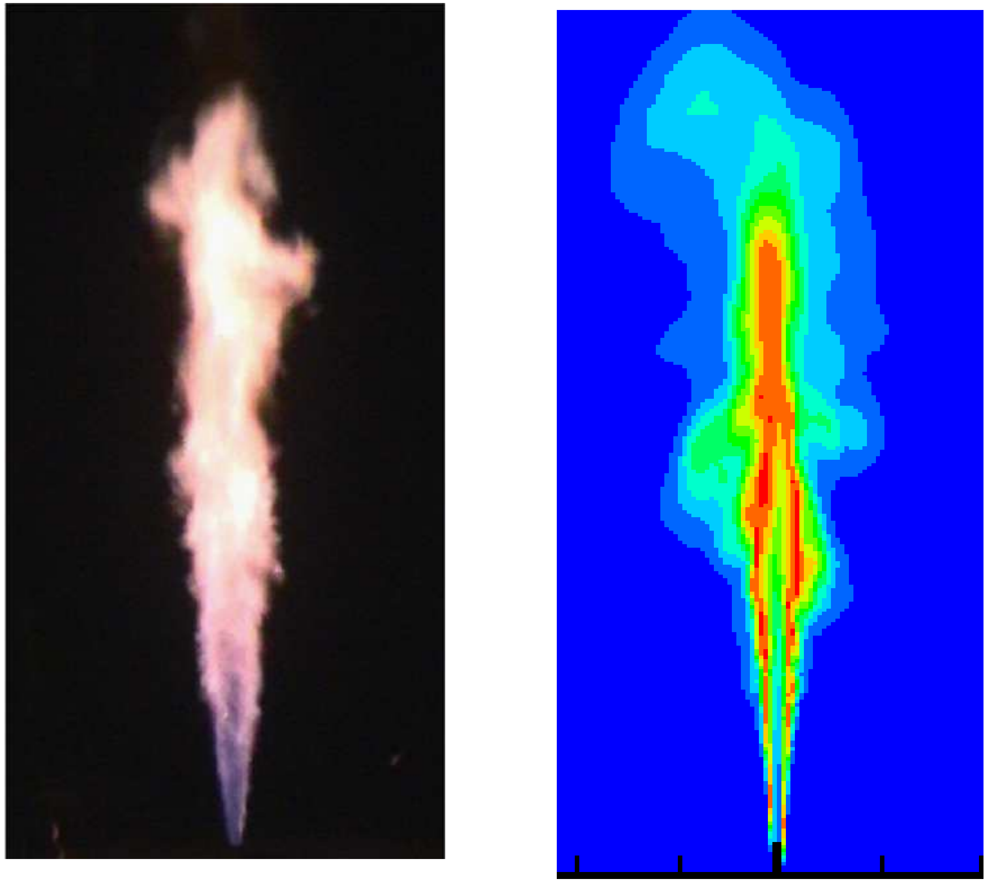
Case	1	2	3	4	5	6
Jet direction (H-horizontal; V-vertical)	V	H	H	H	H	H
Nozzle diameter (mm)	5.08	10	20.9	20.9	20.9	20.9
Tank pressure (bar)	104.8	32.99	59.8	59.8	59.8	59.8
Tank temperature (K)	231.4	276.01	308.7	308.7	308.7	308.7
Fuel	H_2	hydrogen/methane (80%:20%)	H_2	H_2	H_2	H_2
Ambient temperature(K)	293	283.15	280	280	280	280
Ambient pressure(bar)	1.0	1.0	1.022	1.022	1.022	1.022
Wind speed	0	0	2.84	2.84	2.84	2.84
Angle between wind and jet directions (°)	0	0	1.5	1.5	1.5	1.5
Ground reflectance	0	0	0.8	0.0	0.5	0.2
Experimental data	Schefer et al. [2]	Studer et al. [3]	Ekoto et al. [6]	-	-	-

Results and discussions

The under-expanded hydrogen jet fire of Schefer et al.

Schefer, R.W., Houf, W.G., Williams, T.C., Bourne B. and Colton, J., Characterization of High-pressure, Underexpanded Hydrogen-jet Flames, *International Journal of Hydrogen Energy*, **32**, 2007, pp. 2081-2093.

