Chemo-Mechanical Micro Model for Alkali-Silica Reaction

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Acknowledgments

Context

- AAR Modeling: Micro (one aggregate), meso (few aggregates) or macro (structure).

- Micro model brings together two disciplines:

  Material scientists who pretend to know about mechanics.
  Structures Engineers who pretend to know about materials.

  and thus is never perfect ☹

- This presentation
  - Falls in the second category.
  - The model presented is just a model, not 100% correct, neither complete, with some assumptions.
  - Just another paper ☺

- Presentation will be coarse grained, details are left to the article.

Objective/Approach I

Objective Simulate the response of a non reactive mortar bar test starting from the simulation of the gel formation and expansion of a single aggregate.

Approach to the study

- 1. Macro diffusion of ion into a mortar bar
- 2. Micro ion diffusion into a single aggregate
- 3. Formation of gel a) Fill up the pores; b) stress induced expansion
- 4. Randomly locate reactive aggregate inside the bar
- 5. Finite Element analysis of reactive bar with expanding aggregates.
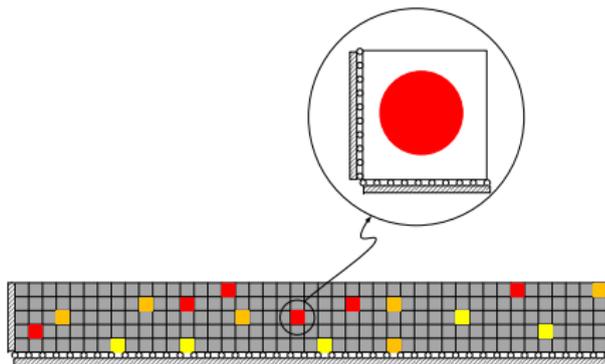
Objective/Approach II

1. select mortar bar size (*L* and *H*) for each aggregate size of reactive aggregate
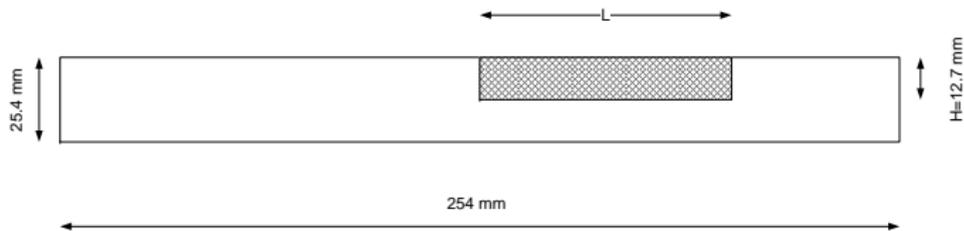
Aggregate size	Diameter (mm)	Micro-model size (RVE) mm	Dist. between agg. and RVE bound.	L (mm)	# of vertical elem. in FE Mesh, n_v
No. 8	2.36	3.335	0.487	126.7	4
No. 16	1.18	1.668	0.244	126.8	8
No. 30	0.60	0.849	0.125	127.4	15
No. 50	0.30	0.426	0.063	126.9	32
No. 100	0.15	0.214	0.032	31.7	64
No. 200	0.075	0.108	0.0167	8.4	128
No. 400	0.038	0.058	0.009	4.1	256

Objective/Approach III

2. The size of element corresponds to the size of the REV (aggregate size dependent) of reactive ASR in the micro model
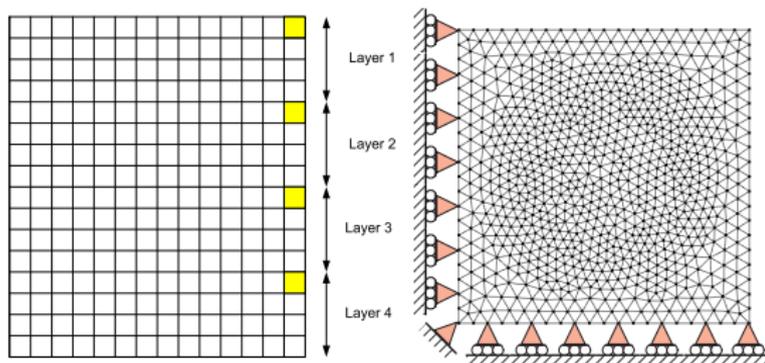

