

### The effect of impurities on the calculation of dehydroxylation fractions

The impurities of kaolinite have a potential impact on the calculation of dehydroxylation fraction, although it was not involved in the calculation in the previous paper as the authors know. In this paper, the dehydroxylation fractions were calculated according to the following equation.

$$\delta = \frac{\Delta m}{m_T} \times 100\%$$

$$\theta = 1 - \frac{\delta_a}{\delta_b} \times 100\% = 1 - \frac{\delta_a}{14\%} \times 100\%$$

Where  $\Delta m$  is the mass loss above 150°C,  $m_T$  is the mass of sample, and  $\delta$  is the mass loss fraction of sample.  $\delta_a$  is the mass loss fraction of calcination product and  $\delta_b$  is the mass loss fraction of kaolinite without calcination (14% in this paper). If there are no impurities in kaolinite, all the mass loss was entirely derived from dehydroxylation. Therefore,  $\delta_a$  is the mass fraction of the residual hydroxyl groups in the product while  $\delta_b$  is the mass fraction of all the hydroxyl groups in the kaolinite, and  $\theta$  is the dehydroxylation fraction under ideal condition without impurities.

Now let's consider the condition of the existence of impurities. The mass fraction of the residual hydroxyl groups in the product and the mass fraction of all the hydroxyl groups in the kaolinite are modified as follows.

$$\begin{aligned} \delta' &= \frac{\Delta m - m_T \cdot \beta \cdot (1 - \eta) \cdot \gamma}{m_T \cdot (1 - \beta)} = \frac{1}{1 - \beta} \cdot \delta - \frac{\beta \cdot (1 - \eta) \cdot \gamma}{1 - \beta} \\ \delta'_a &= \frac{1}{1 - \beta} \cdot \delta_a - \frac{\beta \cdot (1 - \eta) \cdot \gamma}{1 - \beta}, \quad \delta'_b = \frac{1}{1 - \beta} \cdot \delta_b - \frac{\beta \cdot (1 - \eta) \cdot \gamma}{1 - \beta} \\ \theta' &= 1 - \frac{\delta'_a}{\delta'_b} = \frac{\delta'_b - \delta'_a}{\delta'_b} = \frac{\frac{1}{1 - \beta} \cdot (\delta_b - \delta_a)}{\frac{1}{1 - \beta} \cdot \delta_b - \frac{\beta \cdot (1 - \eta) \cdot \gamma}{1 - \beta}} = \frac{\delta_b}{\delta_b - \beta \cdot (1 - \eta) \cdot \gamma} \cdot \theta = \frac{14\%}{14\% - \beta \cdot (1 - \eta) \cdot \gamma} \cdot \theta \end{aligned}$$

Where  $\beta$  is the proportion of impurities in sample,  $\eta$  is the proportion of impurities volatilized during flash calcination and  $\gamma$  is the proportion of impurities volatilized in TG. Because  $\beta$  cannot be obtained, we evaluated its range as follows.

$$\begin{aligned} \frac{0}{m_K - 40\% \cdot m_K \cdot 14\%} < \beta = \frac{m_I}{m_T} < \frac{2\% \cdot m_K}{m_K - 95\% \cdot m_K \cdot 14\%} \\ 0 < \beta < 2.3\% \end{aligned}$$

Where  $m_I$  is the mass of impurities in sample and  $m_K$  is the mass of kaolinite without calcination corresponding to  $m_T$ . The minimum value of  $\beta$  is obtained when the denominator is the largest and the numerator is the smallest. The minimum value of  $\beta$  is obtained when the denominator is the largest and the numerator is the smallest. The corresponding situation is that all the impurities volatilized during flash calcination without residual part in product. The maximum value of  $\beta$  is obtained when the denominator is the smallest and the numerator is the largest. The corresponding situation is that all the impurities were left in product without volatilization during flash calcination (in this paper, the purity of kaolinite was estimated higher than 98% according to the Si/Al mole ratio), and 95% of the hydroxyl groups were removed during flash calcination (95% is the maximum

dehydroxylation fraction in this paper). Consequently, the range of  $\beta$  is from 0 to 2.3%. Considering  $0 < (1-\eta) \cdot \gamma \leq 1$ , the range of the modification factor of dehydroxylation fraction is from 1 to 1.2.

$$\theta \leq \theta' = \frac{14\%}{14\% - \beta \cdot (1-\eta) \cdot \gamma} \cdot \theta \leq 1.2\theta$$

For different products,  $\beta$ ,  $\eta$  and  $\gamma$  are different, so it is unable to use a constant factor to modify all the dehydroxylation fractions. Moreover, these factors are in an acceptable range. Therefore, this paper has to ignore the effect of impurity, otherwise it will not be able to calculate the dehydroxylation fractions and the next kinetics parameters. Maybe it is also the reason why the previous research ignored the effect of impurity on dehydroxylation calculations.