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# LWRS contribution to the RILEM benchmark on materials modeling of ASR – Preliminary results

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# RILEM Benchmark

In order to analyze the current state of modeling capabilities, the RILEM Technical Committee 259 on the 'Prognosis of deterioration and loss of serviceability in structures affected by alkali-silica reactions (ASR)' has launched a benchmark on numerical models for the simulation of ASR at the material and the structural scale.

The context of this benchmark is the following:

> A number of structures worldwide are known to (or will) suffer from chemically induced expansion of the concrete. This includes not only the traditional alkali aggregate reaction (also known as alkali silica reaction) but increasingly delayed ettringite formation (DEF). There are three components to the investigation of structures suffering from such an internal deterioration: a) Chemo-physical characterization focusing primarily on the material; b) Computational modeling of the evolution of damage and assessing the structural response of the structure; and c) aging management of the structure. Focusing on the second aspect, ultimately an engineer must make prediction for the response of a given structure. In particular, he has to provide answers to the following questions: a) Is the structure operational?, b) is it safe?, and c) how the serviceability and safety margins will evolve in time. This task is best addressed through a numerical simulation (typically finite element analysis), which should account for most of the structure's inherent complexities. This is precisely the subject of this document The assessment of finite element codes has been partially assessed within the ICOLD International Benchmark Workshops on Numerical Analysis of Dams, and there were only limited discussion of AAR within the European project Integrity Assessment of Large Concrete Dams, NW-IALAD, In either cases, there has not yet been a comprehensive, rigorous and rational assessment of finite element code prediction capabilities and accuracies. Ultimately, practitioners would like to be able to calibrate their model with the limited historical field observation (typically inelastic crest displacements for dams, or crack maps for reinforced concrete) and then use the model to extrapolate the behavior of the existing or modified structure into the future. In science and engineering, any extrapolation should be based on a fundamentally sound model which ideally should be independently assessed for its capabilities. Unfortunately, expansive concrete (finite element) models have not yet been assessed within a formal framework. The objective of this effort is indeed an attempt to develop such a formal approach for the benefit of the profession. Though we are aware of the importance of the chemical constituents of a reactive concrete (part a above), and their potential impact on the residual swelling, this aspect is not considered in this study. Henceforth, we limit ourselves to the interaction of various mechanical aspects: temperature, relative humidity, chemically induced swelling, and mechanical load. The authors believe that prior to the comparison of analysis of a structure, a battery of basic tests should be undertaken first on the material. Each one of the test problems in turn will highlight the strength (or the deficiency) of the model, one at a time. Then and only then, we could assess a model predictive capabilities for the analysis of a structure. This document will describe such a series of tests, and format in which data should be reported. In order to facilitate comparison, the test problems are of increasing complexity. For the most part we assess one parameter at a time, then two, and then three. Only after such an exercise could we compare full blown structures (shear wall, reinforced concrete beam, and dam for structural analysis.

Seven materials problems and four structural problems have been submitted and published on the RILEM TC-259 webpage `http://www.rilem.org/gene/main.php?base=8750&gp_id=323`. ORNL's contribution to this workshop is currently limited to materials simulations using meso-scale modeling. For the participants using meso-scale models, the following additional information and instructions were provided: The Young modulus and Poisson ration of the aggregate are equal to 60 GPa and 0.2, respectively. The volume fraction of aggregate must be greater than 40% with a maximum of 70%. The maximum aggregate size is 2 mm. The particle size distribution is user-discretionary but must be provided as an additional output. It is requested that the constitutive parameters of the matrix (cement paste or mortar) are calibrated to obtain the mechanical properties of concrete used by the participants using macroscopic homogenous continuum models. Cement paste/mortar parameters must be provided as additional outputs

## AMIE

**Limitations** AMIE was not designed for heat transfer or moisture diffusion problems. Hence, tests involving drying, or drying-wetting cycles, cannot be modeled with AMIE. The proposed modeling strategy is a simplification of the approach proposed by Dunant and Scrivener [1]; Giorla et al. [2]: Aggregates are, here, assumed homogeneous, i.e., without gel pockets/veins, uniformly expanding, i.e., no effect of size or eventual mineralogical composition, and elastic only, i.e., no damage/cracking. These assumption are known to develop higher damage in the cement paste as no energy can by dissipated in the aggregates making the most of the volume fraction of the material.