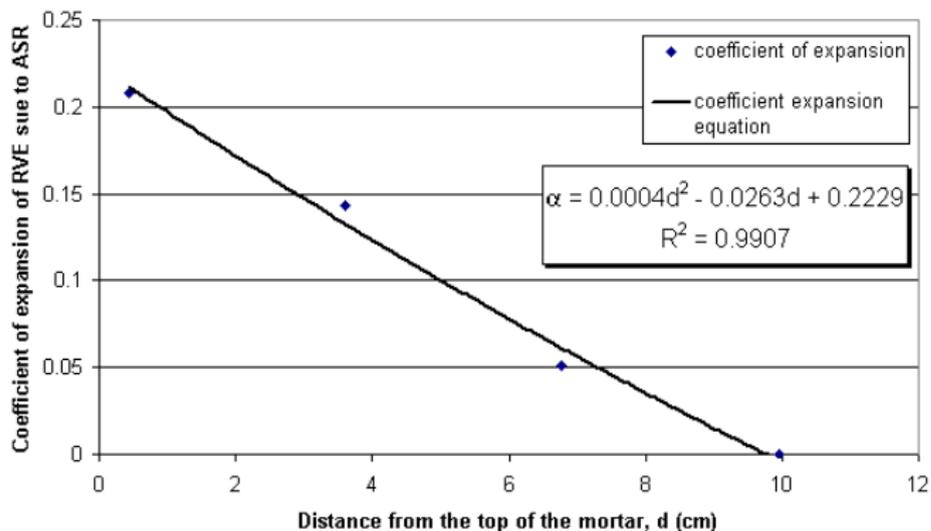3. Perform a macro diffusion analysis of ion into the mortar bar
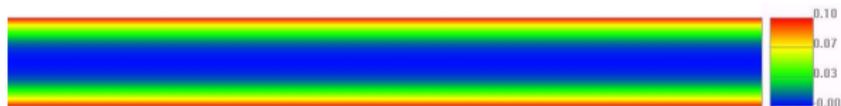
Objective/Approach IV

4. Select four locations, and for each one perform coupled stress (finite element) and diffusion (finite difference) for one reactive cell
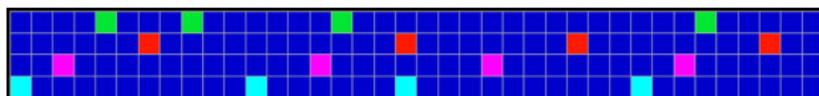
Objective/Approach V

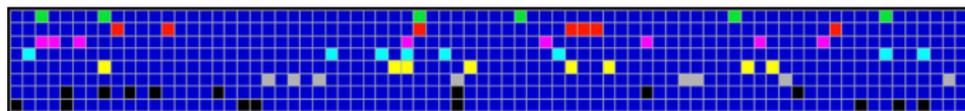**5** Curve fit the expansion in terms of elevation
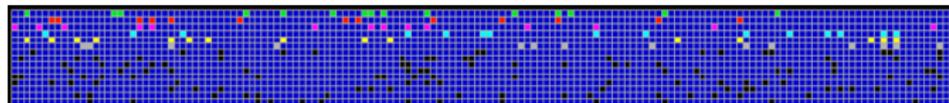
Objective/Approach VI

⑥ Perform a stress analysis of the entire bar with 10% of reactive aggregates randomly distributed. Reactive aggregates will be assigned an equivalent thermal strain from the curve fitted expansion curve.
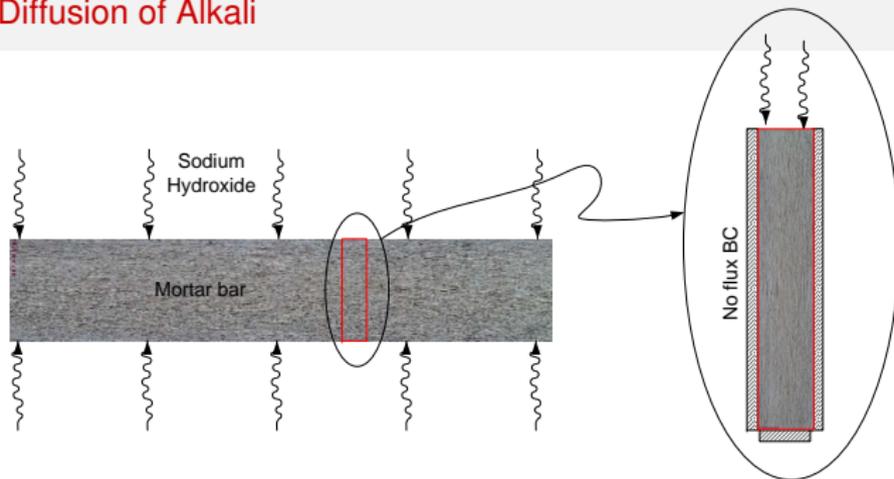

