Clean Hydrogen Partnership

CFD models and predictions for hydrogen fire hazards

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European Hydrogen Safety Panel (EHSP)
Clean Hydrogen JU Webinar "Computational Fluid Dynamics (CFD) for hydrogen safety analysis" 07 December 2022

EUROPEAN PARTNERSHIP

Co-funded by the European Union

In-house CFD codes for hydrogen fire and explosion hazards

HyFOAM

Modified from open source CFD code OpenFOAM for:
- Research
- Consultancy
- Fee paying development for sponsors

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- Predictive tools for LOC scenarios of gaseous hydrogen (GH_2) during transportation
  - Hydrogen spontaneous ignition
  - **Hydrogen jet fires**
  - Hydrogen deflagrations
- Predictive tools for LOC scenarios of liquid hydrogen (LH_2) during transportation
  - LH_2 vapour cloud from sudden catastrophic release
  - LH_2 vapour cloud from jet release
  - Hydrogen jet fires at cryogenic conditions
  - Vapour cloud explosions (VCE)

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Hydrogen jet fires – model outline(1/2)

- HyFOAM code with own modified eddy dissipation concept (EDC) for fires (Chen et al. 2014)
- Finite volume discrete ordinates model (fvDOM)
- Weighted sum of grey gas model for radiation

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

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

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

Zhibin Chen, Jennifer Wen, Baopeng Xu, Siaka Dembele, Large eddy simulation of a medium-scale methanol pool fire using the extended eddy dissipation concept, International Journal of Heat and Mass Transfer, Volume 70, March 2014, Pages 389-408.
Zhibin Chen, Jennifer Wen, Baopeng Xu, Siaka Dembele, Extension of the eddy dissipation concept and smoke point soot model to the LES frame for fire simulations, Fire Safety Journal, Volume 64, February 2014, Pages 12-26.

Hydrogen jet fires – model outline(2/2)

Modelling approach

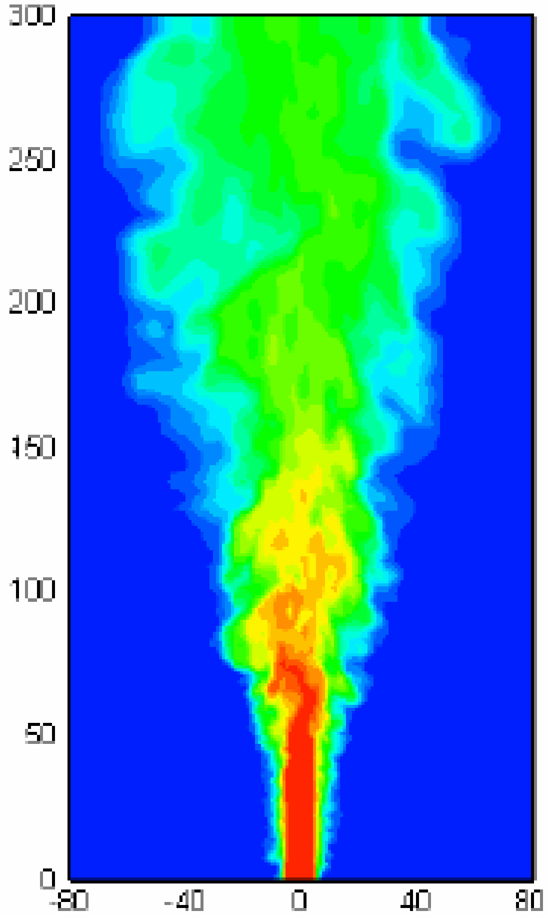
- Pseudo-source approach (Ewan and Modie 1985)
- Leak modelled from downstream as a sonic jet with the same mass flow rate

