

# Modeling of cement-based materials submitted to sulfate attack

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## Objective

External sulfate attack (ESA) and delayed ettringite formation (DEF) are well-known concrete degradation phenomenon induced by crystallization of ettringite. This paper aims to propose a model, based on the homogeneous paste expansion and surface-controlled ettringite growth mechanism, explaining the both phenomenon in a uniform method. The driving force for this mechanism is the pore pressure from the supersaturated sulfate solution, which leads the ettringite forming from the largest pores to the smallest ones, no matter it is in capillary pores (ESA) or gel pores (DEF).

## Modeling

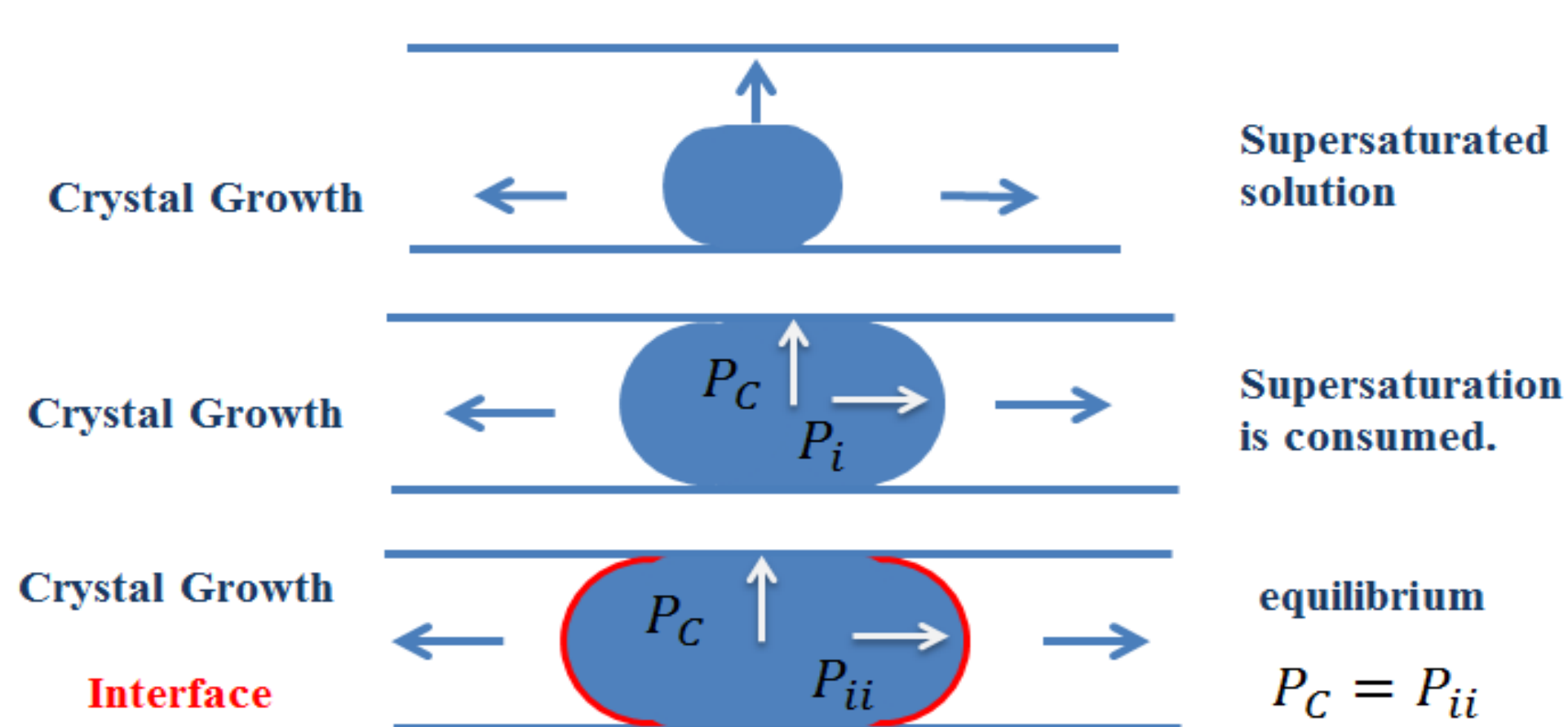


Fig. 1 Crystallization evolution

Poroelasticity theory:

$$\varepsilon_{xx} = \frac{b}{3K} S_C P_C$$

Correns' equation<sup>[1]</sup>:

$$P_C = \frac{RT}{V_C} \ln(\beta_{Aft})$$

Ostwald-Freundlich Equation:

$$\varepsilon_{xx} = \frac{b}{3K} S_C P_C$$

Growth rate mechanism:

$$\frac{d}{dt}(S_C) = a(1 - \exp(-\frac{\beta_{Aft}^{eq}}{\beta_{Aft}}))$$

a: kinetic constant (calibrated)