No. 8 Mortar bar

No 16 Mortar bar

No 30 Mortar bar

⑦ Determine the expansion of the bar, and corresponding anisotropic AAR strain tensor

1. Macro-Ion Diffusion of Alkali

- Mortar bar composed of non-reactive cement
- Diffusion of sodium-hydroxide into mortar bar
  $B_{ion,macro} \frac{\partial C_{ion}}{\partial t} = \nabla(D_{ion,macro}(C_{ion})\nabla C_{ion})$ Finite difference grid (3x31)
- C_{ion} is the free ion concentration of the pore solution inside the concrete, $B_{ion,macro}$ and $D_{ion,macro}$ are the binding capacity and ion permeability of the concrete, respectively.
- Record ion concentration in terms of time and depth ($C_{ion}(y, t)$

2. Micro-Ion Diffusion Model of Alkali

$$B_{ion}\frac{\partial C_{ion}}{\partial t} = \nabla(D_{ion}(C_{ion})\nabla C_{ion}) \qquad D_{ion,micro}(t) = \left(1 - b \cdot \frac{C_{gel}(t)}{C_p}\right)D_{ion,micro}^0$$

Initial aggregate   Diffusion of alkali ions into the aggregate   Volume of reacted aggregate at time t
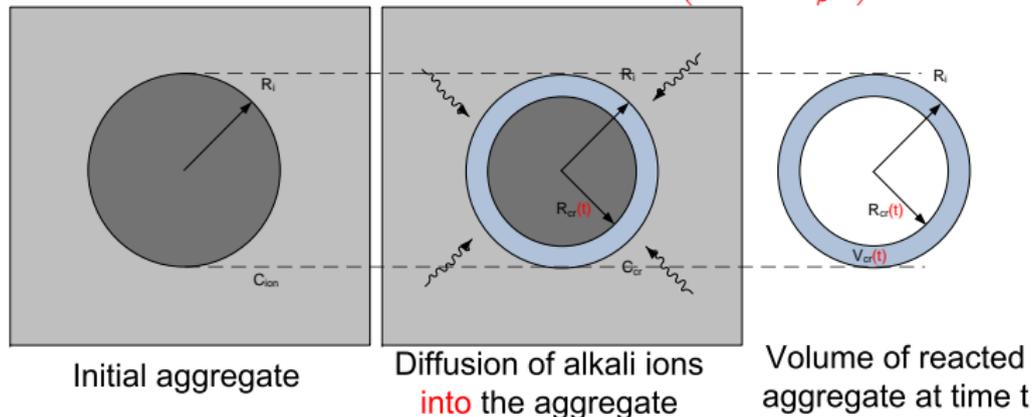
- Diffusion of alkali ions from the pore solution into the aggregate.
- Assumed that ASR occurs only when C_{ion} reaches a critical concentration C_{cr}.
- Dynamic process, moving front where $C_{ion} = C_{cr}$ varies with time t.
- Solve for the ASR depth as a radius $r_{cr}(t)$ by simply replacing C_{ion} with C_{cr}.
- D_{ion} decreases with an increase in ion concentration
- Does not account for the alkali-calcium substitution