## Results

### Constitutive Model Calibration

The geometry of the specimen is a standard cylinder of 16 cm in diameter (x-axis) and 32 cm in height (y-axis). The 2D microstructure is generated automatically by AMIE assuming an axial vertical symmetry Figure 1. For the sake of printing, the presented microstructure is rotated by 90 degrees. Note that on the axis of symmetry, aggregates are potentially cut whereas the 'wall effect' (i.e., aggregates away the surface) from the on the three other sides (actual external surfaces of the cylinder) is reproduced. The total volume fraction of meshed aggregates is 54.3%. A Fuller particle size distribution is adopted, min./max. diameter: 5/20 mm.

**Tensile Strength** The traction test is modeled by assuming no vertical displacement on the lower edge of the mesh and by applying a gradual uniform vertical displacement on the upper edge of the mesh. The macroscopic behavior of the concrete specimen is linear elastic until reaching failure at 3.12 MPa, for a target value of 3.5 MPa. The failure mode Figure 2 is obtained by a propagation of a localized quasi-horizontal fracture as generally observed experimentally under these conditions.

**Elastic Modulus** The elastic modulus of the cement paste is calibrated at 29 GPa in order to obtain a concrete modulus of 37.4 GPa for a given target of 37.3 GPa in the benchmark document.

**ASR Expansion** Aggregates are assumed homogeneous and subjected to a uniform expansion modelled by the classical sigmoid proposed by Larive [3]. The sigmoid parameters are those fitted by Saouma and Perotti [5] on Multon's experimental data: maximum expansion: 0.363%, latency time: 146.5 days, and characteristic time 86.9 days.

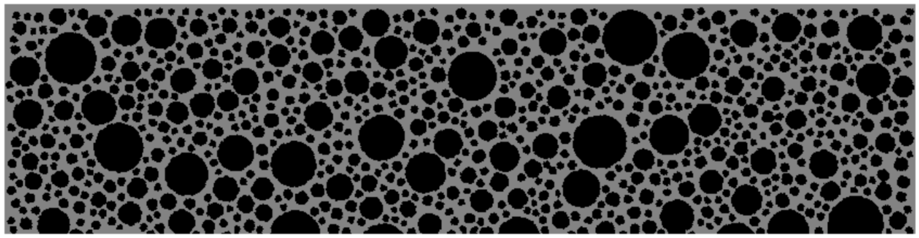


**Figure 1: Concrete microstructure automatically generated by AMIE (axial symmetry): black: aggregate; gray: matrix.**

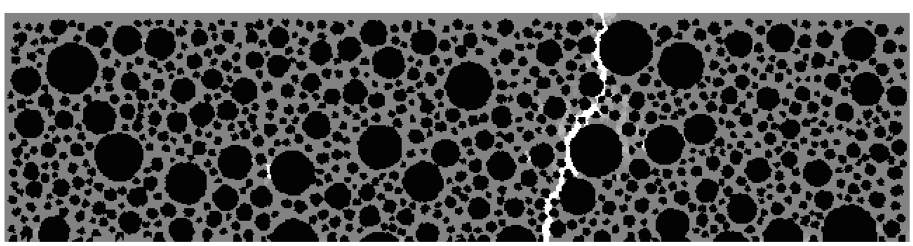


**Figure 2: Failure pattern under uniaxial traction. Cracked area in white.**

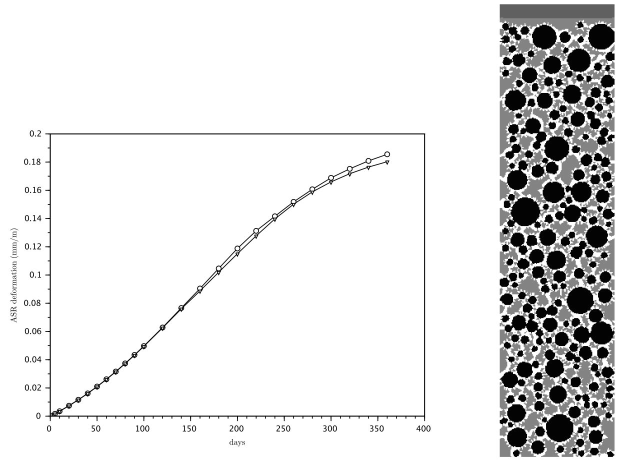



**Figure 3: (Left) ASR deformation at 293 K. ○: axial deformation; ▽: radial deformation; dashed lines: no damage behavior for the matrix. (Right) Damage at the end of the expansion test.**

**Creep** The creep test is calibrated on the uniaxial vertical deformation obtained under constant stresses of 10 MPa or 20 MPa. Figure 4 shows the computed specific creep deformation in the axial and radial directions assuming no damage in the matrix, while Figure 5 shows the creep deformation under 10 MPa assuming a quasi-brittle behavior for the matrix. The simulation was stopped at after day 110 by lack of convergence.