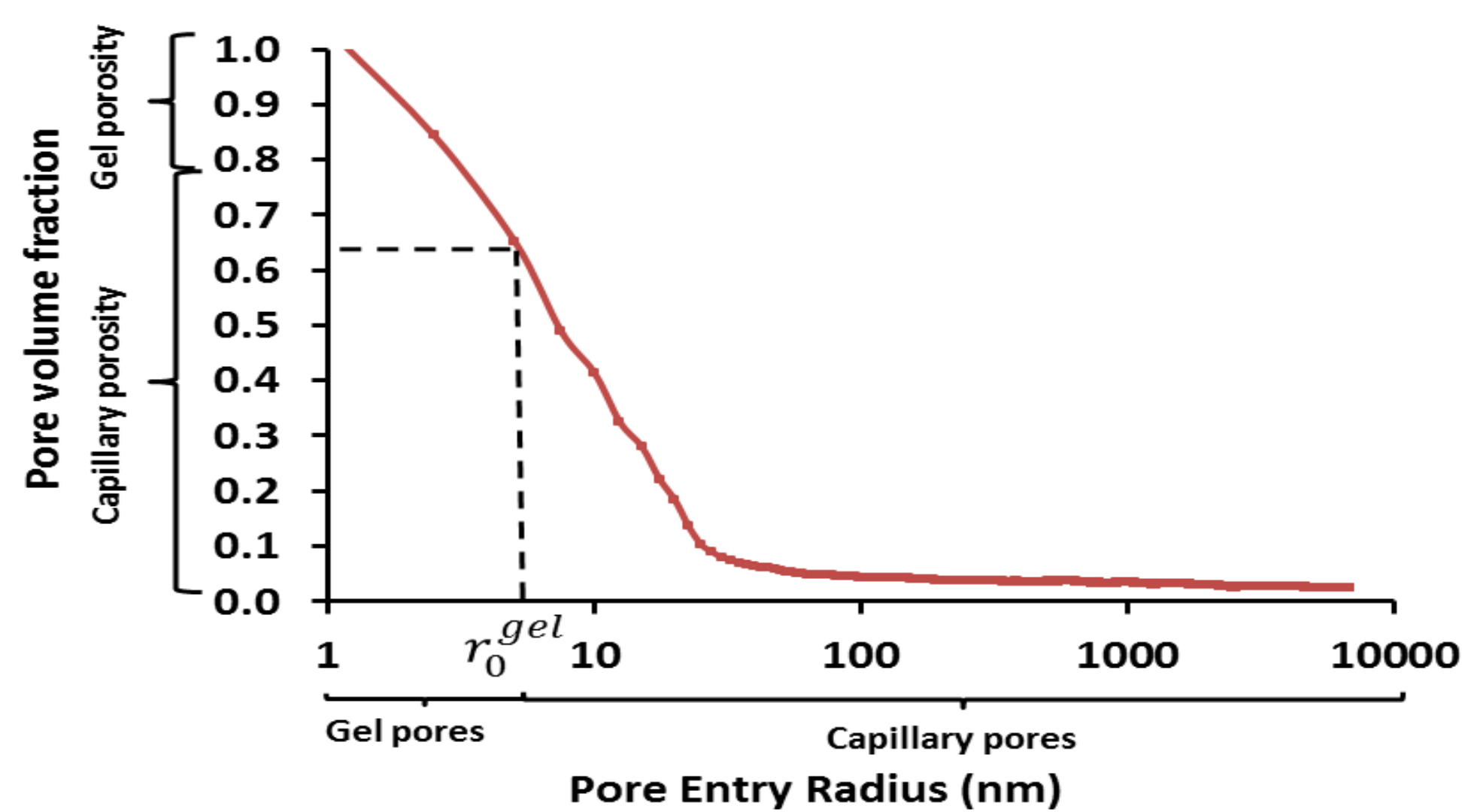


Fig. 2 Evolution of the pore volume fraction with the pore radius

Assumption:

Ettringite (ESA) in capillary pores:

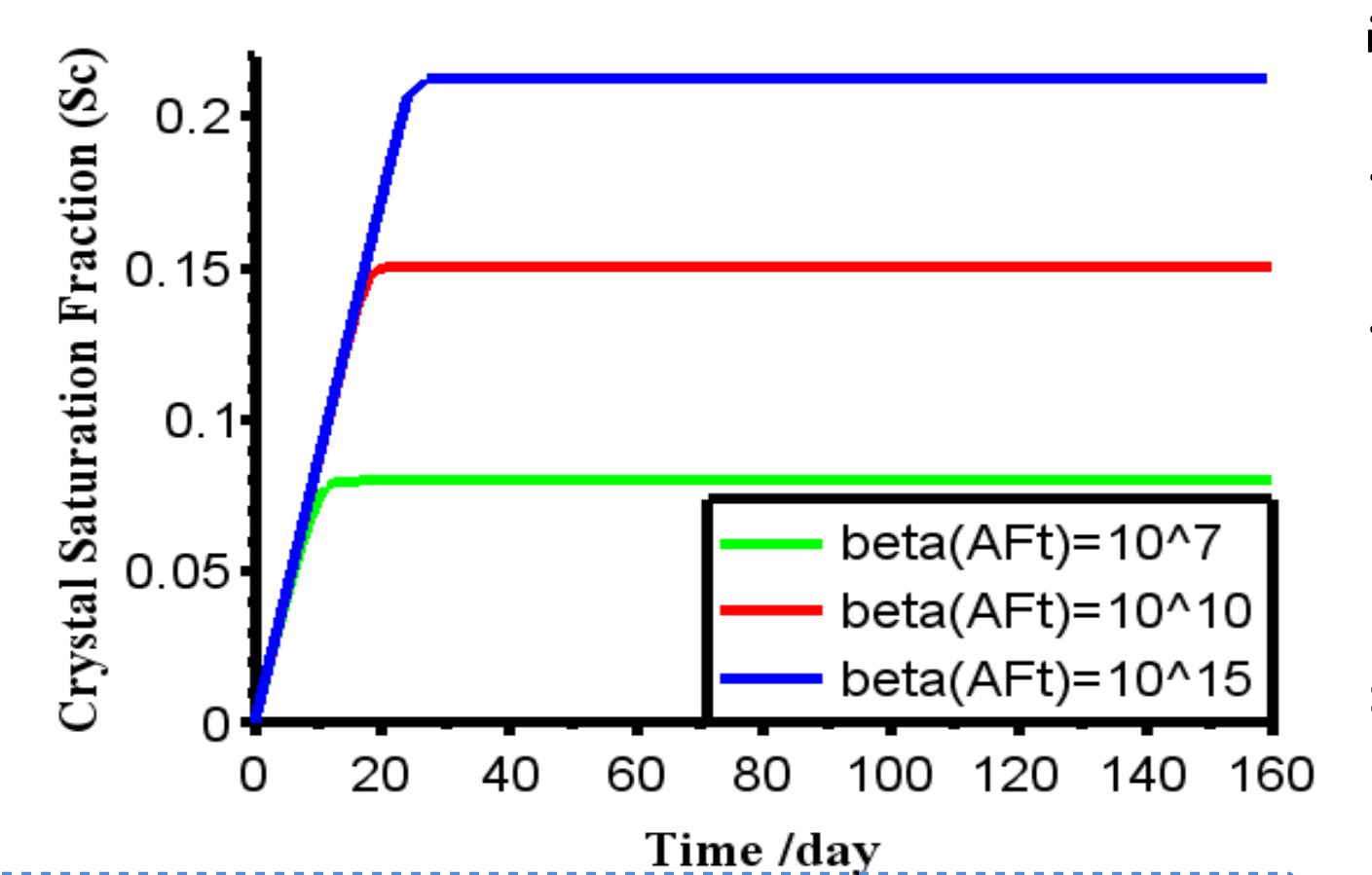
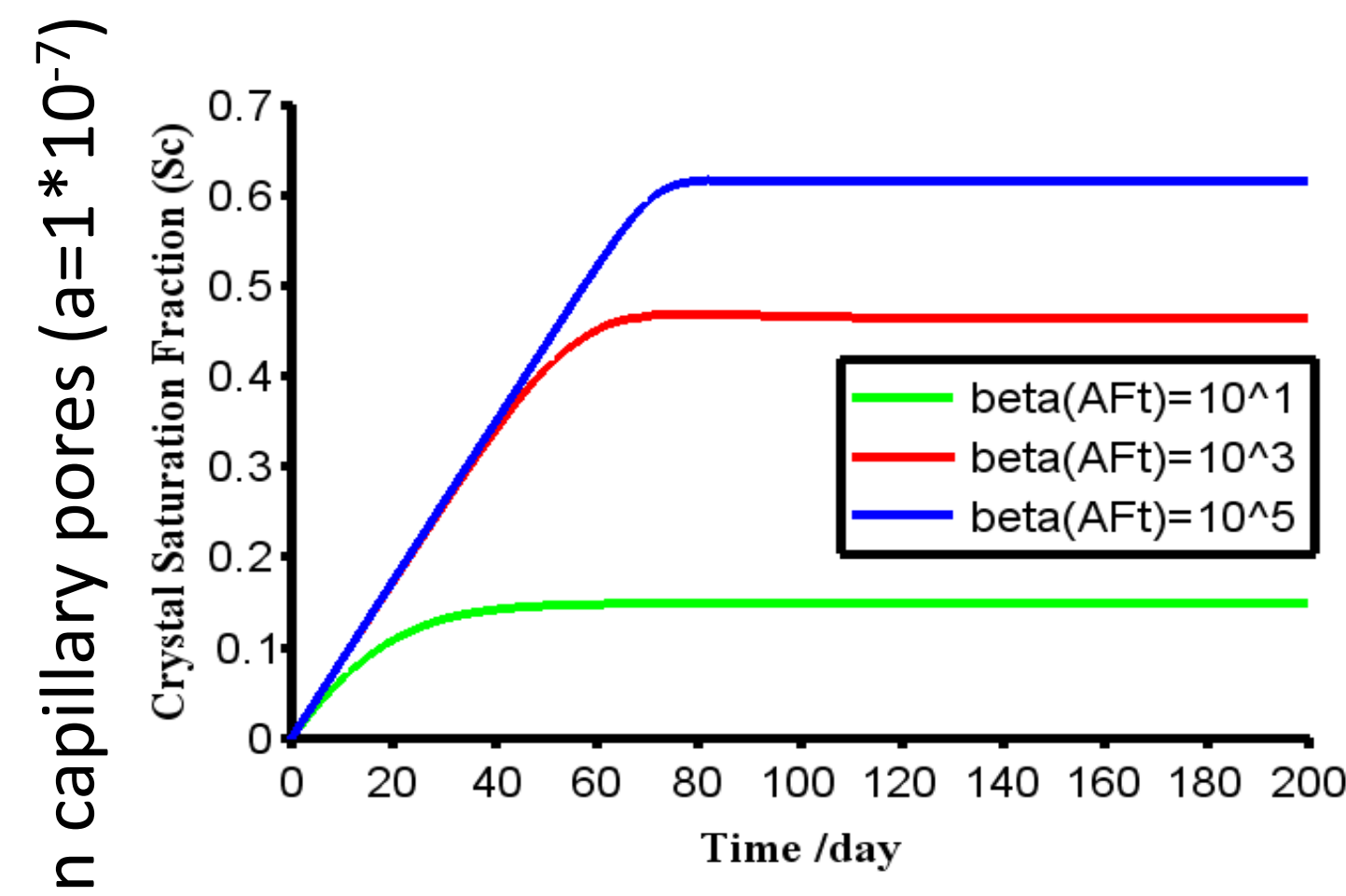
$$S_C^{cap}(r) = 1 - S(r) \quad r > r^{gel}$$