Nozzle Diameter: 5.08mm
Pressure: 104.8atm
Tank temperature:231.4K



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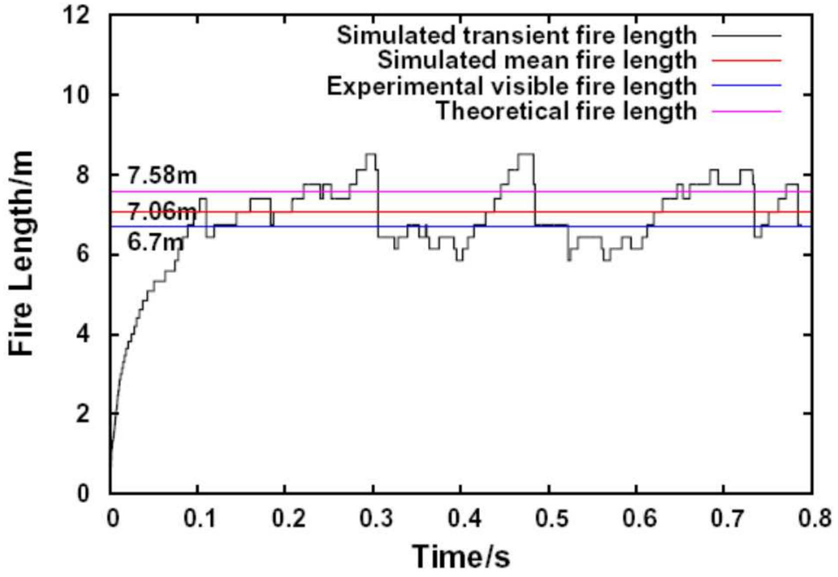
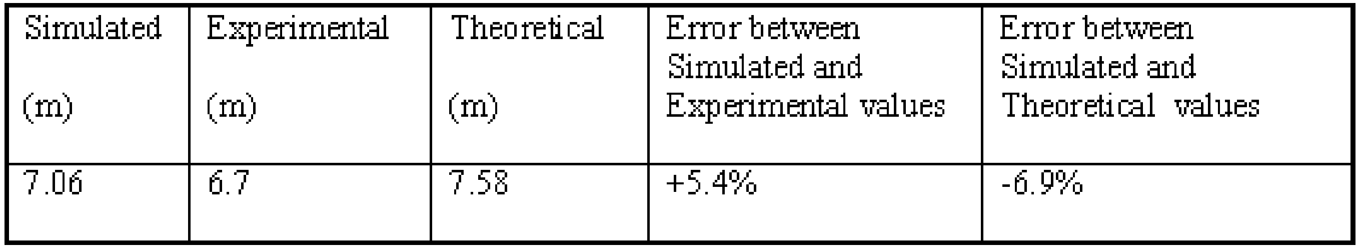


