Appendix A

Equations for Obtaining Some Parameters

A1. Equations for Obtaining Degree of Hydrations of Each Cement Compound

Seangsoy (2002) proposed the equations for calculating degree of hydration of each cement compound at a constant concrete temperature as the function of water to cement ratio and age. The equations are shown as follows.

$$\alpha_{C3A}(t) = \frac{100 \times \{1 - \exp[A \cdot \tan^{-1}\{B \cdot (wb)^{C} \cdot t\}]\}}{1 + \exp[\{D \cdot (wb)^{3} + E \cdot (w/b)^{2} + F \cdot wb + G\} \cdot \tan^{-1}(H \cdot t)]} \tag{A1}$$

$$\alpha_{C3S}(t) = \frac{100 \times \{1 - \exp[\{A/(B + \exp(C \cdot wb))\} \cdot \tan^{-1}(D \cdot t)]\}}{1 + \exp[\{E \cdot (wb)^{3} + F \cdot (wb)^{2} + G \cdot w/b + H\} \cdot t^{\{I/(J + \exp(K \cdot wb))\}}]} \tag{A2}$$

$$\alpha_{C2S}(t) = \frac{100 \times \{1 - \exp[\{A/(B + \exp(C\, wb))\} \cdot \tan^{-1}\{D\,(wb)^{E}\, t\}]\}}{1 + \exp[F \cdot t^{G}]} \tag{A3}$$

$$\alpha_{C4AF}(t) = \frac{100 \times \{1 - \exp[A \cdot \tan^{-1}\{B \cdot (wb)^{C} \cdot t\}]\}}{1 + \exp[\{D\,(wb)^{3} + E\,(wb)^{2} + F\, wb + G\} \tan^{-1}\{H\,(wb)^{I} t\}]} \tag{A4}$$

where $\alpha_{C3A}(t)$, $\alpha_{C2S}(t)$, $\alpha_{C2S}(t)$, and $\alpha_{C4AF}(t)$ are the degree of hydration at time considered of C_3A, C_3S, C_2S, and C_4AF, respectively (%). wb is the water to binder ratio. t is the age of concrete(days). The constant values (i.e. A, B, and C) used in these equations are shown in Table A1 to A4.

Table A1 Constant values used in the equation of degree of hydration of C_3A

T	Constant Values							
(°C)	A	B	C	D	E	F	G	H
10	-4.069	0.049	-0.422	10.095	-14.021	-0.966	0.785	0.334
20	-4.179	0.106	-0.471	7.927	-10.736	-2.570	0.921	0.694
30	-3.399	0.296	-0.553	2.127	-4.107	-4.986	1.088	1.559
40	-2.906	0.769	-0.747	-23.893	21.166	-12.903	1.772	2.873
50	-3.093	1.443	-0.904	-22.598	19.580	-12.705	1.715	3.580
60	-3.242	2.625	-1.088	-21.204	17.693	-12.255	1.614	5.721
70	-4.782	5.612	-1.096	10.309	-8.244	-5.787	1.029	6.892
80	-14.56	6.447	-65.038	16.914	-16.787	-2.703	0.609	12.237
90	-42.614	14.823	-88.549	-256.99	-169.62	124.70	-16.566	50.385

Table A2 Constant values used in the equation of degree of hydration of C_3S

T	Constant Values										
(°C)	A	B	C	D	E	F	G	H	I	J	K
10	-1.082	-0.995	0.014	0.004	-0.629	1.479	-4.657	0.925	0.217	0.439	-1.595
20	-1.671	-0.982	0.060	0.022	-18.35	26.42	-15.51	2.259	0.005	0.015	-12.79
30	-1.502	-0.898	0.273	0.230	-21.18	30.13	-17.67	2.578	0.004	0.010	12.91

40	-0.756	-0.997	0.008	0.022	1.922	0.177	-6.752	1.405	0.009	0.033	-11.43
50	-0.043	-0.998	0.010	0.727	-14.91	20.46	-15.22	2.447	0.002	0.005	-15.19
60	-0.034	-0.998	0.008	1.148	-5.173	7.352	-10.84	2.009	0.001	0.003	-16.73
70	-2.025	-0.900	0.347	1.700	-2.267	2.818	-9.755	1.944	0.001	0.003	-16.03
80	-5.610	-0.770	0.704	2.464	4.733	-5.768	-7.403	1.739	0.001	0.001	-21.85
90	-0.900	-0.955	0.033	2.500	29.08	-42.28	6.552	0.162	0.003	0.006	-11.18

