2019.4.16.

①

월-오후
4~6.
샘플 thm

시멘트 구성 분석

- Bogue equation

$\% C_3S = 4.071C - 7.6S - 6.718A - 1.430F - 2.850\bar{S}$

$\% C_2S = 2.867S - 0.7544\, C_3S$

$\% C_3A = 2.650A - 1.692F$

$\% C_4AF = 3.043F$.

Oxide	#1	#3
S	21.1	21.1
A	6.2	4.2
F	2.9	4.9
C	65	65
$\bar{S}$	2.0	2.0
Rest	2.8	2.8

⇒

	#1	#3
C_3S	52.8	63.3
C_2S	20.7	12.7
C_3A	11.5	2.8
C_4AF	8.8	14.9.

- Gypsum.

$C\bar{S}$, $C\bar{S}H_2$, $C\bar{S}H_{0.5}$.

- Recently amorphous phase was reported in OPC. , CSA...
- Carbonation, Prehydration can be detected.
- Different polymorphs can be quantified.

Monoclinic C_3S, Rhombohedral C_3S ...

~~Ortho~~

Cement hydration

$2C_3S + 7H \rightarrow C_3S_2H_4 + 3CH$ $\quad \Delta H = -500\ J/g$

$2C_2S + 5H \rightarrow C\text{-}S\text{-}H + CH$ $\quad \Delta H = -250\ J/g$

$2C_3A + 21H \rightarrow C_4AH_{13} + C_2AH_8$

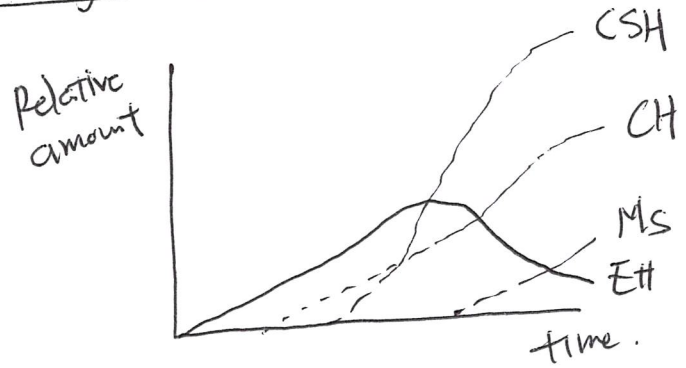
w/ $C\bar{S}$

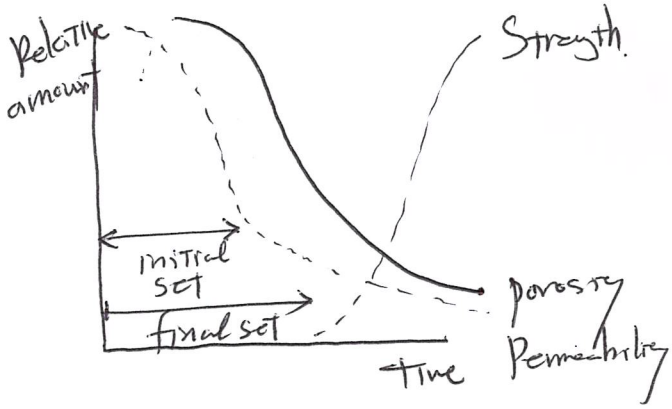
$C_3A + 3C\bar{S}H_2 + 26H \rightarrow C_6A\bar{S}_3H_{32}$

$2C_3A + C_6A\bar{S}_3H_{32} + 4H \rightarrow 3C_4A\bar{S}H_{12}$

Degree of Hydration

Mehta & Monteiro 37p.

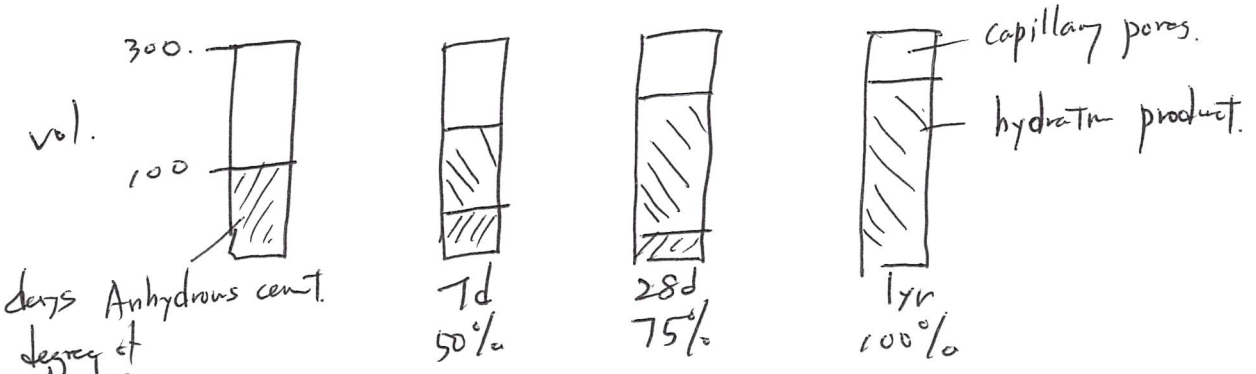




Case A:

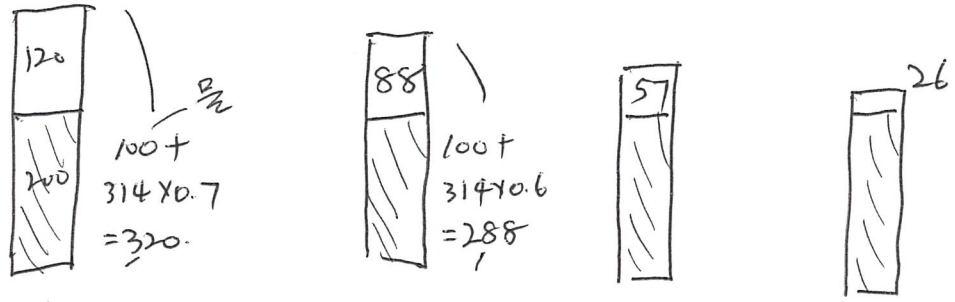
$100\ cm^3$ cement, $w/c = 0.63$

$\frac{V_w \cdot 1}{100 \cdot 3.14} = 0.63$, $V_w = 197.82\ cm^3$



		7d	28d	1yr
degree of Hydra.		50%	75%	100%
porosity	$\frac{200}{300} = 66\%$	50%	$\frac{125}{300} = 42\%$	$\frac{100}{300} = 33\%$

Case B: 100 cm³ of cement, 100% hydration.
varying W/C



W/C	W/C = 0.7	0.6	0.5	0.4
porosity =	$\frac{120}{320}$ = 37%	30% = $\frac{88}{288}$	22% = $\frac{57}{257}$	11% = $\frac{26}{226}$

$$\frac{\rho_w \cdot V_w}{\rho_c \cdot V_c} = 0.7 \; ; \quad \frac{1 \cdot V_w}{3.14 \cdot 100} = 0.7 \; ; \quad V_w = 0.7 \times 314$$

Quantitative XRD

} QXRD range. (cement : C_3S, C_2S, C_3A ... , hydrates ... : C-S-H, CH, Ett, MS ...)

28d.

75%

- Free water 제거 필수는 X.

- 전체 solid 영역에서의 상대 비율 구할 수 있다.

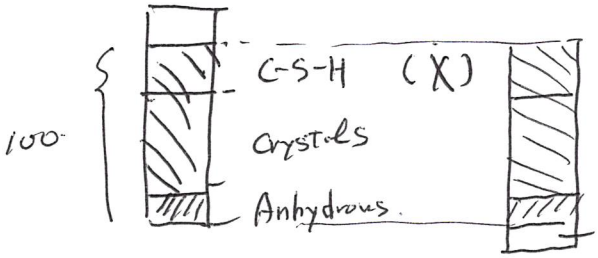
- 비결정질 구하는 방법. - Model base.
  - Internal standard
  - External standard.

- Model base

↕ hump. modeling. ; unit cell 결정, density 결정...

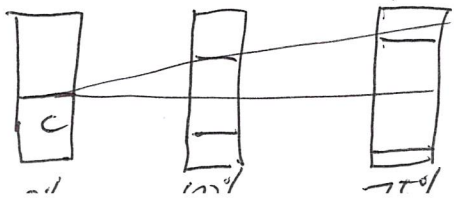
- cannot be applied for overlapped amorphous phase.

- Internal / External standard.



19% internal standard. Al_2O_3, TiO_2, ZnO ...