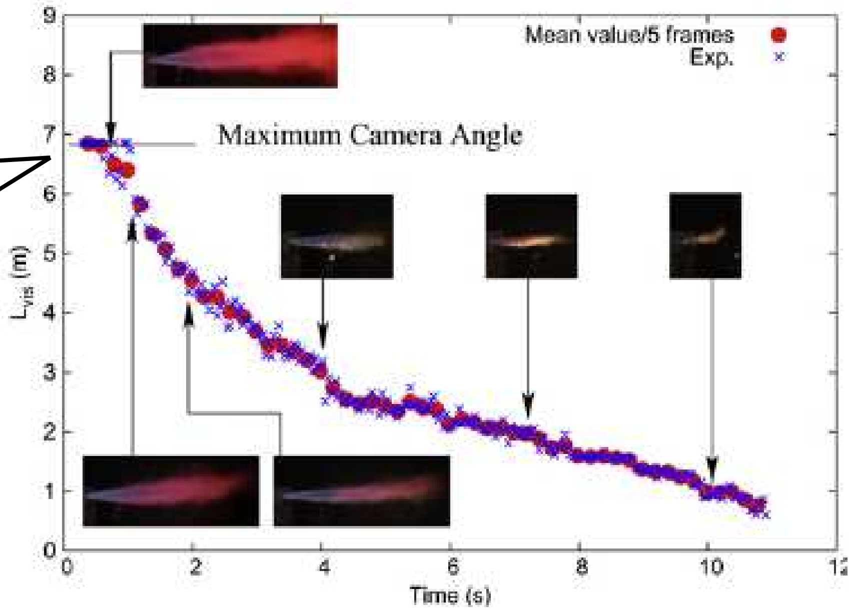


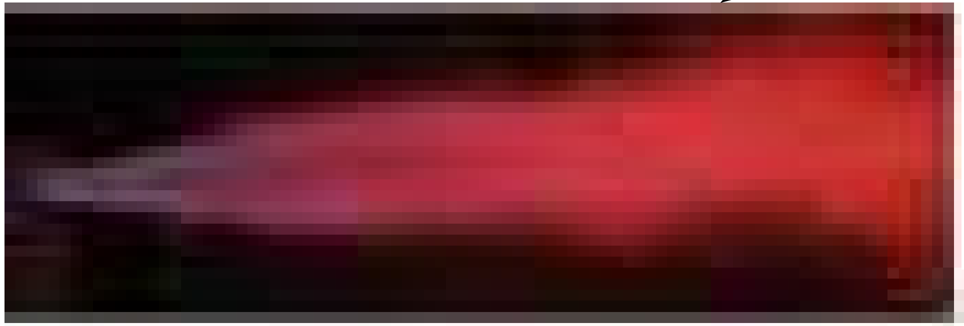
Simulated (m)	Experimental (m)	Theoretical (m)	Error between Simulated and Experimental values	Error between Simulated and Theoretical values
7.06	6.7	7.58	+5.4%	-6.9%

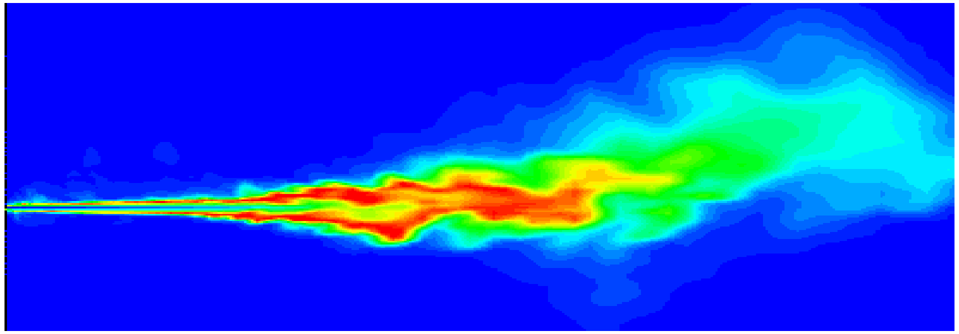
The undere-expanded jet fire of Studer et al.

Studer, E., Jamois, D., Jallais, S., Leroy G., Hebrard J. and Blanchetière, V., Properties of Large-scale Methane/Hydrogen Jet Fires, International Journal of Hydrogen Energy, 34, 2009, pp. 9611-9619.

Pressure: 32.99atm
Tank temperature:276K
Fuel: 80%H2+20%CH4
Nozzle Diameter: 10mm