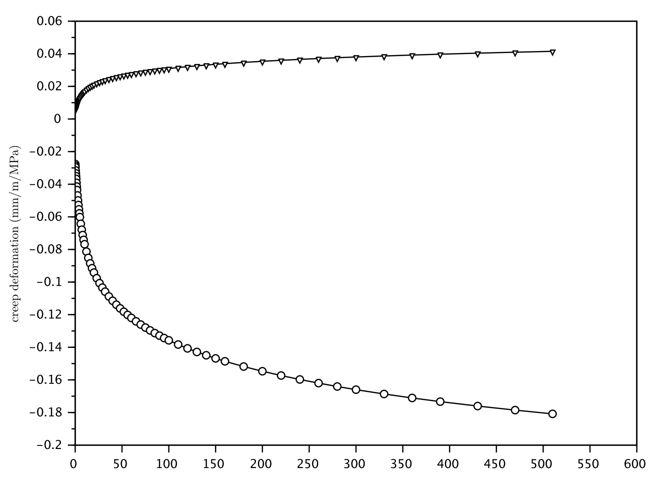



**Figure 4: Specific creep deformation assuming no damage for the cement paste. ○: axial deformation; ▽: radial deformation.**

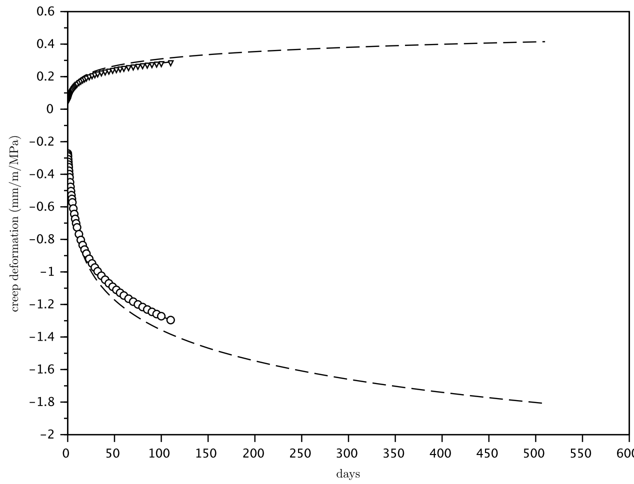



**Figure 5: Creep deformation assuming no damage for the cement paste. ○: axial deformation; ▽: radial deformation; dashed lines: no damage behavior for the matrix.**

### Post-Expansion Elastic Modulus

The mechanical properties of concrete following ASR are known to decrease substantially and monotonically with the expansion level. The simulation consists in applying an internal expansion to a certain degree during 300 days using the characteristic and latency times given by Saouma and Perotti, before applying a small traction to measure the residual elastic properties.

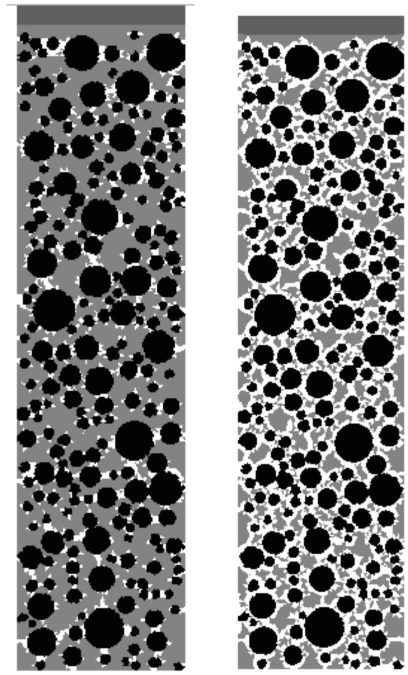
**Table 1: Residual elastic modulus of the concrete sample after ASR-expansion. n.c.: not converged.**

| aggregate expansion ($\mu m\,m^{-1}$) | concrete expansion ($\mu m\,m^{-1}$) | elastic modulus (GPa) | relative value (-) |
|---|---|---|---|
| 200 | 93 | 29.6 | 79.1% |
| 500 | 237 | n.c. | ≈ 0 |
| 1,000 | 500 | n.c. | ≈ 0 |

Compared to Larive's data, the ASR-induced reduction of the modulus of elasticity occurs at much lower level of expansion. These phenomenons are susceptible to provide an explanation: (1) Crack percolation occurs more easily in 2D than in 3D; (2) The adopted constitutive behavior for the matrix in traction is brittle; (3) The aggregates expand uniformly, i.e., no internal cracking allowing some energy dissipation outside of the matrix.