Ettringite (DEF) in gel pores:

$$S_C^{gel}(r) = S(r^{gel}) - S(r) \quad r < r^{gel}$$

$S(r)$  represents the volume fraction occupied by pores having a pore entry radius lower than  $r$ .

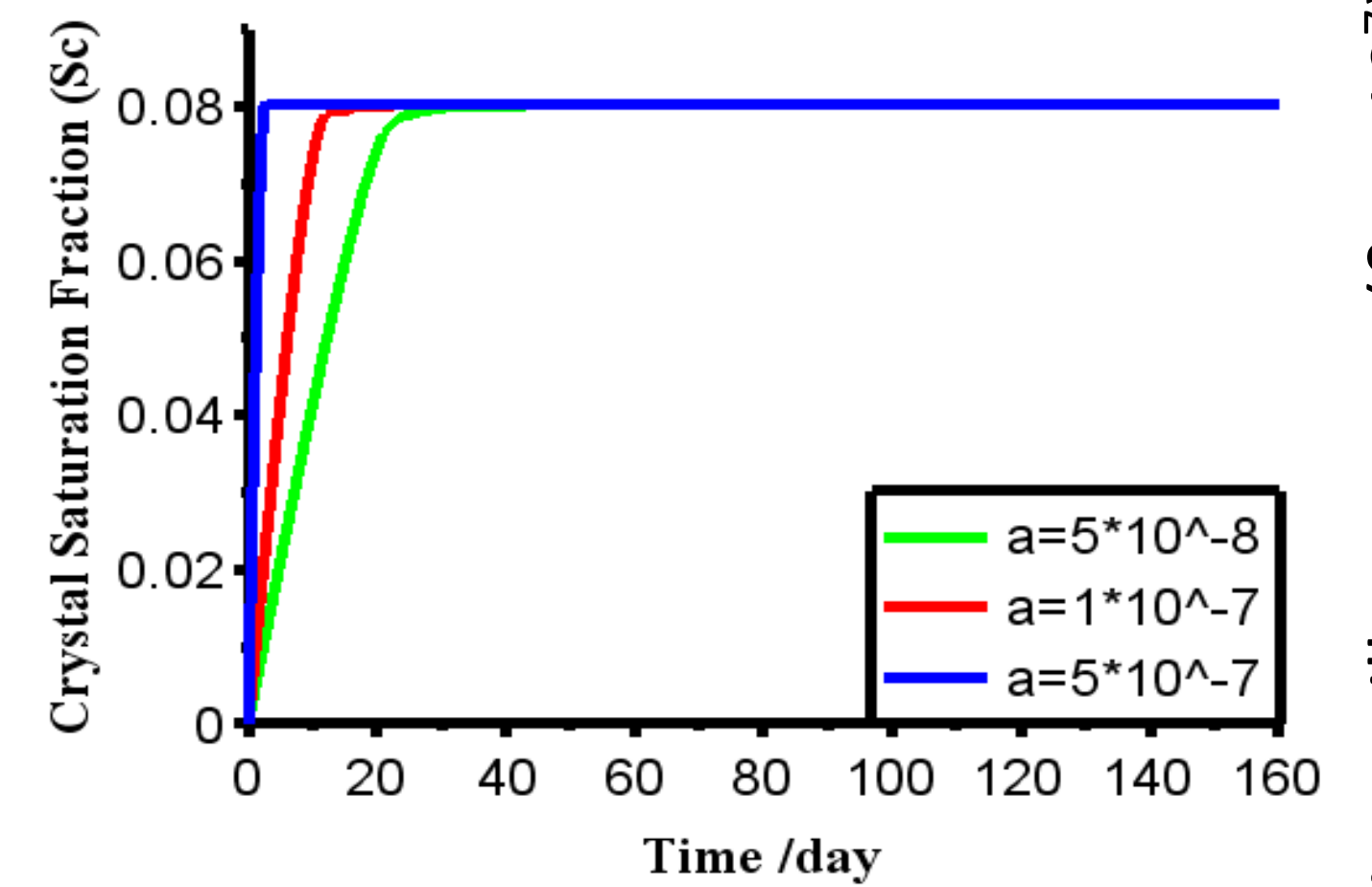
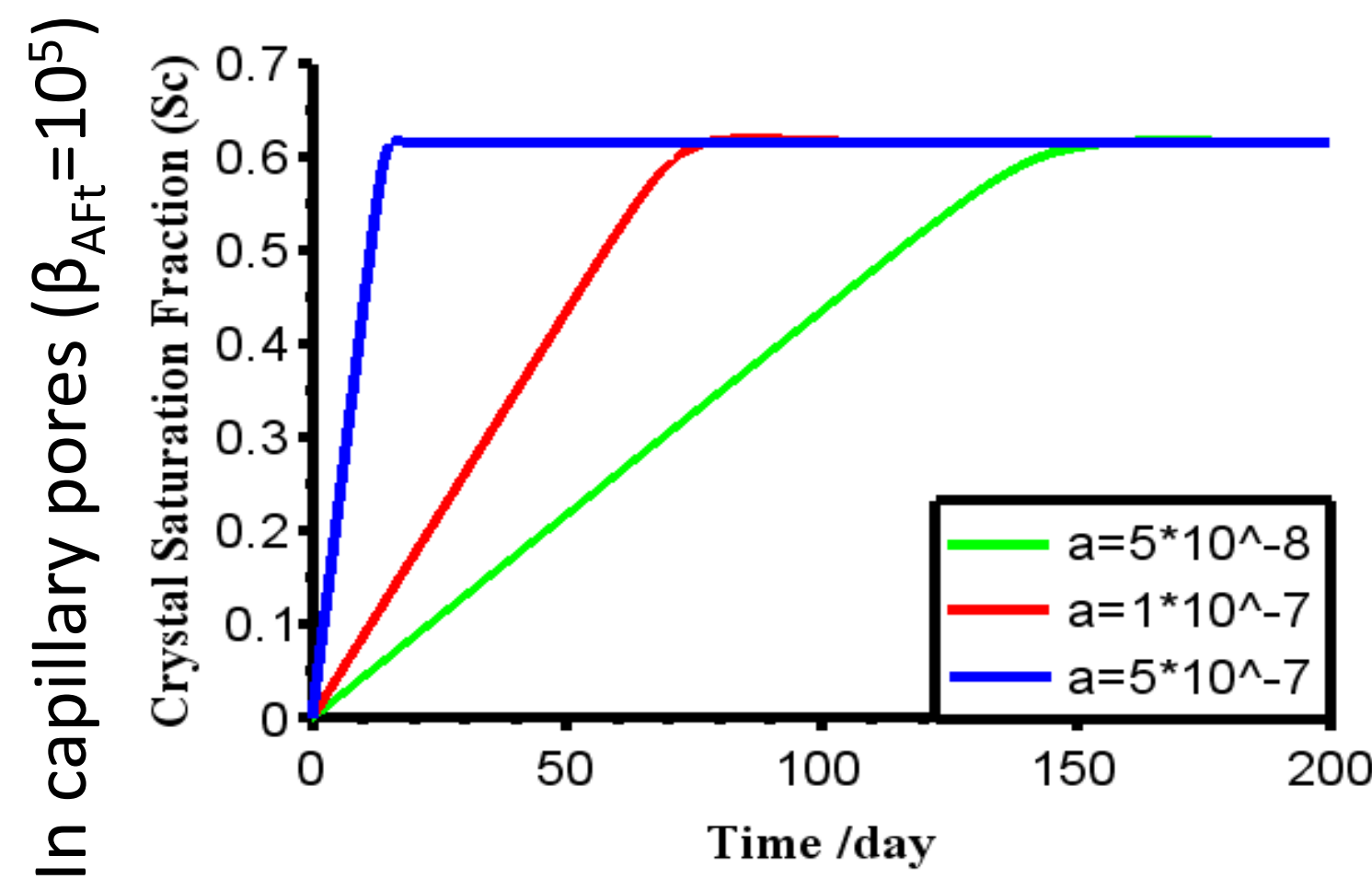
## Sensitivity analysis