$$D_{eq} = D_j (0.536 C_D \frac{P_o}{P_a})^{0.5}$$

$$P_e = P_o (\frac{2}{\gamma + 1})^{\gamma/\gamma - 1}$$

$$\rho_e = \rho_o (\frac{2}{\gamma + 1})^{\gamma/\gamma - 1}$$

$$Y_o = \frac{4.99 D_s}{z} (\frac{\rho_g}{\rho_a})^{1/2} C_D^{1/2}$$



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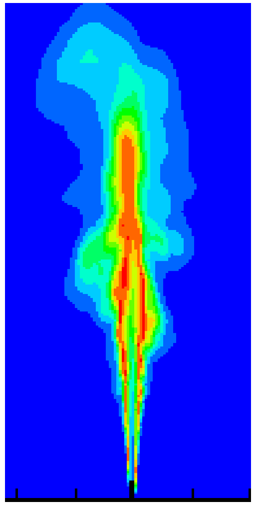
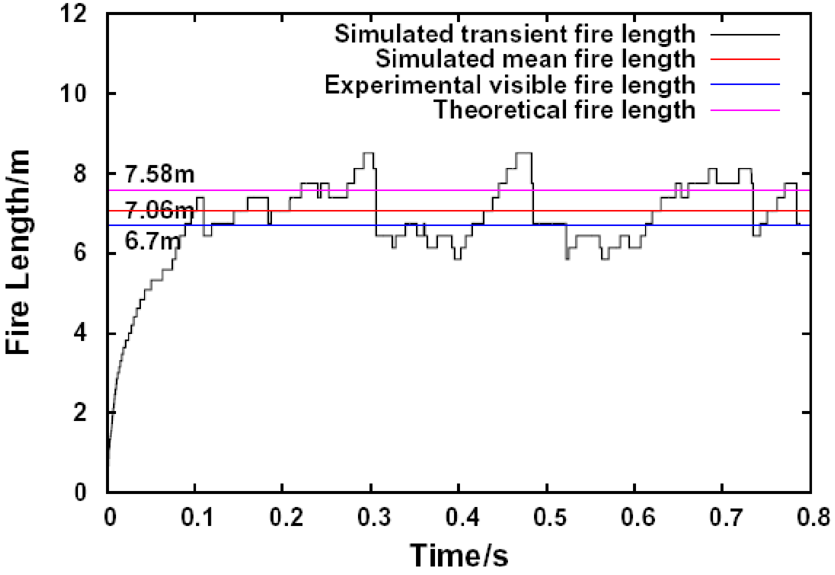
Hydrogen jet fires – validation (1/3)

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

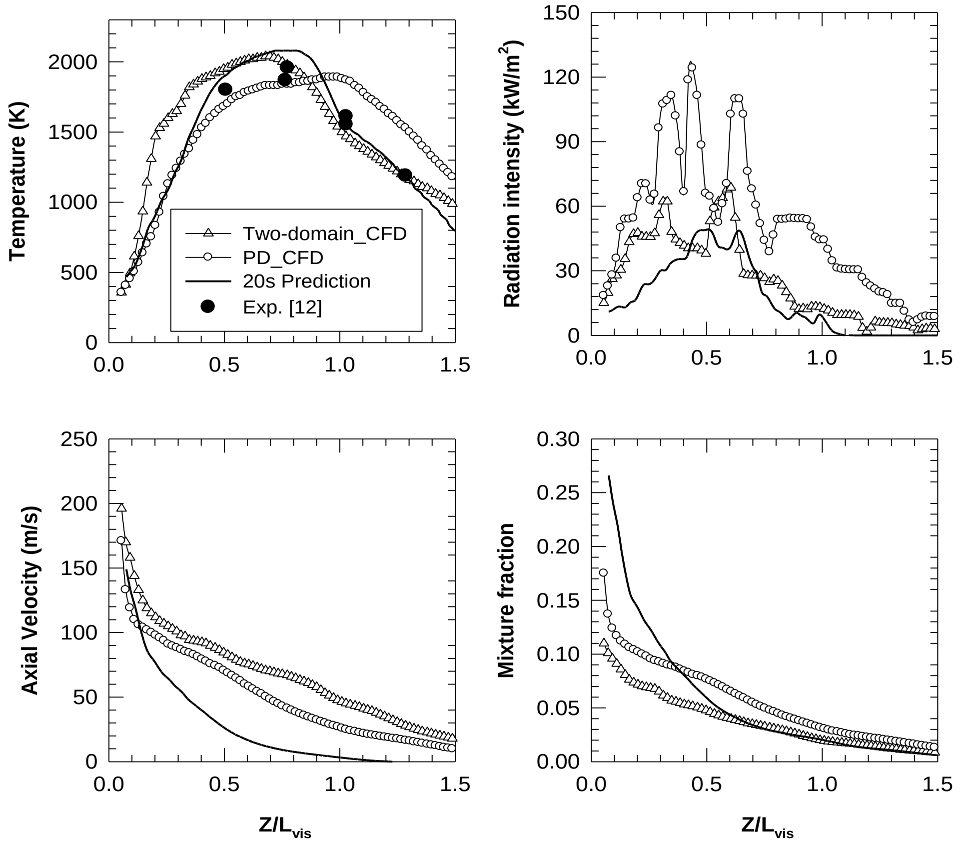




Wang, C. J., Wen, Jennifer X., Chen, Z. B. and Dembele, S. (2014) Predicting radiative characteristics of hydrogen and hydrogen/methane jet fires using FireFOAM, Int. J of Hydrogen Energy, 39 (35).
Schefer, R.W., Houf, W.G., Williams, T.C., Bourne B. and Colton, J., Characterization of High-pressure, Underexpanded Hydrogen-jet Flames, Int. J of Hydrogen Energy, 32, 2007.

