Supplementary materials

Fire Hazard Mitigation in Bi-Continuous Phase Polymer Composites: Surface vs. Bulk and Experimental vs. Computational

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1 Coupling simulation of indoor dynamic fire and personnel evacuation

AutoCAD 2019 is used to construct a 3D building model of 25 × 25 × 3 m, and to divide the mesh model into 0.1 × 0.1 × 0.1 m for modular calculation[1]。Subsequently, it was imported into the Fire Dynamic Simulation (FDS) software PYROSIM 2019 to further simulate indoor smoke, heat, visibility, and other results in fire scenarios, and generate a visual model. Then, by coupling the FDS results (carbon monoxide volume fraction, carbon dioxide volume fraction, oxygen volume fraction, smoke, temperature) with personnel evacuation simulation results, the influence of different materials on the speed of personnel evacuation in indoor fire scenarios is obtained[2]. During the coupling simulation process, the evacuation route of indoor personnel is controlled by the Steering method[3]. The stoichiometric equations for the decomposition products of PVC, HDPE, and CPE are controlled by the following equation (1-3):

$$C_2H_3Cl + 1.53O_2 + 1.53(3.76)N_2 \rightarrow HCl + H_2O + 0.14CO + 0.96CO_2 + 0.90C + 1.53(3.76)N_2\#\ (1)$$

$$C_2H_4 + 3O_2 \rightarrow 2H_2O + 2CO_2\#\ (2)$$

$$C_4H_7Cl + 4.53O_2 + 1.53(3.76)N_2 \rightarrow HCl + 3H_2O + 0.14CO + 2.96CO_2 + 0.90C + 1.53(3.76)N_2\#\ (3)$$

For ease of modeling, PVC, HDPE, and CPE were considered as C2H3Cl, C2H4, and C4H7Cl, respectively, and defined as traceable raw materials. O_2, N_2, HCl, H_2O, CO, CO_2, and Soot C were defined as untraceable raw materials.

Table S1 Information of different pyrolysis models

Model		P/H	N-CPE	H-CPE	Cl-CPE
Phase 1	Density ($g \cdot cm^{-3}$)	0.91	1.45	1.51	1.45
	Heat of combustion ($MJ \cdot kg^{-1}$)	60.00	15.76	20.05	17.19
	Thermal conductivity ($W \cdot m^{-1} \cdot K^{-1}$)	0.41	9.34	3.78	7.81
	Smoke yield ($m^2 \cdot s^{-1}$)	0.05	0.07	0.10	0.07
Phase 2	Density ($g \cdot cm^{-3}$)	1.40	1.40	1.40	1.32
	Heat of combustion ($MJ \cdot kg^{-1}$)	5.00	5.00	3.00	5.00
	Thermal conductivity ($W \cdot m^{-1} \cdot K^{-1}$)	0.17	0.17	0.17	0.17
	Smoke yield ($m^2 \cdot s^{-1}$)	0.21	0.21	0.21	0.18
Absorption Coefficient (m^{-1})		5×10^4	5×10^4	5×10^4	5×10^4
External heat flux (kW)		35	35	35	35
Burner area (m^{-2})		9	9	9	9
Initial indoor temperature (℃)		20	20	20	20
Number of occupants		10	10	10	10

Note: the above data (phase 1 and phase 2) are sourced from experiments.