Conclusion:

$S_C^{final}$  is determined by  $\beta_{Aft}$  only.

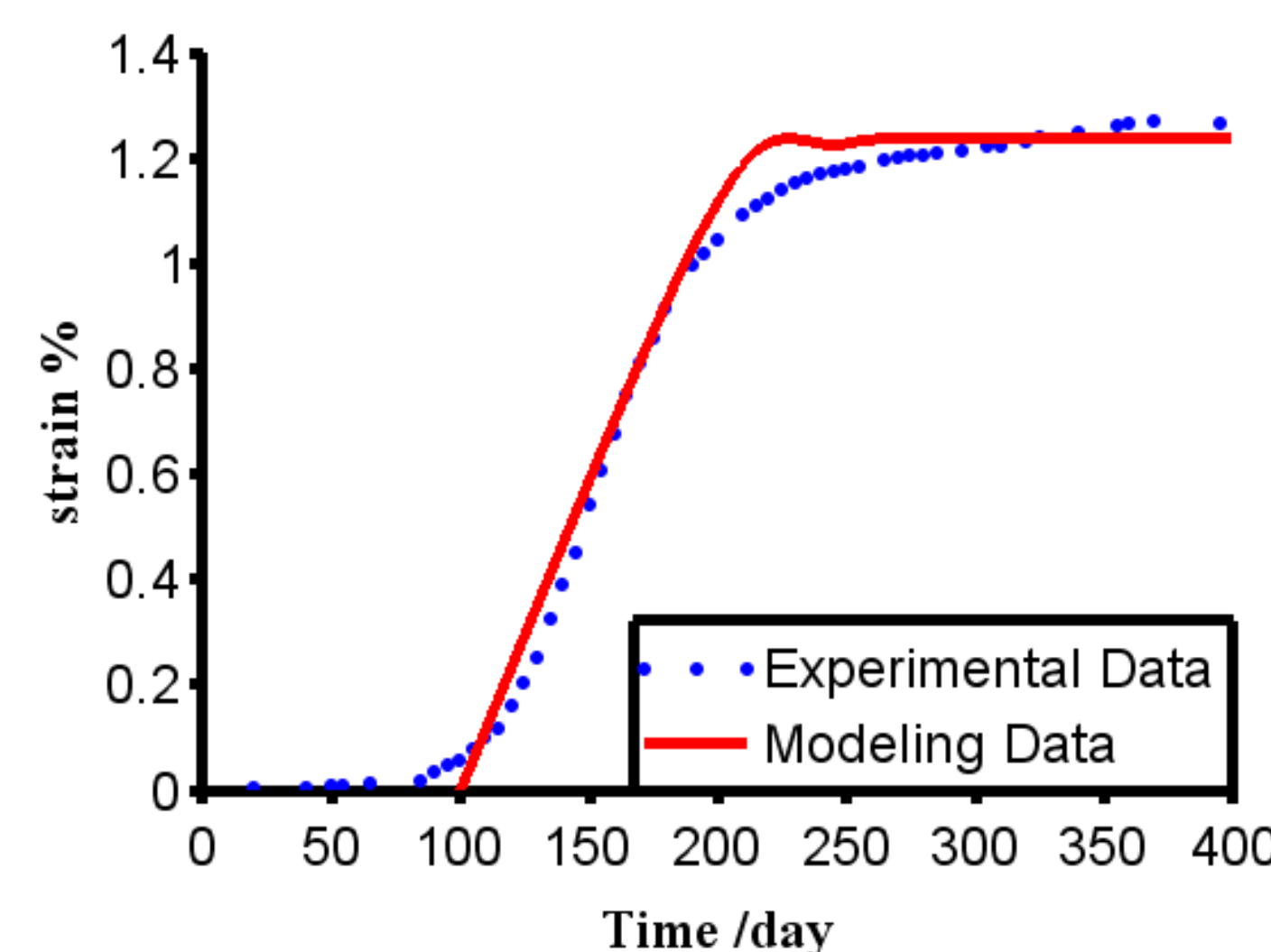
In addition to Correns' equation, the  $\beta_{Aft}$  could be calibrated by final swelling.



## Comparison Results

DEF<sup>[2]</sup> Mortar bars: 16 \* 16 \* 160mm<sup>3</sup>

Preheating: 20 C for 4h, 90 C for 12 h (with heating rates of 30-35 C/h), cool naturally to 20 C over about 5 h and in water afterwards.