3.a Micro Diffusion of Gel

| Aggregate saturated with gel | Gel diffusing into adjacent pores | Pores saturated with gel |
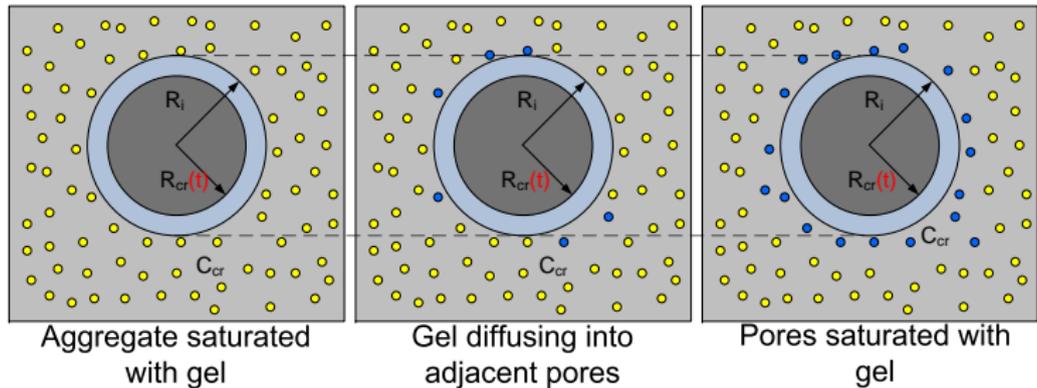
- gel formation first fills up the pores.

3.b Micro Diffusion of Gel I

Pores saturated with gel, formation of gel around the aggregate's Interface Transition Zone
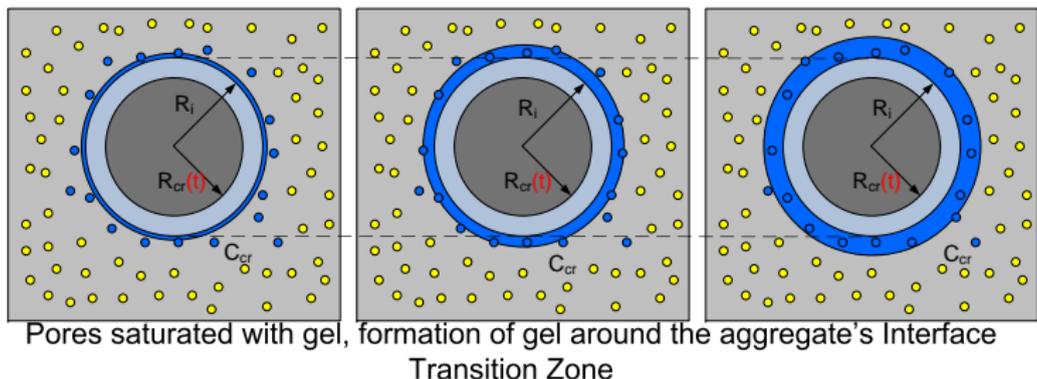
- Once the gel has saturated the pores, formation of gel along ITZ.
- Effective volume of gel $V_{gel,eff}^{R_i}(t) = V_{gel}^{*R_i}(t) - V_{pore}^{R_i}$ where $V_{gel}^{*R_i}$
- When $V_{gel,eff}^{R_i}(t)$ becomes positive, the interfacial pressure initiates and drives the gel diffusion through the porous cement paste.

3.b Micro Diffusion of Gel II

- Darcy's law for a viscous flow: $\frac{\partial C_{gel}(t)}{\partial t} = \nabla \left(\frac{K_{gel}}{\eta_{gel}} \nabla P_{gel}(t) \right) C_{gel}(t)$ and η_{gel} are the concentration and viscosity of the gel, respectively. K_{gel} is the gel permeability of the porous cement paste; $P_{gel}(t)$ is the interface pressure distribution due to ASR gel (thus depends on the degree of saturation of the pores). At the boundary of the aggregate, the interface pressure around the aggregate, $P_{int}(t)$ due to ASR gel is applied

- Chemo-mechanical equation, We assume (neglecting diffusion of the gel into the cement paste) $C_{gel}(t) = \frac{C_p}{f_t^p} P_{gel}(t)$

- Determine $P_{int}(t)$ from stress analysis.

- Total volume change due to ASR in all the aggregates with size R_i, is equal to the volume of ASR gel beyond the accommodating capacity of their interface zone: $\Delta V_{gel}^{R_i}(t) = V_{gel,eff}^{R_i} - V_{pg}(t)$, where $V_{pg}(t)$ is the total gel which permeated into the cement paste and $\Delta V_{gel}^{R_i}(t)$ will cause the transient internal pressure between the aggregate and the cement paste matrix, $P_{int}(t)$.