Hydrogen jet fires – validation (2/3)

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%



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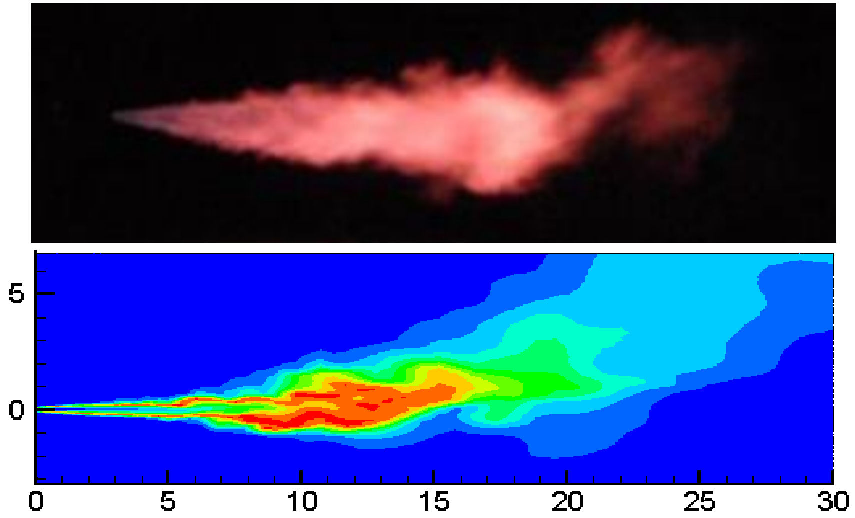
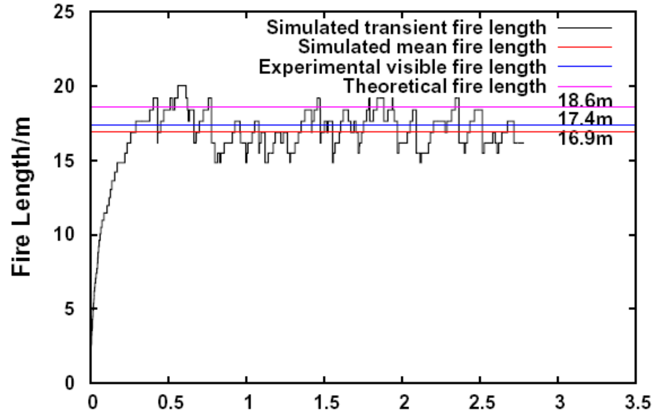
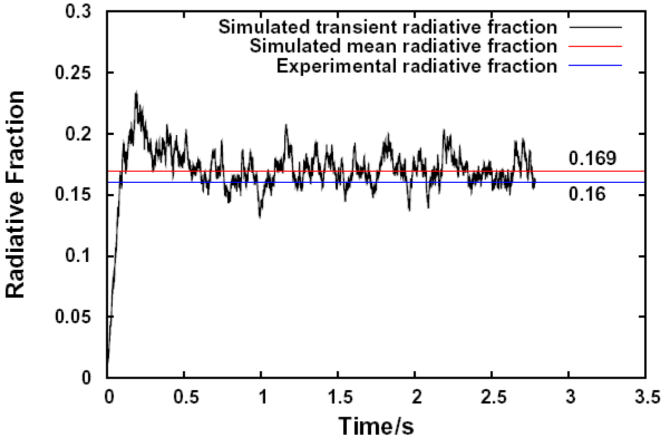
Hydrogen jet fires – validation (3/3)