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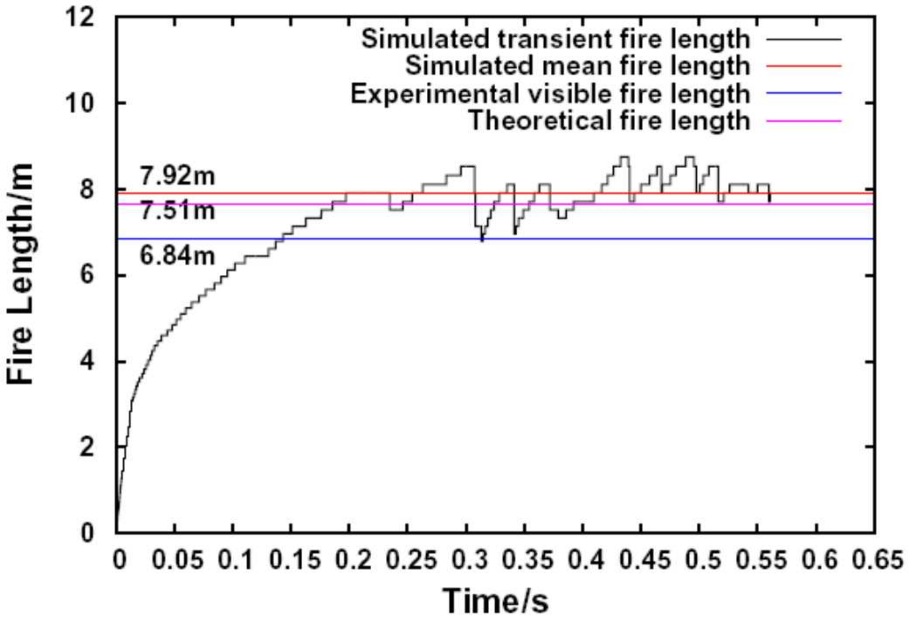
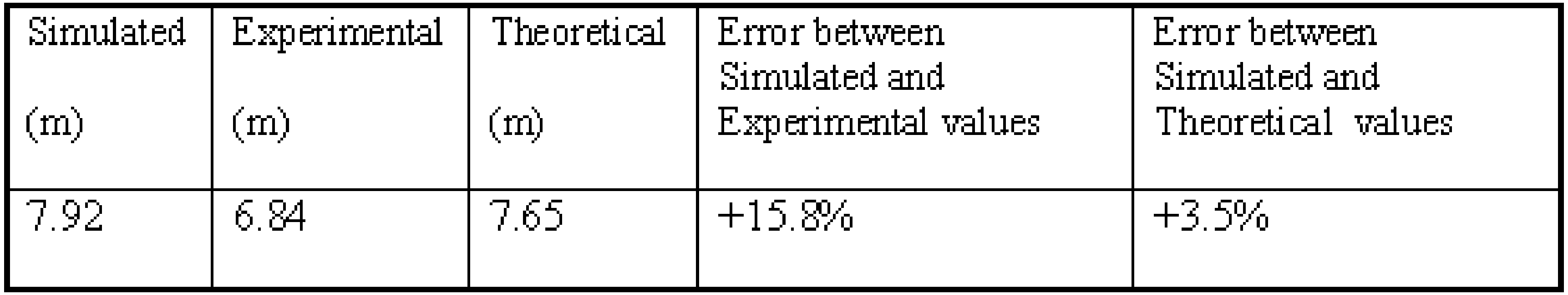


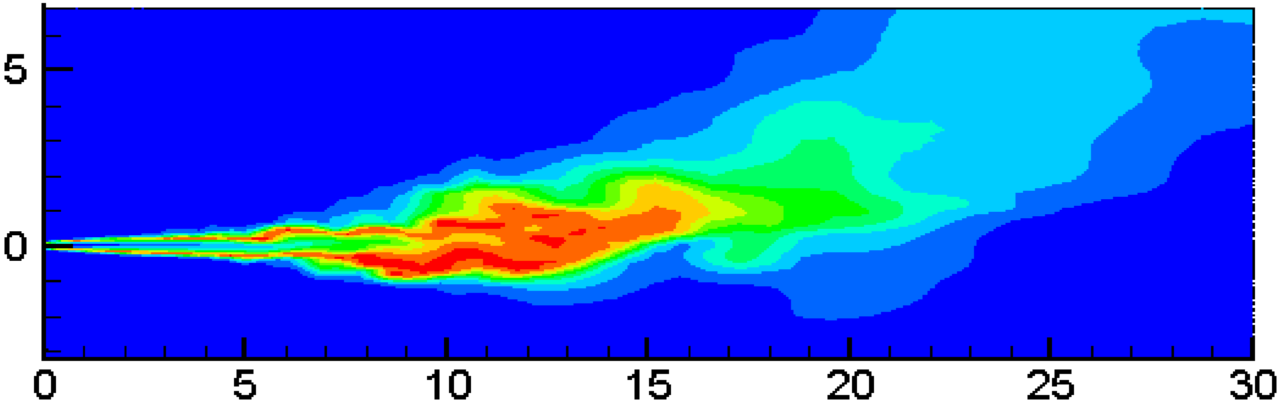


Simulated (m)	Experimental (m)	Theoretical (m)	Error between Simulated and Experimental values	Error between Simulated and Theoretical values
7.92	6.84	7.65	+15.8%	+3.5%

The under-expanded hydrogen jet fire of Ekoto et al.