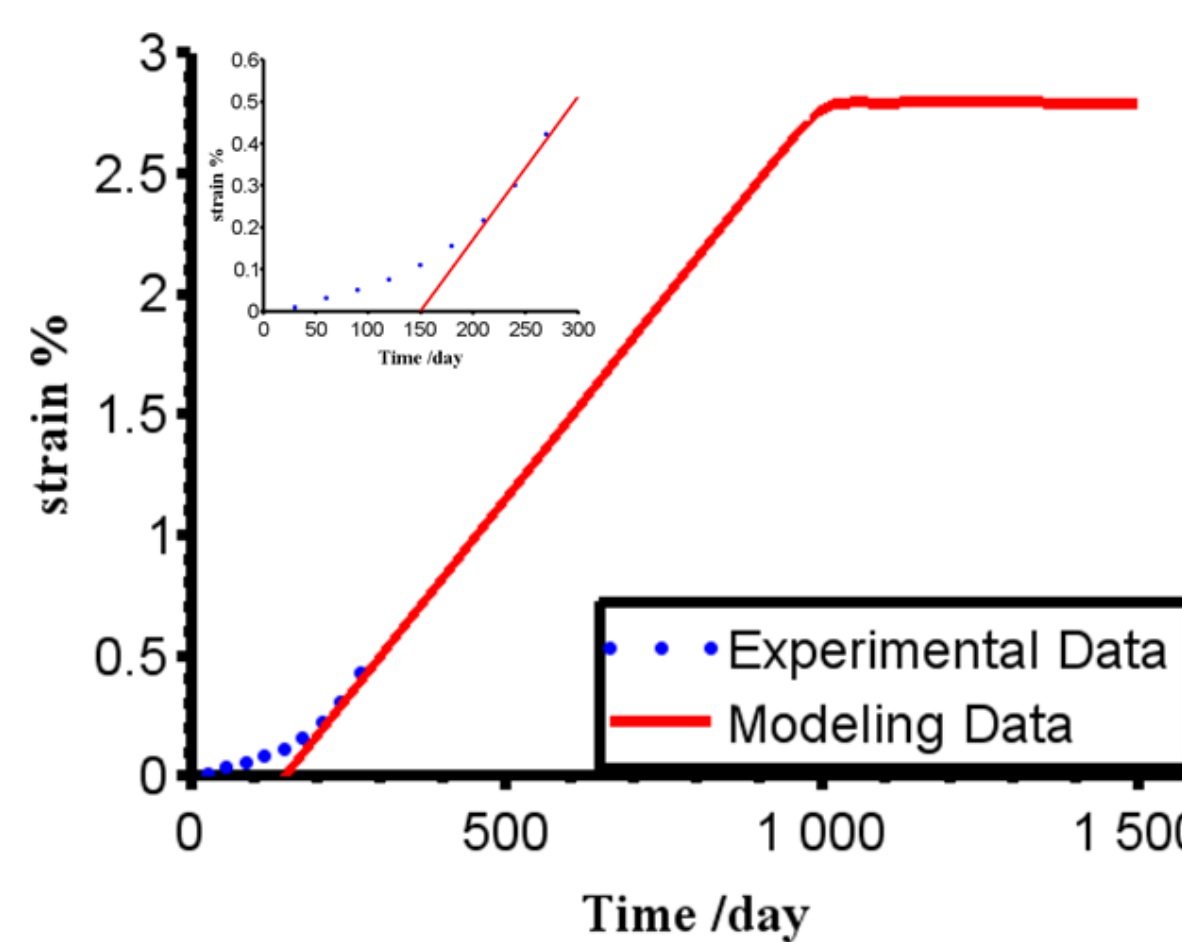


Storage conditions: a) 20°C

$a_1 = 1.25 \cdot 10^{-8}$ ,  $\beta_{Aft} = 10^{8.2}$ ,  $K = 0.2\text{GPa}$ ,  $b = 1$

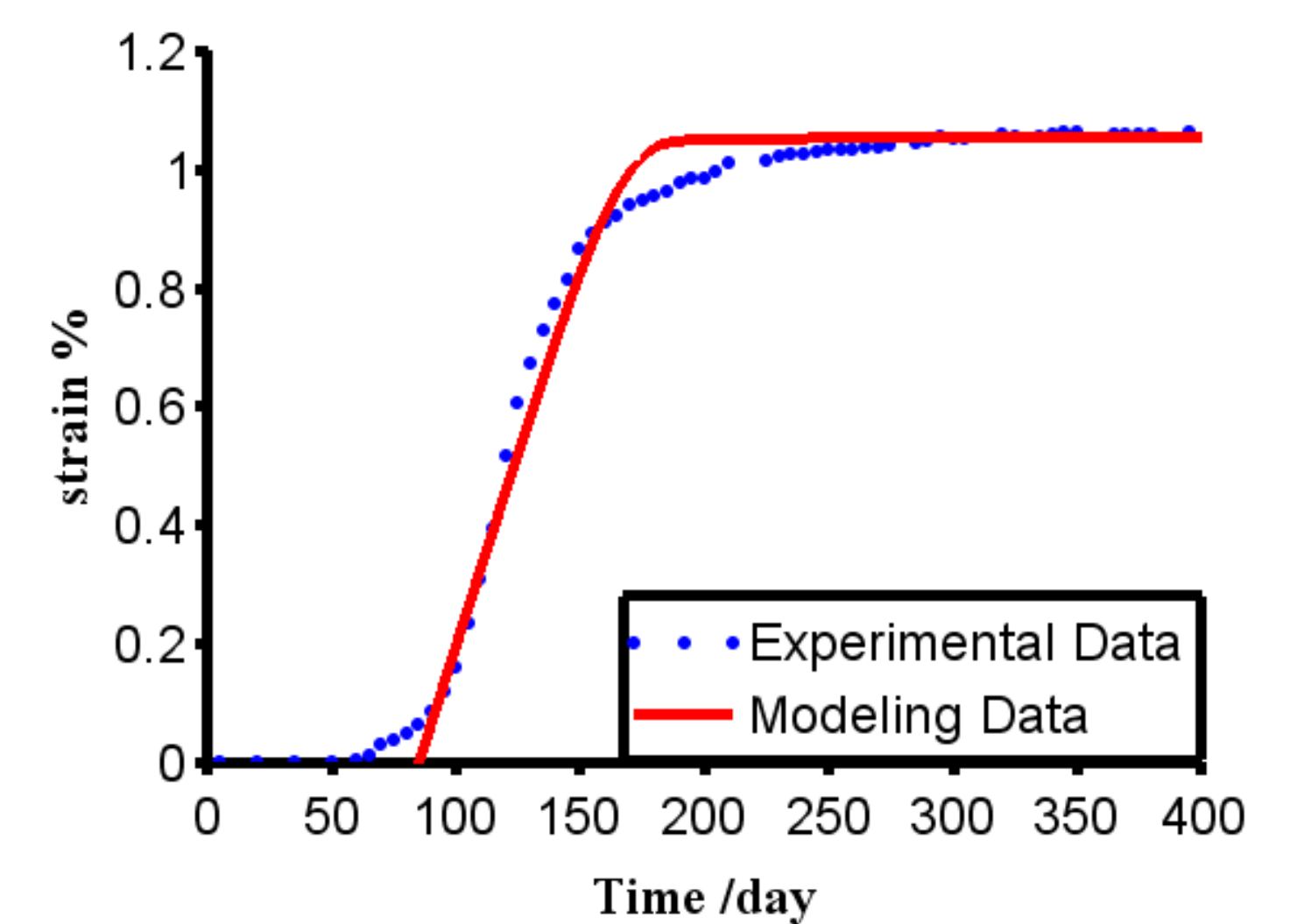
ESA<sup>[3]</sup>

Sulfate solution: 4.3% magnesium sulfate and 2.5% sodium sulfate (by weight)