Table A3 Constant values used in the equation of degree of hydration of C_2S

T	Constant Values						
(°C)	A	B	C	D	E	F	G
10	-0.104	0.0096	-6.537	0.019	-2.419	-1.587	0.270
20	-0.094	0.0075	-6.593	0.026	-2.650	-1.680	0.226
30	-0.089	0.0057	-6.560	0.039	-2.966	-1.239	0.313
40	-0.085	0.0042	-6.512	0.056	-3.304	-0.921	0.450
50	-0.081	0.0029	-6.511	0.072	-3.652	-0.851	0.539
60	-0.077	0.0016	-6.509	0.086	-4.053	-0.857	0.618
70	-0.071	0.0012	-6.618	0.110	-4.299	-0.913	0.689
80	-0.062	0.0007	-6.828	0.120	-4.622	-1.034	0.714
90	-0.058	0.0002	-6.942	0.126	-5.145	-1.158	0.769

Table A4 Constant values used in the equation of degree of hydration of C_4AF

T	Constant Values								
(°C)	A	B	C	D	E	F	G	H	I
10	-3.888	0.039	-0.381	27.130	-20.26	11.194	-1.899	-0.058	-1.952
20	-3.671	0.067	-0.487	14.122	-8.984	8.350	-1.731	-0.177	-1.074
30	-3.663	0.215	-0.158	-0.053	10.656	1.298	-1.031	-0.048	-1.880
40	-3.626	0.411	-0.135	7.971	6.050	2.082	-1.097	-0.048	-2.180
50	-3.518	0.651	-0.125	-11.70	-3.532	-2.745	1.190	0.064	-2.265
60	-3.455	1.002	-0.111	-15.73	-0.564	-3.616	1.313	0.085	-2.324
70	-3.410	1.485	-0.103	-27.77	9.639	-6.580	1.630	0.101	-2.476
80	-3.255	2.204	-0.199	-496.8	428.3	-127.3	12.831	0.016	-4.300
90	-3.316	3.185	-0.179	-602.9	523.1	-154.8	15.454	0.018	-4.368

A2. Equations for Obtaining Degree of Pozzolanic Reaction

The degree of pozzolanic reaction of paste is defined as the weight fraction of already reacted fly ash per total fly ash in the paste mixture. Seangsoy (2002) also proposed the equations for calculating the degree of pozzolanic reaction as the function of by water to binder ratio, contents of calcium oxide and silicon dioxide both in cement and fly ash, and fineness of fly ash. The equations are shown as follows.

$$\alpha_{poz}(t) = \frac{\tan^{-1}[(0.049 \cdot T^{0.496} - 0.186 \cdot wb - 0.135) \cdot t]}{\tan^{-1}[(0.049 \cdot T^{0.496} - 0.186 \cdot wb - 0.135) \cdot 365]} \cdot \alpha_{poz}(365) \quad \text{(A5)}$$

$$\alpha_{poz}(365) = \left[100 - \left\{ \begin{matrix} (102 - 0.1 \cdot T) \cdot (0.416 + 0.0088 \cdot wb^{-1.822}) \cdot \\ \tan^{-1}\left\{ (7.92\, wb^{-1.55} - 15.70) \left(\frac{SiO_2}{CaO_{eff}} - \frac{\%SiO_{2c}}{\%CaO_c} \right) \right\} \end{matrix} \right\} \right] \quad \text{(A6)}$$

$$\times \left(1 - \frac{\%LOI}{100} \right) \times \left[0.948 \cdot \tan^{-1}(7.227 \times 10^{-4} \cdot F_f) \right]$$

$$SiO_2 = [(W_c \cdot \%SiO_{2C}) + \varphi\,(W_f \cdot \%SiO_{2c}] / 100 \quad \text{(A7)}$$

$$CaO_{eff} = [(W_c \cdot \%CaO_C) + \varphi\,(W_f \cdot \%CaO_f)] / 100 \quad \text{(A8)}$$

$$\varphi = \frac{1 - \exp(-a \cdot \%CaO_f)}{1 + \exp(-a \cdot \%CaO_f)} \quad \text{(A9)}$$

$$a = 0.0048\,(F_f / 300)^{3.0734} + 0.0245 \quad \text{(A10)}$$

where $\alpha_{poz}(t)$, and $\alpha_{poz}(365)$ are the degree of pozzolanic reaction at any age of paste and at 365 days of paste, respectively (%). t is the age of paste (days). T is the concrete temperature (°C). w/b is the water to binder ratio. $\%CaO_c$, and $\%SiO_{2c}$ are the calcium oxide content and silicon dioxide content in cement, respectively (% by weight of cement). $\%CaO_f$, and $\%SiO_{2f}$ are the calcium oxide content and silicon dioxide content in fly ash, respectively (% by weight of fly ash). CaO_{eff} is the effective unit calcium oxide content in paste (kg/m^3). SiO_2 is the silicon dioxide content in paste (kg/m^3). W_c, and W_f are the weight of cement and fly ash in paste, respectively (kg/m^3). φ is the effectiveness of calcium oxide in fly ash, and F_f is the fineness of fly ash (m^2/kg).