Ekoto, I.W., Houf, W.G., Ruggles A.J., Creitz, L.W. and Li, J.X., Large-scale Hydrogen Jet Flame Radiant Fraction Measurements and Modelling, Proceedings of the 2012 9th the International Pipeline Conference, Calgary, Alberta, Canada, 2012, Paper IPC2012-90535, 2012.

Jet	d_j [mm]	$\dot{m}$ [kg/s]	p_0 [barg]	T_0 [K]	RH [%]	T_{amb} [K]	p_{amb} [mbar]	u_{wind} [m/s]	φ_{wind} [°]	L_{vis} [m]
1	20.9	1.0	59.8	308.7	94.3	280	1022	2.84	68.5	17.4



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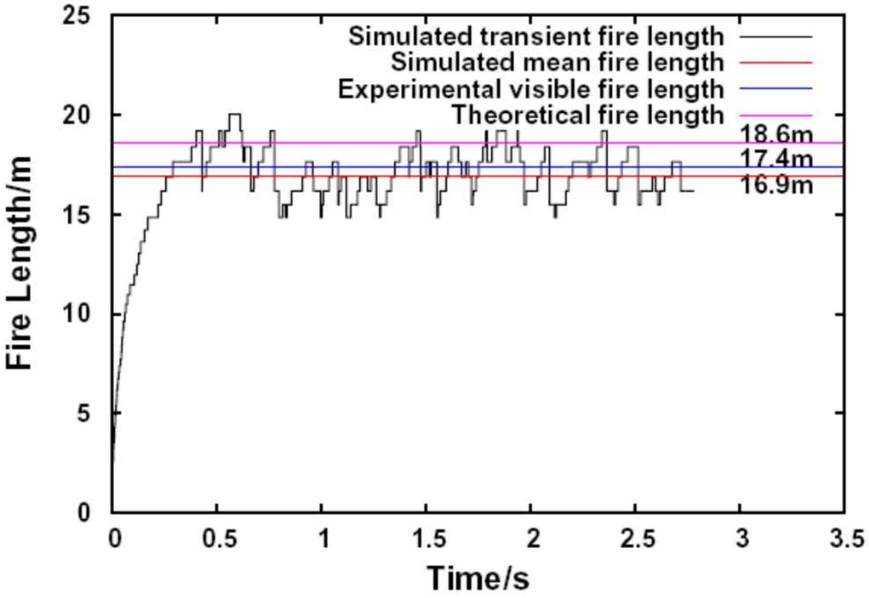

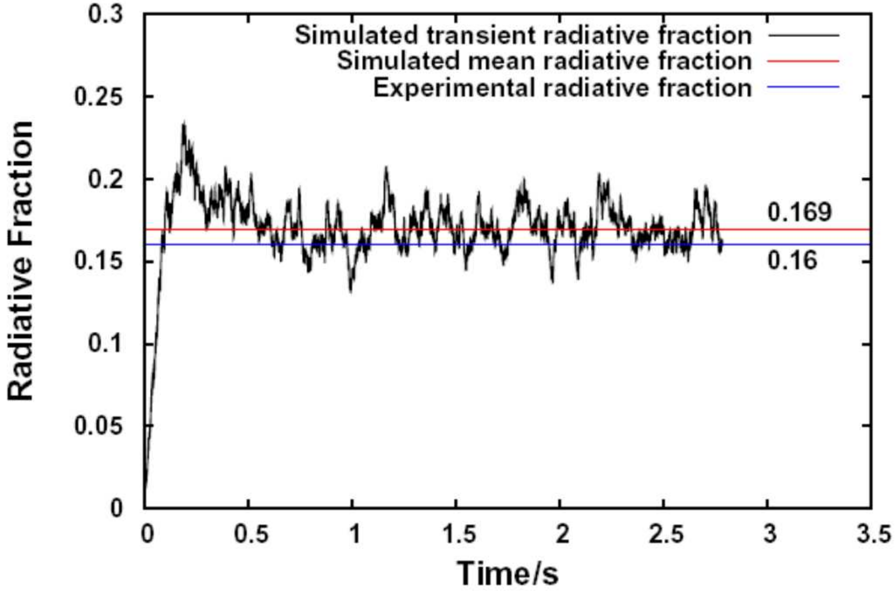

Simulated (m)	Experimental (m)	Theoretical (m)	Error between Simulated and Experimental values	Error between Simulated and Theoretical values
16.9	17.4	18.6	-2.9%	-9.1%