3.b Micro Diffusion of Gel III

- Coefficient of ASR expansion for an aggregate with radius R_i can be determined from $\alpha_i^{R_i}(t) = \frac{\Delta V_{gel}^{R_i}(t)}{V_a^{R_i}} = \frac{V_{gel,eff}^{R_i}(t) - V_{pg}^{R_i}(t)}{V_a^{R_i}} = \frac{V_{gel}^{R_i}(t) - V_{pore}^{R_i} - V_{pg}^{R_i}(t)}{V_a^{R_i}}$

- Total coefficient of expansion is the sum of all individual aggregate expansions (each one depending on its size). The interface pressure determined this way must be equal to the pressure obtained from the state equation. Nonlinear iterative formulation

Algorithm
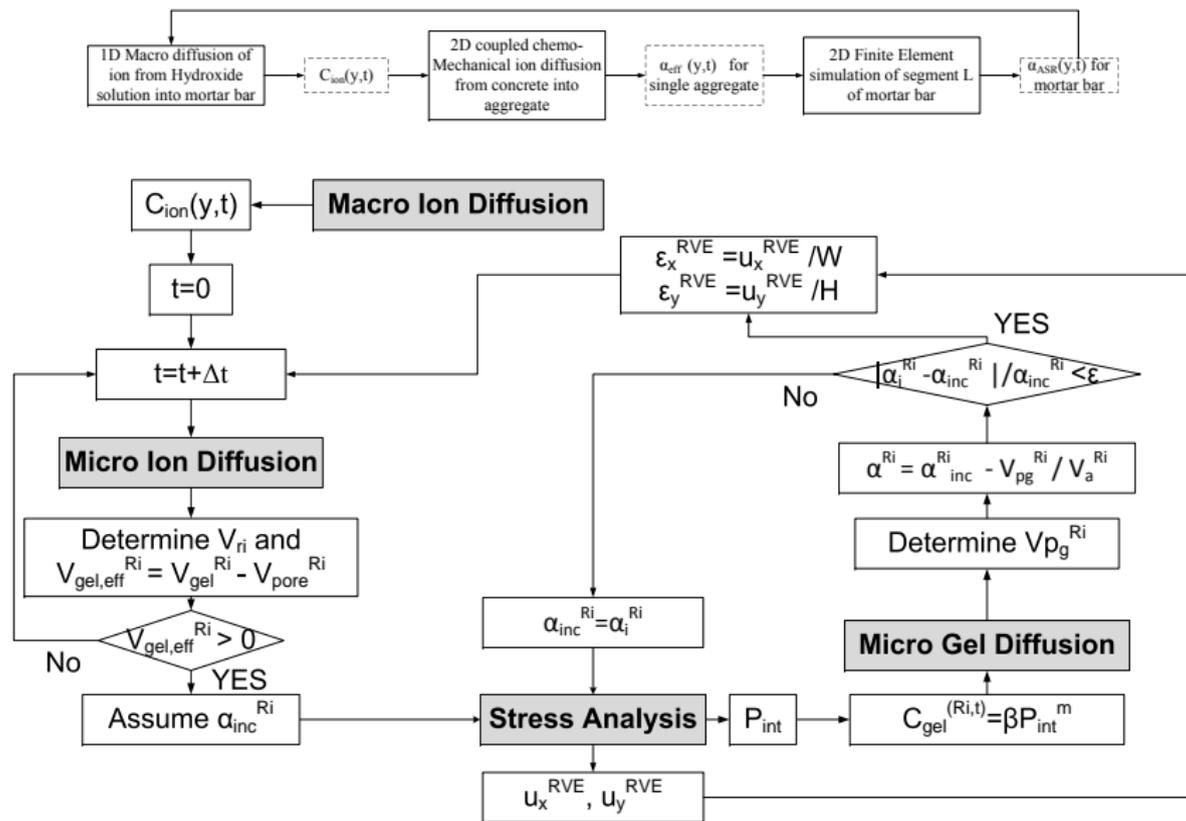
Parameters

| Parameter	Value
Maximum time (in days)	14
Step size (in *seconds*)	10,000
Volume fraction of aggregate	0.65
Volume fraction of matrix	0.35
D_{ion}/B_{ion} (mm^2/sec)	1×10^{-10}
ν_{gel} (mm^2/sec)	1×10^{-10}
Critical ion concentration, C_{cr}	0.005
Constant ion concentration, C_o	0.1
Volume ratio η	1.75
V_{unit} (mm^3/mm^2)	0.002
Porosity, $C_p(\%)$	40

Pressure and Expansion *vs* time

- 10 % of No. 30 reactive aggregate.