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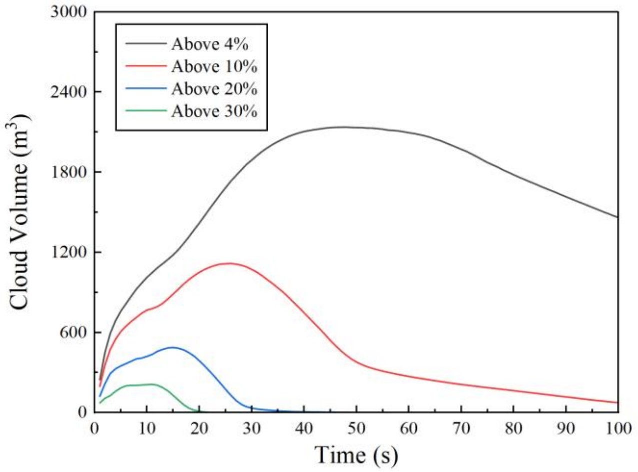
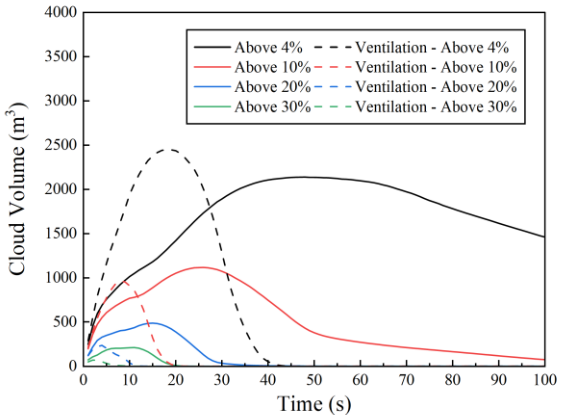
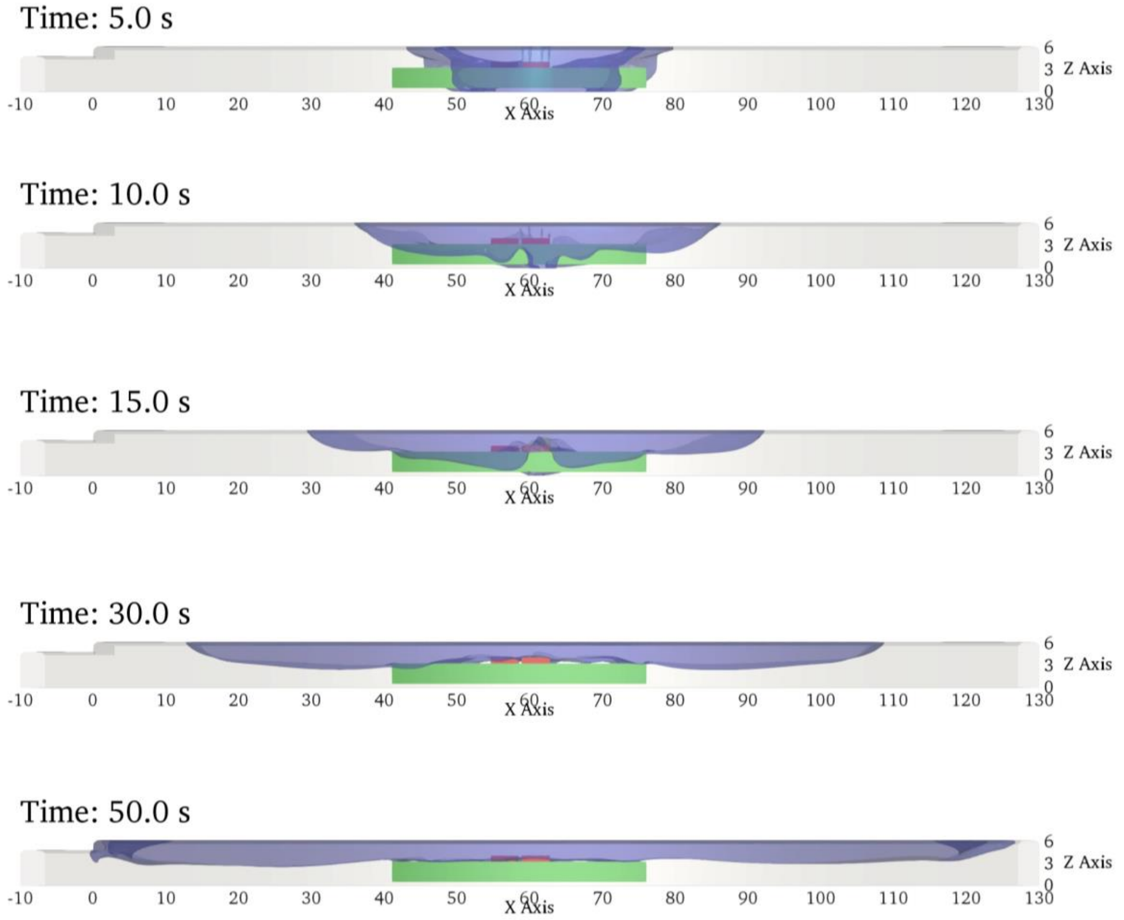
Ekoto, I.W., Houf, W.G., Ruggles A.J., Creitz, L.W. and Li, J.X. (2012) Large-scale Hydrogen Jet Flame Radiant Fraction Measurements and Modelling, Proc. 9th Int. Pipeline Conference, Calgary, Alberta, Canada, Paper IPC2012-90535.

Dispersion simulation in preparation for modelling multiple hydrogen jet fires in a tunnel (1/5)