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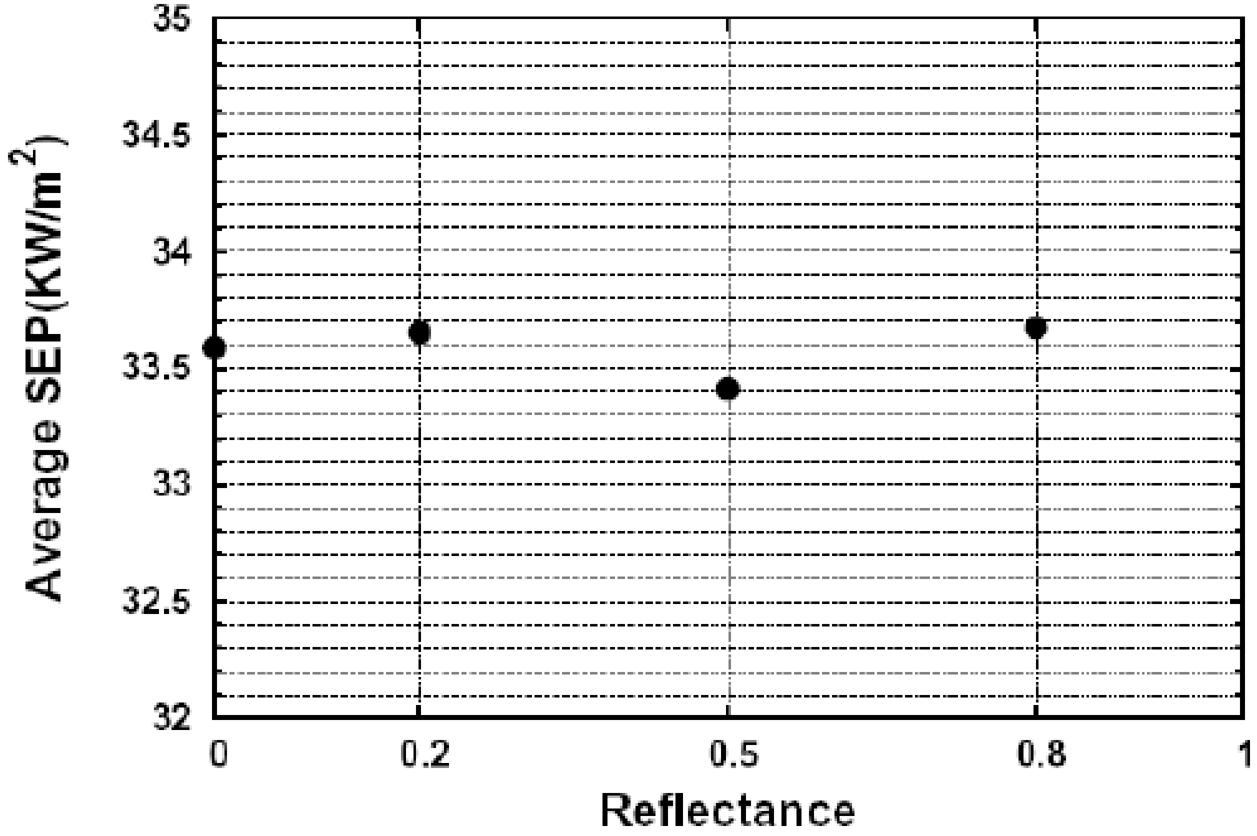
The predicted mean surface emissive power *vs* ground surface reflectance