- Problem in time-dependent QXRD



Chemically bound water (BW)

Q.XRD

A	20%	20%/15% ×10 = 13.3	13.3 × 100/90 = 14.8
B	50%	50%/15% ×10 = 33.3	33.3 × 100/90 = 37
C	15%	15%/15% ×10 = 10	10 × 100/90 = 11.1
IS	15%	15%/15% ×10 = 10	
		56.7	

AC

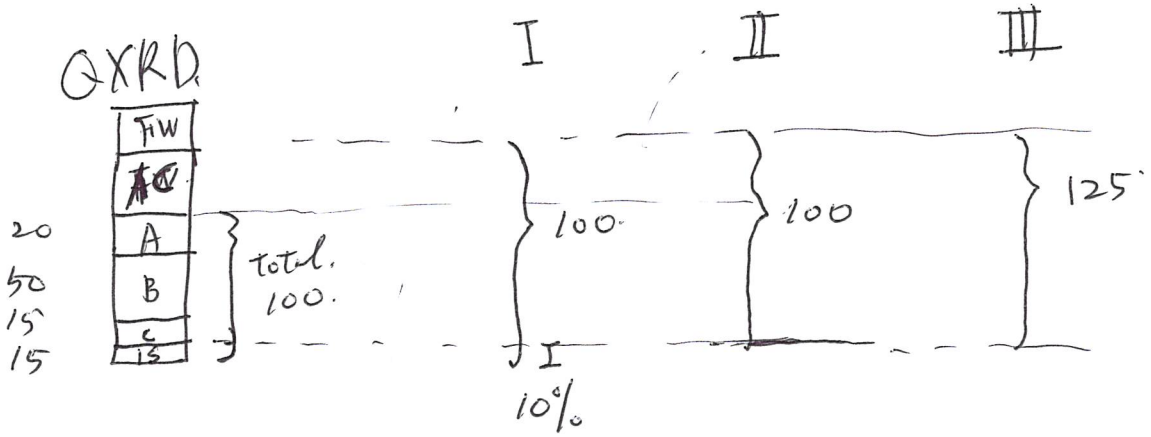
AC = 33.3 → 33.3 × 100/90 = 37

100 → 100

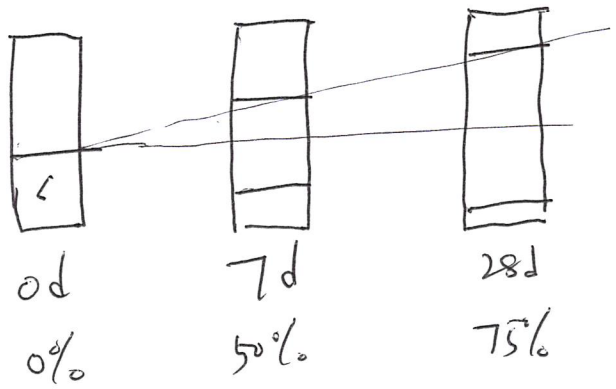
BW(%) = 20. 보정.

Normalize to anhydrous

A	14.8 / {(100−20)/100}	= 18.52
B	37 / "	= 46.3
C	11.1 / "	= 13.9
AC	37 / "	= 46.3
		125



- Problem in time-dependent QXRD



chemically bound water. (BW)

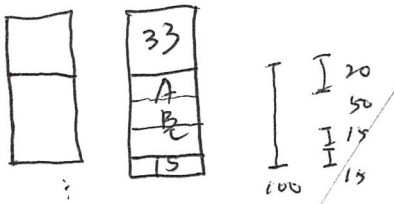
~~Example~~.

- W/ 10% IS, below QXRD result obtained.

A	20%
B	50%
C	15%
IS	15%

Amorphous content in (Solid + 10%) $= 100\% - \left(\frac{10\%}{15\%} \times 100 - 10\%\right) - 10\%$

$= 33\%$



Amorphous content $= 33 \times \frac{1}{0.9} = 37\%$

$A = \frac{20}{20+50+15+33} = 17\%$

$B = \frac{50}{20+50+15+33} = 42\%$

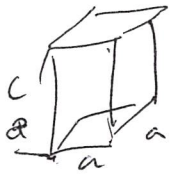
$C = \frac{15}{20+50+15+33} = 13\%$

Unit cell vol. from XRD

Bravais symmetry

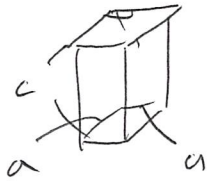
Cubic : $\frac{1}{d^2} = \frac{h^2+k^2+l^2}{a^2}$

unit cell vol. $V = a^3$



Tetragonal : $\frac{1}{d^2} = \frac{h^2+k^2}{a^2} + \frac{l^2}{c^2}$

$V = a^2c$



120° Hexagonal / Trigonal : $\frac{1}{d^2} = \frac{4}{3}\left(\frac{h^2+hk+k^2}{a^2}\right) + \frac{l^2}{c^2}$

$V = \frac{\sqrt{3}a^2c}{2}$

$Ca(OH)_2$	(h, k, l)	d.	Int.	
	0 0 1	4.911	292	$\rightarrow c = 4.911$.
	1 0 0	3.10817	73	
	1 0 1	2.62635	584	
	0 0 2	~~2.655~~ 2.4556.	12	$c^2 = l^2 \cdot d^2$.