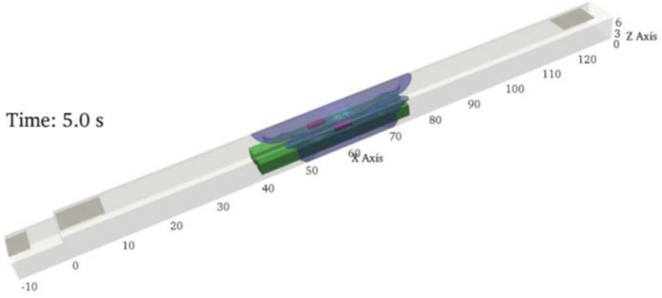


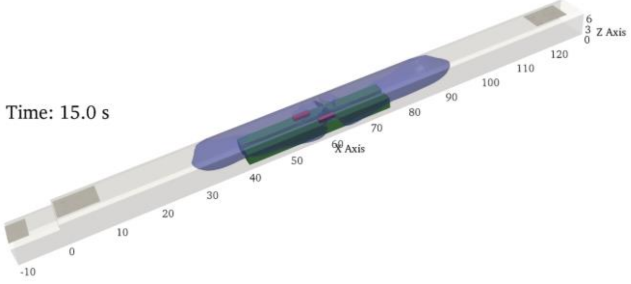
Cloud （above 4% - view 1 ）

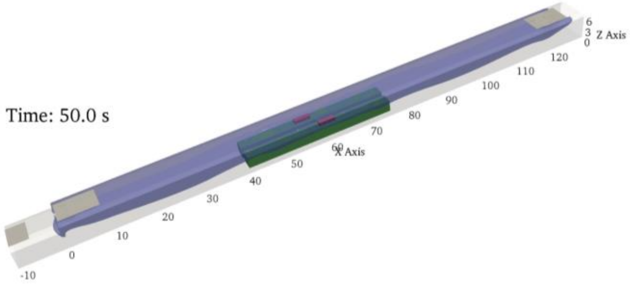


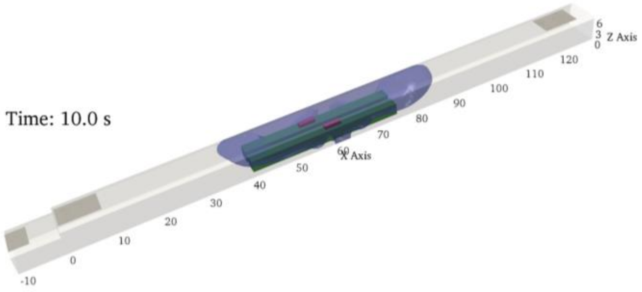
Dispersion simulation in preparation for modelling multiple hydrogen jet fires in a tunnel (2/2)