- Only the results of the RVE at the top layer (of the mortar bar) is shown

- At first, the rate of gel formation is faster than the diffusion capability of the cement paste around the aggregate, thus there is a gradual build-up of pressure around the aggregate.

- Once this pressure reaches the tensile strength of the cement paste (3.0 MPa), then micro-cracks form, and they release the pressure increase by allowing further diffusion of the gel.
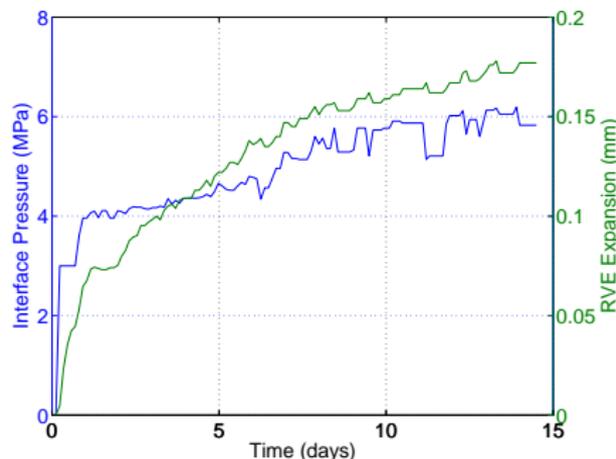
- Interface pressure stabilizes as a result of strain-softening.

- Determine the coefficient of expansion due to ASR gel on the No. 30 reactive RVE of the top element in all 4 considering layers.

Anisotropic Expansion
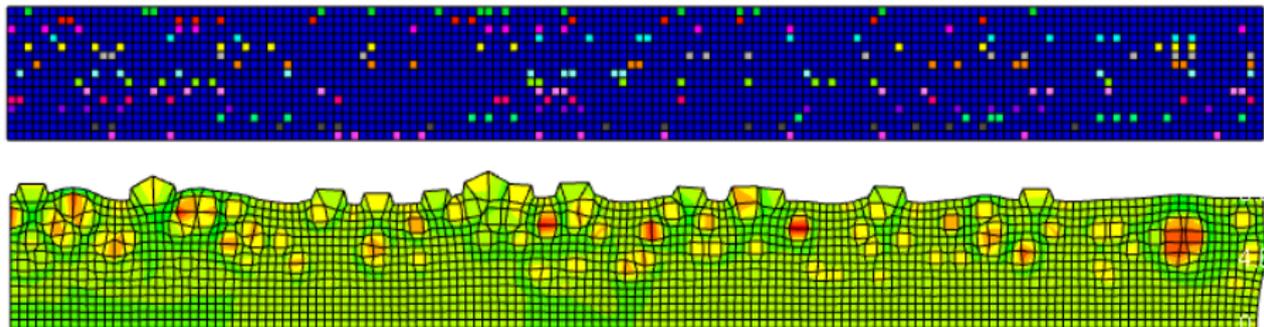
- In the macro level, the random locations of RVE of the 10% No. 30 reactive aggregate inside the mortar bar result in an anisotropic deformation.

ASR Expansion Coefficients in terms of Aggregate Size

- Unanticipated oscillation for aggregates of size 100 or smaller.

- This can be explained by revisiting
$\alpha_i^{R_i}(t) = \frac{V_{gel}^{R_i}(t) - V_{pore}^{R_i} - V_{pg}^{R_i}(t)}{V_a^{R_i}}$ which depends on the volume of non-absorbed gel.

- But gel permeation depends on the distance between the aggregate and RVE boundaries. For aggregate size equal or lower than No. 100, this is less or equal to 0.032 mm.