A3. Equations for Obtaining Free Water Content

The free water content reduces with time due to water consumption in hydration process. Tangtermsirikul and Seangsoy (2002) and Seangsoy (2002) proposed the free water content at a certain age as in the following equation.

$$W_{free}(t) = W_t - W_{hp}(t) - W_{gel}(t) \tag{A11}$$

where $W_{free}(t)$, $W_{hp}(t)$, and $W_{gel}(t)$ are the weight of free water, weight of water consumed by hydration and pozzolanic reactions, and weight of gel water, respectively in the mixture at age t (kg/m3). W_t is the unit water content of the mixture (kg/m3). The weight of water consumed by hydration and pozzolanic reactions and the weight of gel water were proposed as follows.

$$W_{hp}(t) = (1-r)\cdot\theta_{hpc}\cdot W_c\cdot\frac{\alpha_{hy}(t)}{100} + r\cdot\theta_{hpf}\cdot W_f\cdot\frac{\alpha_{poz}(t)}{100} \tag{A12}$$

$$\begin{aligned} W_{wgel}(t) = &\left(0.013 + \frac{0.0026}{-1.01+\exp(0.14\,wb)}\right) W_c\,\frac{\alpha_{hy}(t)}{100} \\ &+ (6.18r^2 + 9.68r)(8.87\,wb^{8.44} + 0.12)\,W_f\,\frac{\alpha_{poz}(t)}{100} \end{aligned} \tag{A13}$$

$$\theta_{hpc} = 0.21 \tag{A14}$$

$$\theta_{hpf} = \frac{0.984}{3.688 + \exp(2.112\cdot r)} \tag{A15}$$

where θ_{hpc} is the minimum ratio of water to cement for completing hydration reaction. θ_{hpf} is the minimum ratio of water to pozzolanic material for attaining the maximum pozzolanic reaction (it is not possible to achieve 100 % degree of pozzolanic reaction). W_c and W_f are the weight of cement and fly ash in mixture, respectively (kg/m^3). r is the replacement ratio by weight of fly ash in total binder. wb is the water to binder ratio. α_{hy} (t) is the average degree of hydration of cement in the paste (%). α_{poz} (t) is the degree of pozzolanic reaction of fly ash in the paste at time t (%). t is the age of paste (days).

A4. Equations for Obtaining Average Pore Diameter and Porosity of Paste

Sumranvanich and Tangtermsirikul (2003) and Sumranvanich (2004) proposed the empirical equations for estimating the average pore diameter and the porosity of cement-fly ash paste. Those equations were formulated to have relationship with the average degree of reaction, water to binder ratio, fly ash to binder ratio, and some chemical composition in cement and fly ash as follows.

$$d(t) = \exp\left[7.5(wb-0.195)^{0.085} - 2.9(wb-0.195)^{-0.19} \times \frac{\alpha_{av}}{100}\right] \times \left[\frac{153}{F_c^{1.02}} + 0.53\right] \times \left[\left(\frac{C_3A}{100}\right)^{-0.06} - 0.14\right] \times \beta_{df} \quad \text{(A16)}$$

$$\beta_{df} = \begin{cases} 1 & \text{if } r = 0 \\ 1 - r(2.15-1.4r)\cdot(1.03-0.0033\cdot\%CaO_f & \text{if } r \geq 0 \end{cases} \quad \text{(A17)}$$

$$n(t) = [23.9\cdot\ln(wb) + 77.4] \times \frac{27.6}{26.5 + \exp\left[(0.86\cdot wb^{-1.43} + 1.2)\cdot\frac{\alpha_{av}(t)}{100}\right]} \times \left[\frac{153}{F_c^{1.02}} + 0.57\right] \times \left[\left(\frac{C_3A}{100}\right)^{-0.065} - 0.15\right] \times \beta_{nf} \quad \text{(A18)}$$

$$\beta_{df} = \begin{cases} 1 & \text{if } r = 0 \\ (1-0.25r^{0.5})\cdot(1.03-0.0033\cdot\%CaO_f & \text{if } r \geq 0 \end{cases} \quad \text{(A19)}$$

where d(t) and n(t) are the average pore diameter (nm) and the total porosity (% by volume), respectively of cement-fly ash paste at time t. $\alpha_{av}(t)$ is the average degree of reaction at time t (%). wb is the water to binder ratio. r is the fly ash to binder ratio. F_c is the Blaine fineness of cement (m^2/kg). C_3A is the content of C_3A in cement (%by weight of cement). $\%CaO_f$ is the calcium oxide content of fly ash (% by weight of fly ash). t is the age of paste (days).