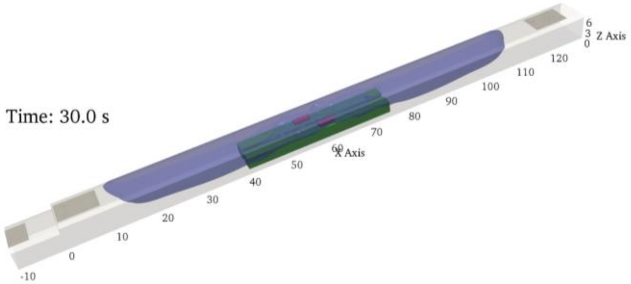
Cloud （Above 4%） - view 2





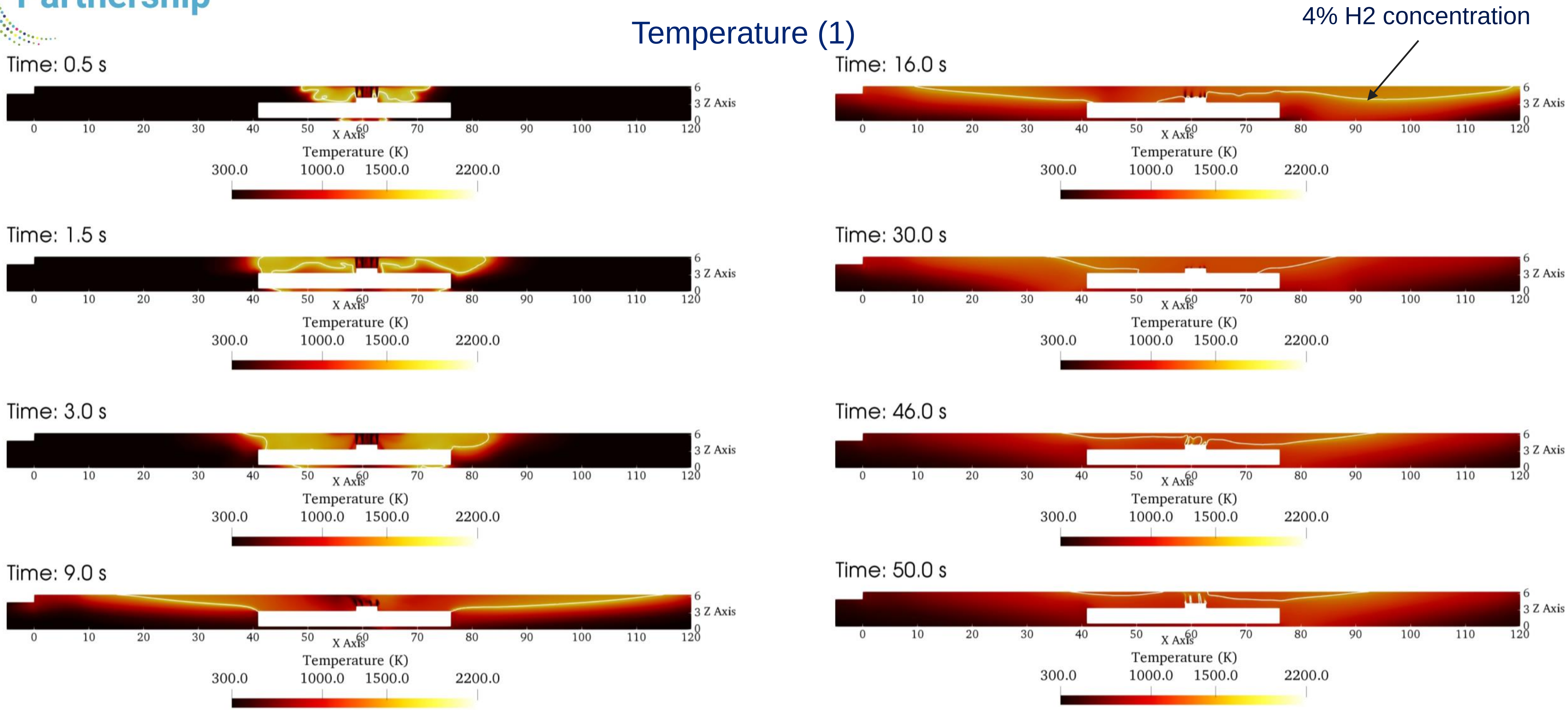






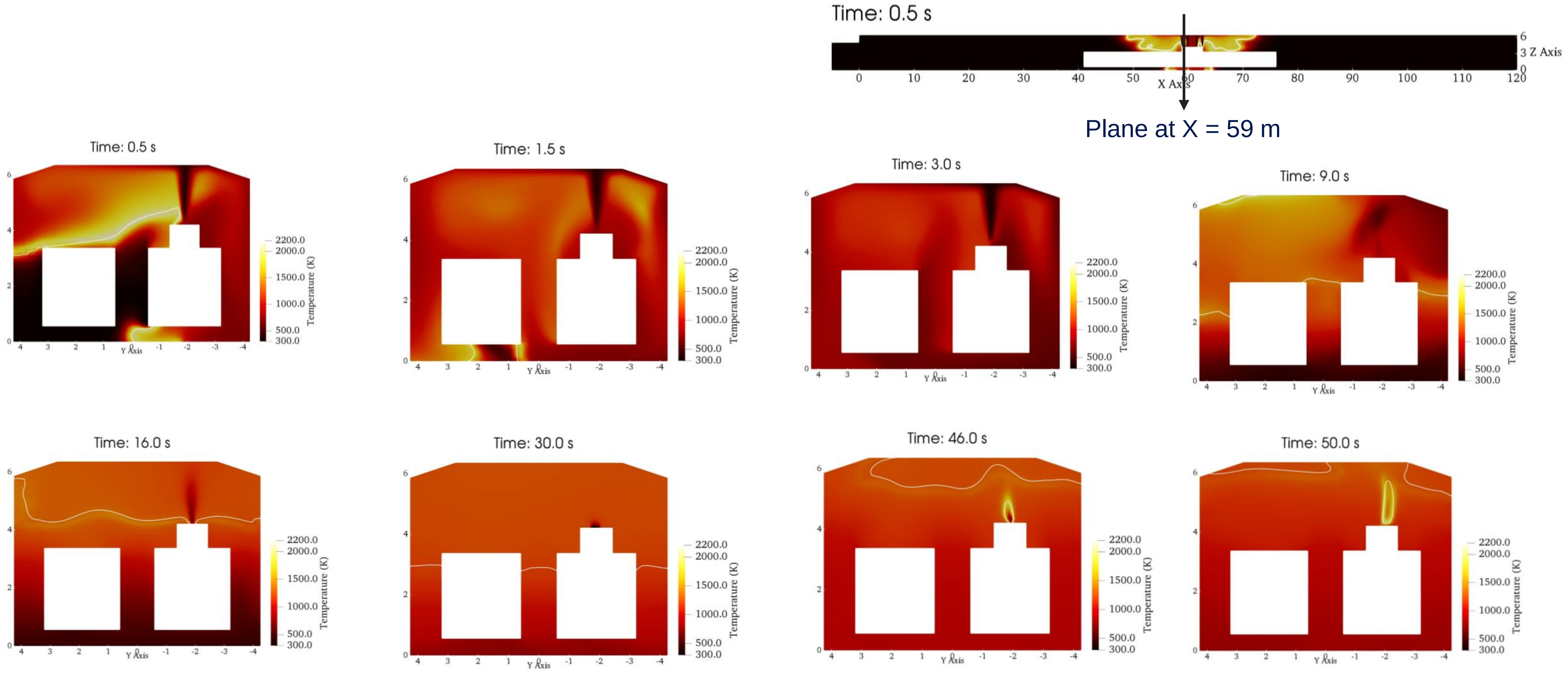
Multiple hydrogen jet fires in a tunnel (1/4)

Temperature (1)