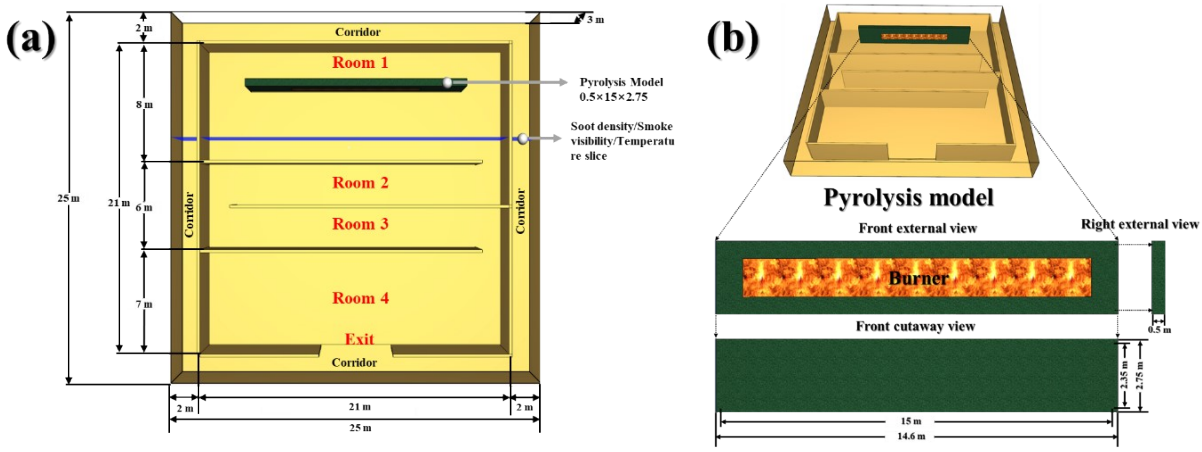

Figure S1 3D models of dynamic fire simulation: (a) building model and (b) pyrolysis model.

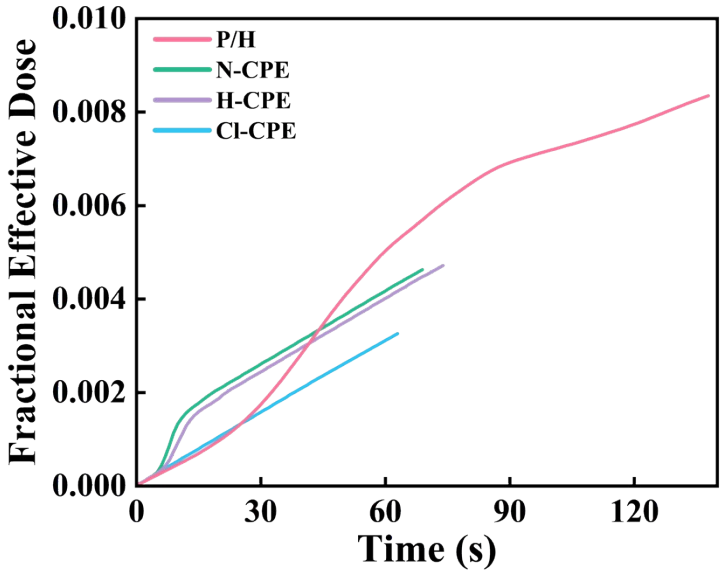

Figure S2 Real-time Fractional Effective Dose during coupling simulation.

2 Detailed data information in section 3.9

Table S2 Comparison of detailed parameters in different composite systems

Sample	$T_{d,5}$ (°C)	TSP (m^{-2})	SD (%)	Visibility of 200 s in simulation (m)	LOI (%)	Heat release ($kW \cdot m^{-2}$)	FDS coupled personnel evacuation (s)
N-CPE	283.7	13.3	51.18	17.8	37.5	450	69
H-CPE	291.7	13.7	62.81	8.7	39.7	565	74
Cl-CPE	286.7	12.6	50.35	30	33.9	334	63

Table S3 Comparison of the bulky chlorine, surface chlorine and surface EG content of different systems

Sample	Surface chorine content[a]	Bulky chorine content (wt%)	Surface EG content[a]
N-CPE	3rd	20.5	1st
H-CPE	1st	24.2	3rd
Cl-CPE	2nd	17.0	2nd

a-EG content and surface chlorine content were analyzed using Raman and FTIR spectroscopy, respectively. However, due to limitations in quantitative analysis, only the order was provided.

References

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