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Numerical benchmark campaign of COST Action TU1404 – microstructural modelling

Supplementary material
Model 7 – HYMOSTRUC3D

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1 Introduction

In this document the input data for *Model 7- HYMOSTRUC3D* used in the numerical benchmark [1] is presented as a supplementary material. The input data file is attached as a separate file.

2 Input data Model 7 – HYMOSTRUC3D

The chemical composition of PC is listed in Table 1. The mineral composition of Portland cement (PC) is: 60.8% C_3S, 12.5% C_2S, 4.32% C_3A and 9.9% C_4AF. The density of PC is 3.15 g/cm^3. The water to cement ratio (w/c) of the cement paste is 0.3. As shown in Fig. 1, the particle size distribution of PC follows the Rosin Rammler Bennett (RRB) distribution: $G(x) = 1 - exp(-bx^n)$. $G(x)$ is the cumulative weight, x is the particle diameter, n and b are the fitting parameters.

Table 1 Chemical compositions of PC

Raw materials	Chemical composition (wt. %)							
	CaO	SiO_2	Al_2O_3	Fe_2O_3	MgO	K_2O	Na_2O	SO_3
PC	63	20	4.5	2.9	1.9	0.95	0.19	2.8

3 Model parameters

3.1 Model parameters for hydration process and microstructure development

K_0 and δ_{tr} are two important model parameters in HYMOSTRUC3D. K_0 is the initial penetration rate of the reaction front of hydrating C_3S, C_2S, C_3A, C_4AF. δ_{tr} is the transition thickness when the hydration mechanism of C_3S, C_2S, C_3A, C_4AF change from *phase boundary reaction* to *diffusion-controlled reaction* (See details of the definitions of

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K_0 and δ_{tr} in [2]). The values of K_0 and δ_{tr} of C_3S, C_2S, C_3A, C_4AF are calculated with the equations listed in Table 2. Table 3 lists the calculated values of K_0 and δ_{tr} for the PC presented in Table 1.

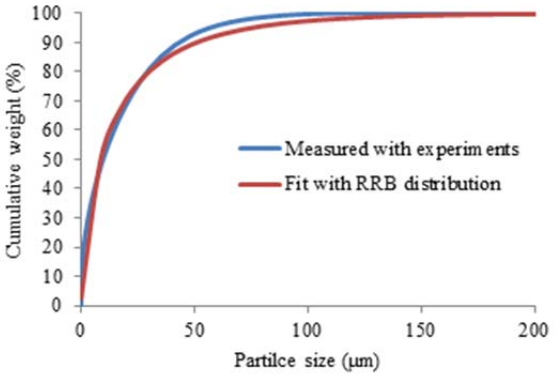

Figure 1. Particle size distribution of PC (n = 0.67588, b = 0.16112)

3.2 Model parameters for heat release

The total heat release of PC is calculated from the degree of hydration of the components in PC (see Eq. (5)).

$$Q(PC) = \alpha(C_3S) \times f(C_3S) \times Q(C_3S) + \alpha(C_2S) \times f(C_2S) \times Q(C_2S) \\ \alpha(C_3A) \times f(C_3A) \times Q(C_3A) + \alpha(C_4AF) \times f(C_4AF) \times Q(C_4AF) \quad (5)$$

where $Q(PC)$ is the total heat release [J/g], $\alpha(C_3S), \alpha(C_2S), \alpha(C_3A)$ and $\alpha(C_4AF)$ are the simulated degree of hydration of C_3S, C_2S, C_3A and C_4AF, respectively. $f(C_3S), f(C_2S), f(C_3A)$ and $f(C_4AF)$ are the mass fraction of C_3S, C_2S, C_3A and C_4AF, respectively. $Q(C_3S), Q(C_2S), Q(C_3A)$ and $Q(C_4AF)$ are the heat release of C_3S, C_2S, C_3A and C_4AF when they completely hydrate [J/g]. In this study $Q(C_3S), Q(C_2S), Q(C_3A)$ and $Q(C_4AF)$ are equal to 570, 260, 840 and 125 [J/g] according to the Woods' report, see [2].

3.3 Model parameters for compressive strength, dynamic Young's modulus and shear modulus

In HYMOSTRUC3D the contact areas between particles are calculated (see the concept of contact areas in [3]. The contact areas are used to calculate the compressive strength, Young's modulus and Shear modulus of cement paste (see Eq. (6) to Eq. (8)).

$$\sigma = 349.3A_{SEC} - 2.0049 \quad (6)$$

$$E = -402.25(A_{SEC})^2 + 206.63A_{c-eff} \quad (7)$$

$$G = -145.09(A_{SEC})^2 + 79.787A_{c-eff} \quad (8)$$

where σ [MPa], E [GPa] and G [GPa] are the calculated compressive strength, Young's modulus and Shear modulus of cement paste, respectively. A_{SEC} is the simulated specific effective contact area.

References

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Table 2 Equations to calculate the hydration parameters K_0 and δ_{tr} for different components of PC [Nguyen, 2011]

No.	Phase	K_0 [μm/h]	δ_{tr} [μm]	
1	C_3S	0.0635 + 0.0195×(1 - % C_3S)	2.1199 + 1.4707×(1 - % C_3S)	(1)
2	C_2S	0.0033 + 0.0020×(1 - % C_2S)	2.0730 + 1.1528×(1 - % C_2S)	(2)
3	C_3A	1.2118 - 1.1714×(1 - % C_3A)	2.3280 + 1.2758×(1 - % C_3A)	(3)
4	C_4AF	0.02	1.19	(4)

Table 3 Calculated hydration parameters K_0 and δ_{tr} for different components of PC particles

No.	Phase	K_0 [μm/h]	δ_{tr} [μm]
1	C_3S	0.071	2.696
2	C_2S	0.005	3.081
3	C_3A	0.091	3.549
4	C_4AF	0.020	1.190