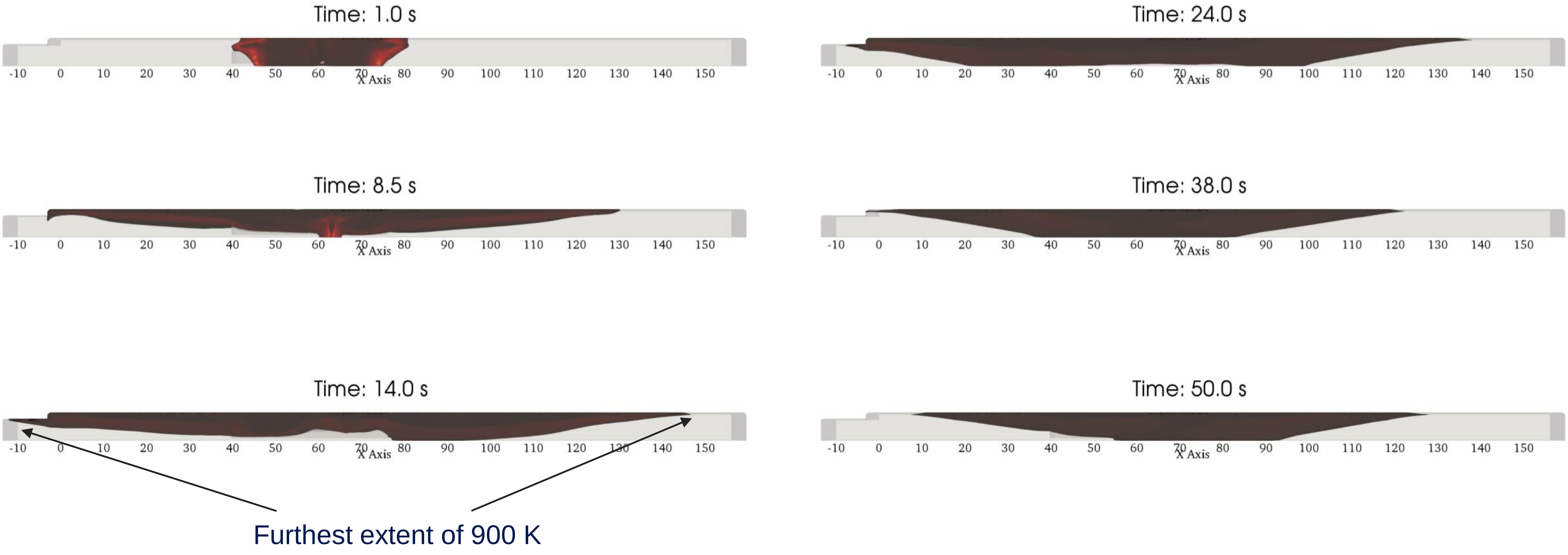
Multiple hydrogen jet fires in a tunnel (2/4)

Temperature (2)



Multiple hydrogen jet fires in a tunnel (3/4)

Cloud above 900 K



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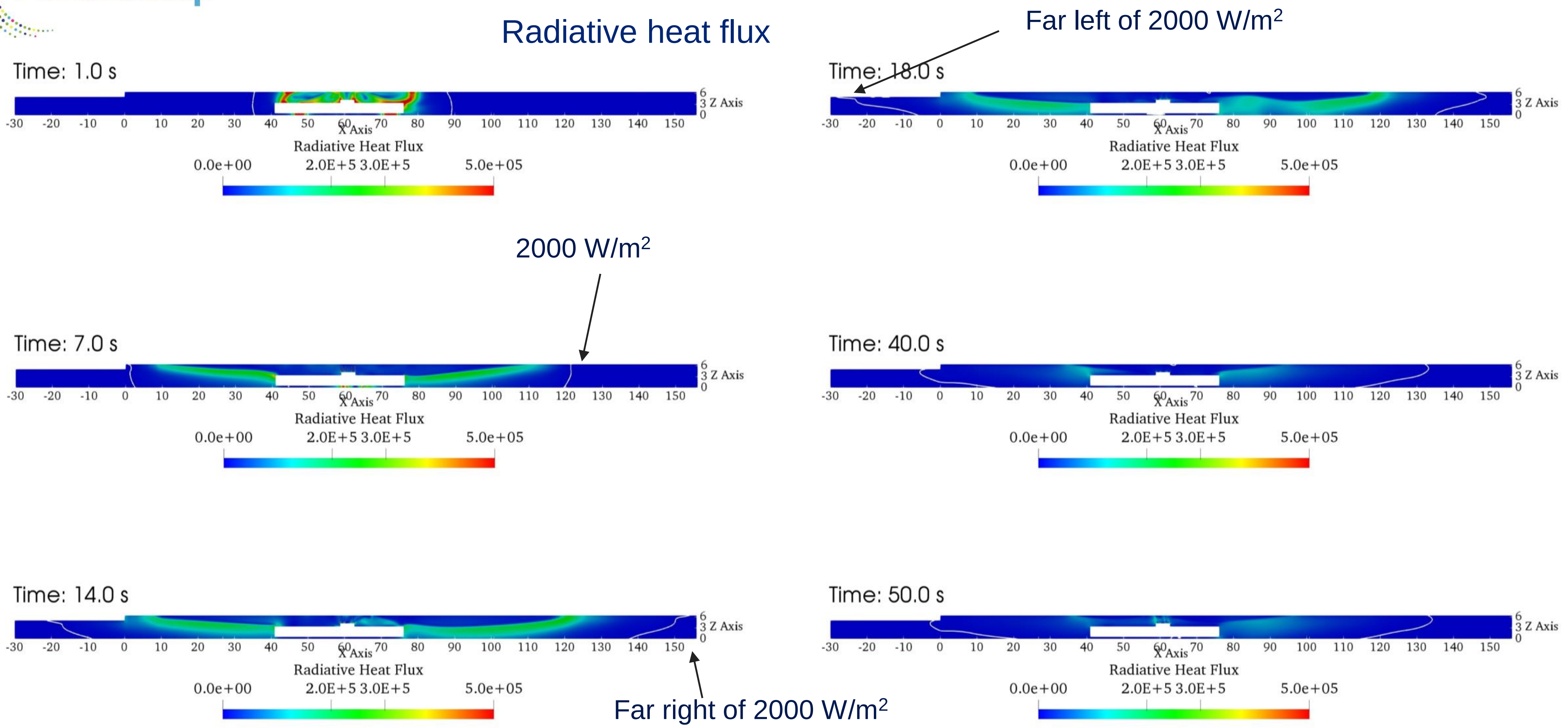
Multiple hydrogen jet fires in a tunnel (4/4)