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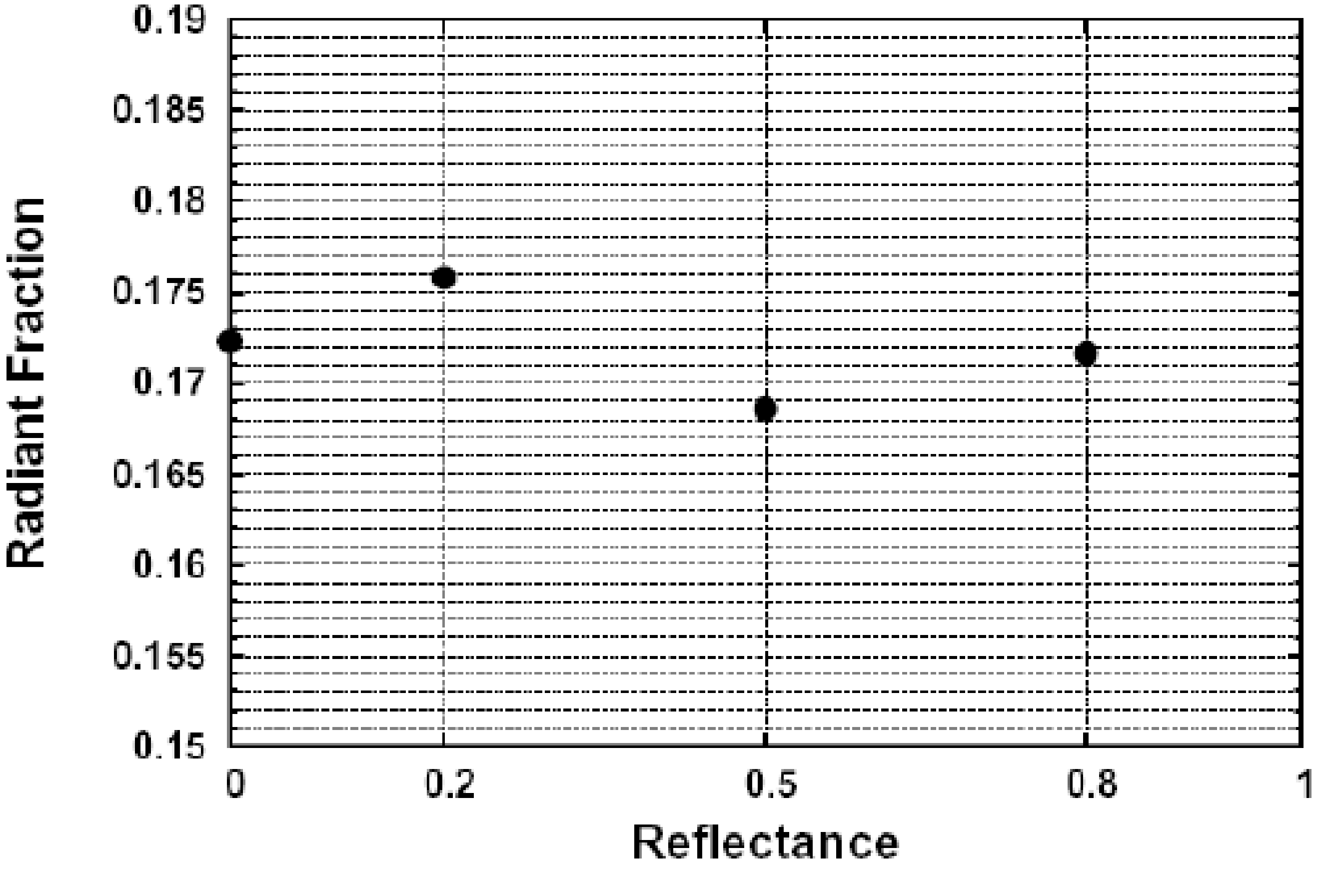
The predicted mean radiant fraction *vs* ground surface reflectance



Concluding remarks

- FireFOAM code has been used to simulate six cases of under-expanded hydrogen and hydrogen/methane jet fires.

- The relatively good agreement with the published experimental data has demonstrated good potential of the FireFOAM code as a reliable predictive tool for hazard analysis of hydrogen and hydrogen/methane jet fires.

- The ground surface reflectance was found to have only minor effect on the surface emissive power of the jet fire. However, the radiant fraction exhibits more sensitivity and ranges from 0.168 to 0.176, which fluctuates close to the suggested value of 0.16 by Ekoto et al.[6].

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Thanks for your attention