- This is a form of size effect ☺
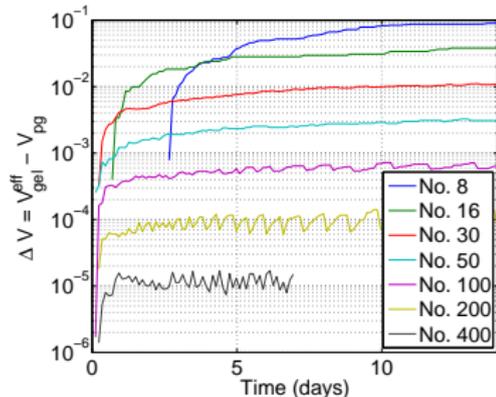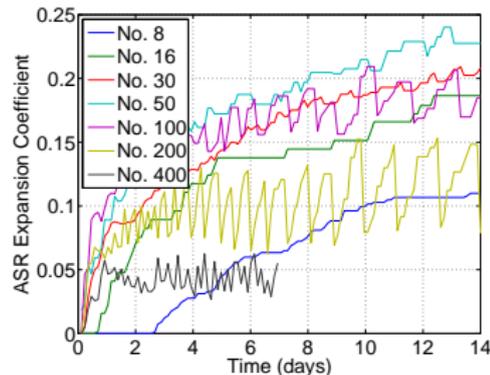
Micro to Macro

- Larive proposed this semi-analytical kinetics curve

$$\xi(t,\theta) = \varepsilon_{ASR}^{\infty} \frac{1-e^{-\frac{t}{\tau_c(\theta)}}}{1+e^{-\frac{(t-\tau_l(\theta))}{\tau_c(\theta)}}}$$

- Experimental tests were conducted at at 80^oC for 14 days. Larive's model (with $\varepsilon_{ASR}^{\infty}$, τ_L and τ_C corresponding to 0.108, 4.5 days and 2 days respectively) is superimposed on the expansion kinetic obtained from the presented numerical model.

- Adequate correlation can be achieved with reasonable parameters.

- This transition from micro to macro requires further studies.
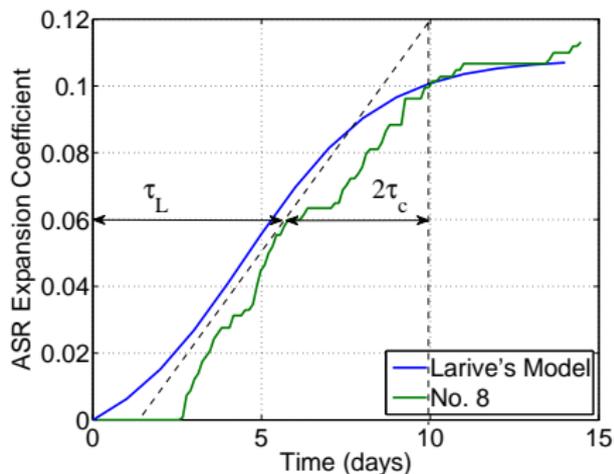
Expansion *vs* fittness

- Numerically simulated ASR expansions of the seven aggregate sizes is compared with the experimental results and the numerical model obtained by Suwito & Xi after 14 days.

- Proposed model provides an adequate correlation
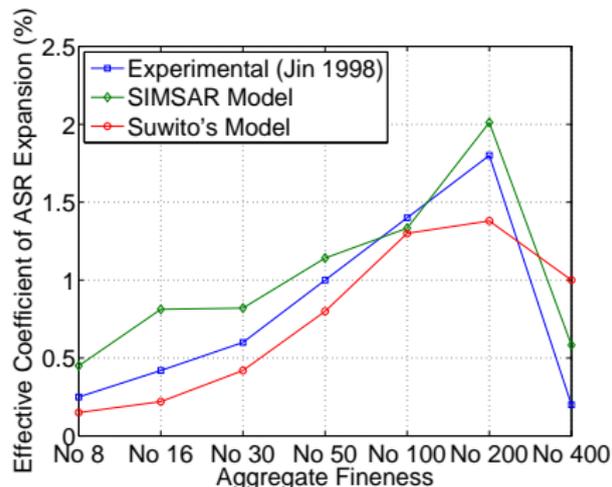
Conclusions

- It is just a model
- Physically sound yet incomplete, with approximations.
- Predictions are realistic
- Results compare reasonably well with laboratory experiments.
- Timid attempt to connect micro (diffusion based) models with macro ones.

Thank You

Thank you for your attention.
Questions?