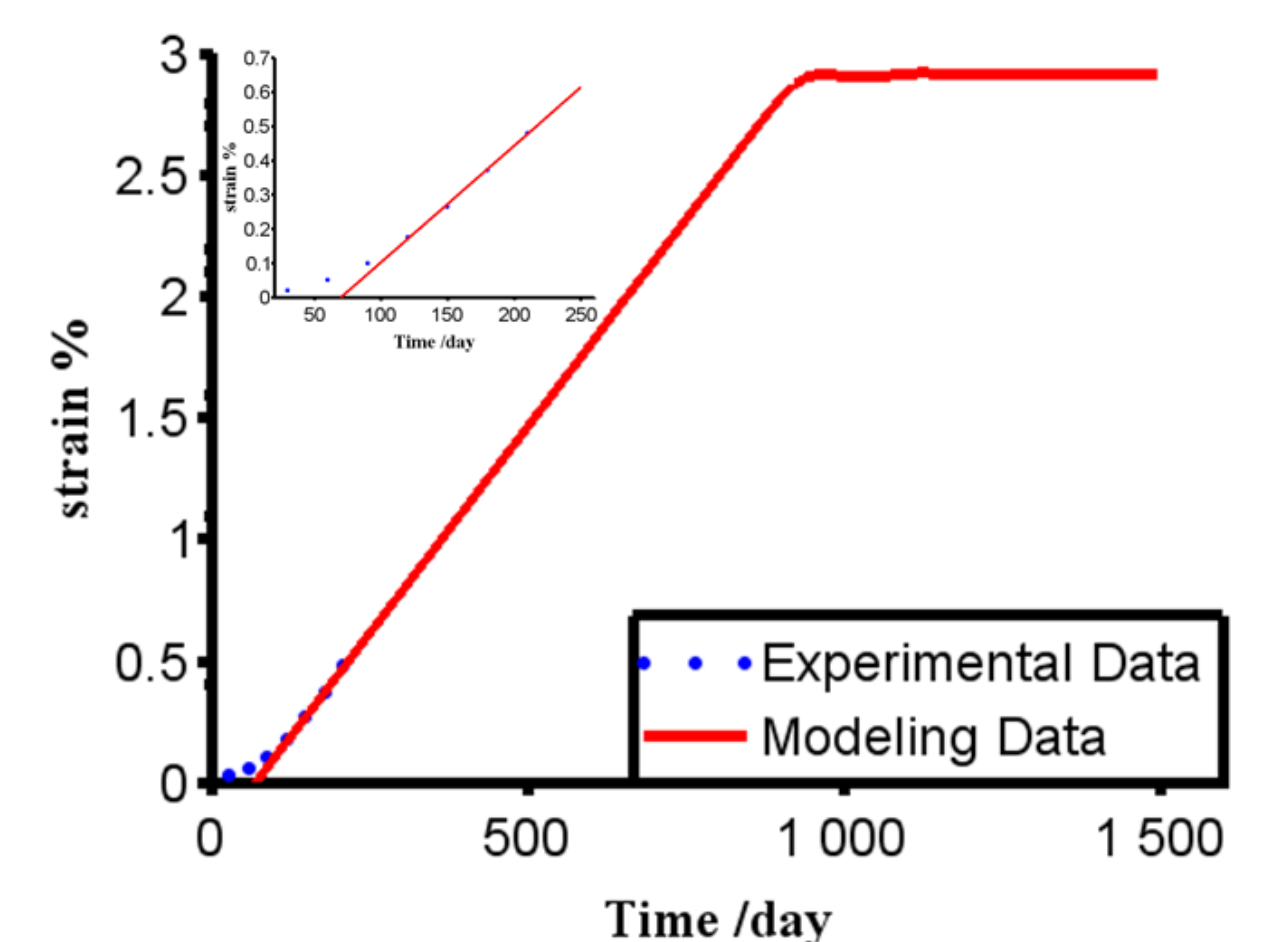
$C_3A$  content (weight) : 8.8%

$a_1 = 1 \cdot 10^{-8}$ ,  $\beta_{Aft} = 10^{8.8}$ ,  $K = 0.6\text{GPa}$ ,  $b = 1$



b) 20°C 98 days and then 38°C.

$a_2 = 1.5 \cdot 10^{-8}$ ,  $\beta_{Aft} = 10^{7.75}$ ,  $K = 0.2\text{GPa}$ ,  $b = 1$



$C_3A$  content (weight) : 12%

$a_2 = 1 \cdot 10^{-8}$ ,  $\beta_{Aft} = 10^{8.8}$ ,  $K = 0.6\text{GPa}$ ,  $b = 1$

## Discussions

- The calibrated  $\beta_{Aft}$  for DEF is between  $10^{7.5}$  to  $10^{8.5}$ , and  $10^{8.2}$  to  $10^{8.5}$  for ESA, which are acceptable.
- The bulk modulus used in the model are 0.2 and 0.6GPa, which are smaller than the predicted ones. A plasticity theory is considered to modify this model.
- The diffusing and leaching of the ions contribute to the saturation index of ettringite. This effect will be added into the model in the further step.

## References:

[1]Correns, Carl W. "Growth and dissolution of crystals under linear pressure." *Discussions of the Faraday society* 5 (1949): 267-271.

[2] Famy, Charlotte. *Expansion of heat-cured mortars*. Diss. Imperial College London (University of London), 1999.

[3] Ouyang, Chengsheng, Antonio Nanni, and Wen F. Chang. "Internal and external sources of sulfate ions in Portland cement mortar: two types of chemical attack." *Cement and Concrete Research* 18.5 (1988): 699-709.