## Creep

**Variable Axial Loading** This test consists in applying an axial load of 5 MPa during the first 105 days, then increase it gradually to reach 10 MPa at 112 days. This load in maintained until day 280, before being decreased within a week time period, to return to the initial 5 MPa loading. The final loading is maintained



(a) (b)

**Figure 6: Concrete microstructure damage by ASR before the traction test. Aggregate expansion: (a) at 200 $\mu\mathrm{m\,m^{-1}}$, (b) at 1000 $\mu\mathrm{m\,m^{-1}}$.**

until day 350.

Figure 7 shows the response to this loading scenario assuming no damage for the cement paste.

## Conclusions

Among the proposed tests of the RILEM benchmark, a few material tests have been selected to evaluate the capabilities of AMIE. Based on the obtained results, it appears that AMIE provides reasonable results for (1) free-ASR expansion, accounting for damage and creep, and, (2) creep without damage. The residual (post-ASR) mechanical properties (modulus, strength) appear underestimated as the result of 2D-crack percolation, the brittleness of the matrix and the uniformity of aggregate expansion. On a more theoretical level, the question of the definition of an accurate failure criterion both in strain and in stress for creep-fracture interaction appears to be requiring further investigation.

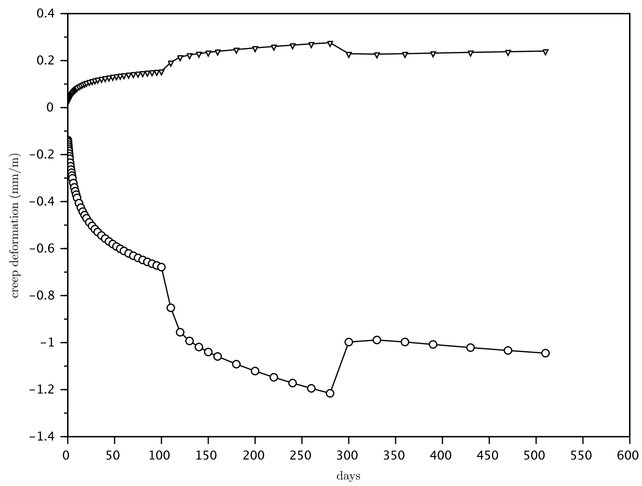



**Figure 7: Specific creep deformation assuming no damage for the cement paste. ○: axial deformation; ▽: radial deformation.**

# References

[1] C. Dunant and K. Scrivener. Micro-mechanical modelling of alkali–silica-reaction-induced degradation using the amie framework. *Cement and Concrete Research*, 40(4):517–525, 2010.

[2] A. Giorla, K. Scrivener, and C. Dunant. Influence of visco-elasticity on the stress development induced by alkali–silica reaction. *Cement and Concrete Research*, 70:1–8, 2015.

[3] C. Larive. *Apports combinés de l'expérimentation et de modélisation à compréhension de l'alcali-réaction et de ses effets mécaniques*. PhD thesis, Laboratoire Central des Ponts et Chaussées, 1997. in French.

[4] S. Multon. *Evaluation expérimentale et théorique des effets mécaniques de l'alcali-réaction sur des structures modèles*. PhD thesis, Laboratoire Central des Ponts et Chaussées, 2003. in French.