Radiative heat flux



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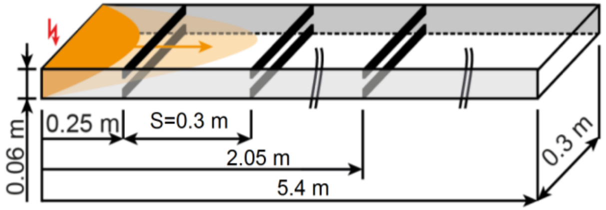
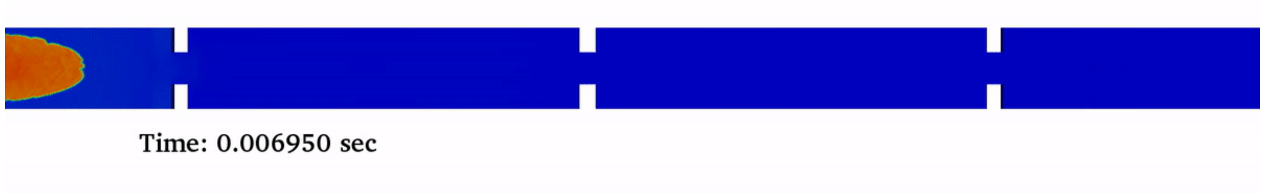
HyFOAM simulations of explosions and DDT

Hydrogen flame acceleration and deflagration to detonation transition (DDT)

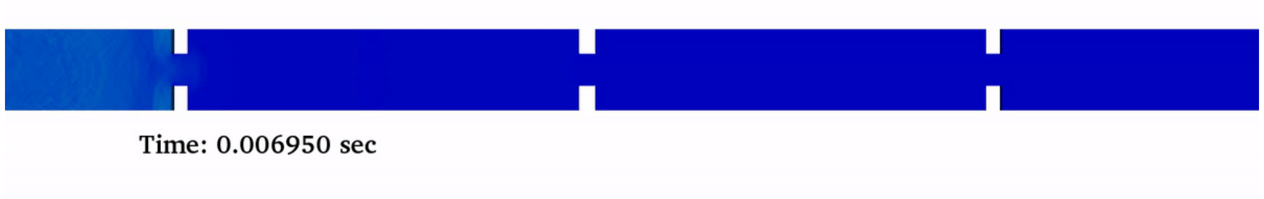


Numerical Schlieren

Temperature (K)

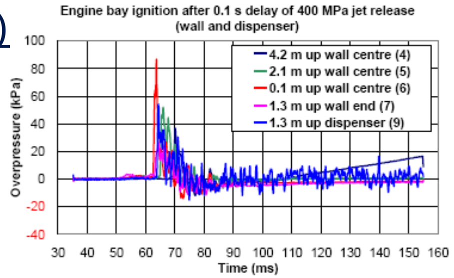


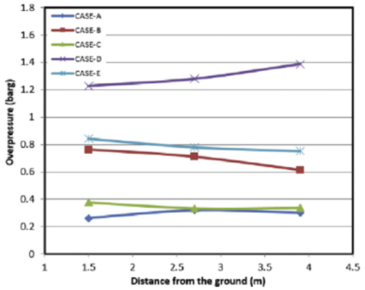
Pressure (pa)



X=0.55m X=0.85m X=1.15m

Hydrogen explosions





DDT in a full scale tunnel (423.9 m^3)

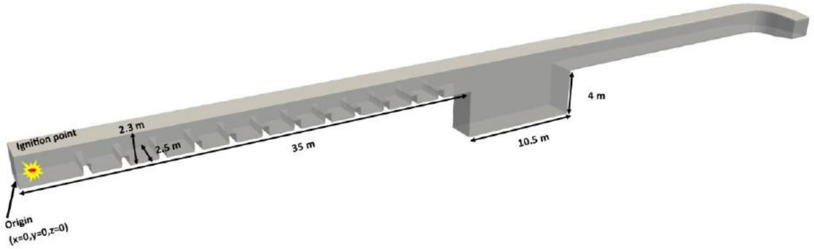
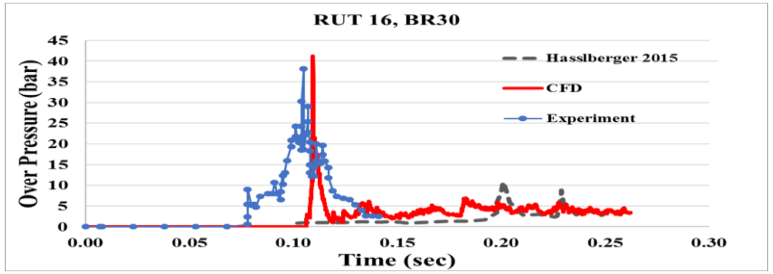


Figure 7-2: RUT 16 geometry configuration; 30% blockage ratio.



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