[5] V. Saouma and L. Perotti. Constitutive model for alkali-aggregate reactions. *ACI Materials Journal*, 103(3):194–2002, May-June 2006.

```
# AMIE input file for the RILEM simulations
#
# global parameters
.define
..path = 1_tension_post_asr # directory in which additional files are read
                            # and results are written
#
# mesh parameters
.discretization
..sampling_number = 32           # number of points on the edge of the sample
..order = LINEAR_TIME_LINEAR     # element type
..surface_sampling_factor = 1.5 # fineness of the mesh around the inclusions (> 1)
..sampling_restriction = 0.002  # minimum inclusion size (m)
#
# time step controls
.stepping
..time_step = 0.000001                 # initial time step to set things up,
                                       # will be overridden during calculation
..list_of_time_steps = time_steps.dat # file containing list of time steps
..minimum_time_step = 1e-9             # time between two damage instants
..maximum_iterations_per_step = 10     # number of damage algorithm iterations
..solver_precision = 1e-7              # for solver convergence
#
# cement paste
.sample
..input = dimensions.ini # file containing the dimensions of the sample
..behaviour
...young_modulus = 29e9             # CALIBRATED WITH 0_calibration_modulus
...poisson_ratio = 0.2              # typical value for concrete
...creep_characteristic_time = 1.5 # CALIBRATED WITH 2_creep
...creep_modulus = 15e9             # CALIBRATED WITH 2_creep
...creep_poisson = 0.2              # visco-elastic Poisson ratio assumed equal
                                    # to elastic in absence of data
...recoverable_modulus = 20e9       # CALIBRATED WITH 2_creep
...creep_activation_energy = 5000  # typical value for concrete, suggested by Bazant 2003
                                    # actual value might vary between 3000K (Fahmi 1972)
                                    # and 16000K (Bengougam 2003)
...imposed_deformation = 0                   # initialization value
...temperature = 293                         # --
...temperature = temperature.dat(t)          # file containing temperature variation
...temperature_reference = 293               # --
...thermal_expansion_coefficient = 20e-6    # typical value for cement paste
...tensile_strength = 4.5e6                  # CALIBRATED WITH 0_calibration_tension
...tensile_strain = 0.00016                  # = tensile_strength / young_modulus
...tensile_ultimate_strain = 0.00064         # should be CALIBRATED WITH
                                             # 0_calibration_tension
...material_characteristic_radius = 0.00015 # calibrated on size of smallest aggregate
...damage_increment = 1.00000 # numerical parameter
                              # reduce for higher accuracy (longer calculation time!)
...time_tolerance = 0.01 # numerical parameter
                         # reduce for higher accuracy (longer calculation time!)
```

```
...residual_stiffnes_fraction = 0.0001 # numerical parameter to help the solver converge
...input = paste_behaviour.ini # file containing additional paste information
...fracture_criterion = SpaceTimeNonLocalMaximumStrain
...damage_model = SpaceTimeFiberBasedIsotropic
...execute = CreepArrhenius                        # creep depends on temperature
...execute = ThermalExpansion                      # adds thermal expansion
#
# inclusions
.inclusions
..family = FileDefinedPolygon
...number = 1
...file_name = top_plate.dat
...behaviour
....young_modulus = 37.3e9
....poisson_ratio = 0.2
..family
...particle_size_distribution = PSDFuller
...number = 2000
...radius_maximum = 0.01   # maximum aggregate radius
...radius_minimum = 0.0025 # minumum --
...surface_fraction = 0.55 # target volume fraction
...placement
....spacing = 0.0005       # minimum distance between aggregates
....tries = 100000
....input = placement.ini  # file containing the dimensions of the box
                           # where the aggregates are placed
...behaviour
....young_modulus = 60e9                           # fixed
....poisson_ratio = 0.2                            # fixed
....imposed_deformation = 0                        # initialization value
....temperature = 293                              # --
....temperature = temperature.dat(t)               # --
....temperature_reference = 293                    # --
....thermal_expansion_coefficient = 10e-6          # typical value for aggregates
....input = aggregate_behaviour.ini # file contaning additional aggregate information
....execute = ThermalExpansion      # adds thermal expansion
#
# boundary conditions
.boundary_conditions
..boundary_condition # left edge (symmetry axis) is fixed in horizontal direction
...condition = FIX_ALONG_XI
...position = LEFT_AFTER
..boundary_condition # bottom edge is fixed in vertical direction
...condition = FIX_ALONG_ETA
...position = BOTTOM_AFTER
..input = boundary_conditions.ini # file containing additional boundary condition info
#
# output average data
.output
..file_name = rilem # name of the file where the results are stored
..time_step
```

```
...at = ALL
..instant = AFTER
..field = STRAIN_FIELD
..field = REAL_STRESS_FIELD
..field = SCALAR_DAMAGE_FIELD
#
# output mesh files
.export
..time_step
...at = ALL
..svg = FALSE
..file_name = rilem_mesh # name of the file where the mesh files are stored
..instant = AFTER
..field = TWFT_STIFFNESS
..field = STRAIN_FIELD
..field = REAL_STRESS_FIELD
..field = SCALAR_DAMAGE_FIELD
..field = TWFT_CRITERION
# end of file
```