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MARS – A Multiphysics Framework for the Analysis of Cast and Printed Concrete

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Abstract. *Predicting the time-dependent responses of concrete and concrete structures remains a challenging task in the construction sector. While experimental investigation serves as an essential cornerstone for concrete research, by itself it only offers limited insights into the complex time-dependent behaviour of concrete. The complexity is due to the multiple coupled hygro-thermo-chemo-mechanical processes. In the last two decades MARS, a special purpose computational software developed by ES3, has shown the capability of turning such insights accessible. This paper aims to provide a state-of-the-art of the MARS capabilities in concrete modelling, enriched with a discussion of some meaningful examples. The multiphysics framework today available in MARS already allows to simulate a wide range of complex phenomena, featuring the long-term performance of ordinary and advanced cementitious materials.*

Keywords: *Durability; Multiphysics Modelling; Concrete; MARS; Lattice Discrete Particle Model; Hygro-Thermo-Chemical Model.*

1 Introduction

Predicting the time-dependent responses of concrete and concrete structures remains a challenging task in the construction sector. Recent advances in the field of low carbon concretes, recycled aggregate concretes, new blended binder systems as well as printed mortars and concretes have introduced numerous new challenges, which will keep the concrete engineering community busy for the foreseeable future. While experimental investigation serves as an essential cornerstone for concrete research, by itself it only offers limited insights into the complex time-dependent behaviour of concrete. The complexity is due to the multiple coupled hygro-thermo-chemo-mechanical processes.

In the last two decades MARS (Multi-scale Multiphysics Analysis on Responses of Structures), a special purpose computational software developed by ES3 (Engineering and Software System Solutions, Inc.), has shown the capability of turning such insights accessible. As a matter of fact, it offers a comprehensive set of readily available modelling features including finite elements (FEM), lattice discrete particle elements (LDPM), and discrete elements (DEM) for the mechanical analysis of both plain and reinforced concrete, along with dedicated modules for the analysis of creep, shrinkage, alkali-silica reaction (ASR). MARS also allows to simulate the evolution of the hydration degree-dependent mechanical properties and their spatial variability. Based on either FE or lattice discrete particle mesh, this software permits also to run hygro-thermo-chemical (HTC) analyses, in order to simulate not only the heat and moisture transport phenomena, but also the evolution of the chemical activity featuring the ageing of cement-based materials. In case of lattice discrete particle mesh, HTC numerical implementation relies on a discrete conduit-based formulation, which is anchored yet dual to LDPM geometry generation.

Recently, this approach has been further expanded through the HTC-LDPM coupling, either one- or two-way. The former has been used for the simulation of creep, shrinkage, thermal expansion and material ageing, intended as strength and stiffness build-up from casting onwards. The one-way coupling has been conceived as a runtime update of both mechanical properties and variables, based on HTC results. The two-way coupling, instead, allows to modify HTC governing parameters depending on the LDPM results. This has enabled to model the effect of damage on the material permeability and cracks self-healing.

Furthermore, a novel and computationally efficient 2-phase shrinkage model, formulations for printed concrete as well as steel fibre and macro-synthetic fibre reinforcement, taking into account the effects of visco-elastic fibre materials, and a modelling framework for (particle filled) thermosets considering curing, cure-dependent mechanical properties, chemical shrinkage and hydrolytic aging complete the set of available model features.

All above-mentioned features are available within the civil engineering plugin for MARS which runs natively on macOS, Windows, Linux and high-performance computing (HPC) systems with openMP and MPI parallelization. All features are available for customisation and user development including user defined materials, elements and one- or two-way coupling modules.

This paper aims to provide a state-of-the-art about the MARS capabilities in concrete modelling, enriched with a discussion of some meaningful examples.

2 Multiphysics Modelling of Cementitious Materials

The MARS software features some unique techniques, such as the LDPM, Lattice Discrete Particle Model (Cusatis et al. 2011a) and its extension to fibre reinforced concrete (Schauffert and Cusatis 2012) as well as the adaptive re-meshing algorithms for shell and solid meshes, which facilitate the solution of problems involving structural break-ups, fragmentation, and post-failure response under extreme loading conditions. Thanks to its object-oriented architecture, it is possible to add new capabilities in an efficient and systematic fashion. In recent years, this proneness to new implementations has permitted to significantly increase its potential through successful collaborations with several universities and research institutions worldwide.

Numerical analysis of concrete structures requires a material model which performs realistically in simulating the damage growth in a wide range of scenarios.

Although, at present, continuum-based approaches are more suited and widely adopted for structural analyses, the discrete ones appear more appropriate to provide a deeper insight of concrete failure mechanisms (Bažant and Planas 2019). This makes the latter particularly appealing to model the durability of cementitious materials, which requires the use of multiphysics models coupling the simulation of mechanical, chemical, and transport phenomena. Discrete models become even more attractive in case of advanced cement-based composites (e.g., fibre-reinforced composites, engineered mixtures) as their response is strongly affected by local mechanisms at micro- or meso-scale. As an example, the discrete models allow to better capture the multi-cracking scenario featuring the response of fibre-reinforced composites (Figure 1). A continuum approach would likely fail in simulating this phenomenon accurately, due to the limit of having the damage smeared over a given process region and the deformation described by uniform strain fields.

Among the particle-based lattice models, the LDPM was calibrated and validated against a number of different quasi-static and dynamic loading regimes, showing superior predictive capability. This model has been used to simulate the mechanical behaviour of quasi-brittle granular materials such as concrete (Cusatis et al. 2011b, Smith et al. 2014) and fibre-reinforced concrete (Schauffert et al. 2012, Rezakhani et al. 2021), sulfur based Martian Concrete (Wan et. al. 2016), mortar (Han et al. 2020), or irregular masonry (Mercuri et al. 2020, Angiolilli et al. 2021) at the mesoscopic scale where the cementitious composite is modelled as composed of two phases: the coarse aggregates and the embedding mortar matrix.

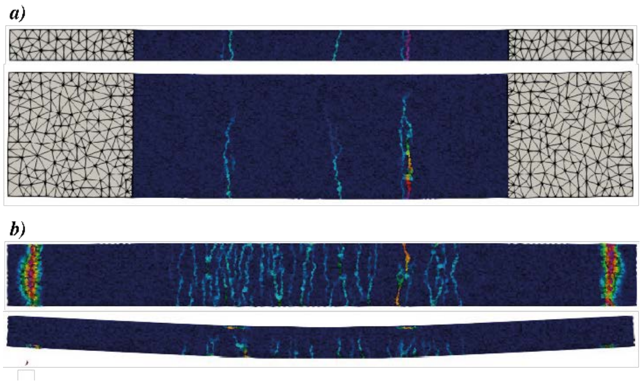

Figure 1. Simulation of the multicracking scenario in FRC samples with different thickness: (a) deep (t=100 mm) and (b) thin (t=25 mm) (Cibelli 2022).

Since the numerical simulation of complex phenomena - such as material ageing, moisture and transport phenomena in uncracked and cracked state, aggressive agents penetration, creep and shrinkage, self-healing, alkali-silica reaction, etc. - requires the combined exploitation of diffusion-chemical and mechanical models, in MARS numerical framework, HTC model (Di Luzio and Cusatis 2009a,b, Di Luzio and Cusatis 2013) and LDPM are required to mutually interact.

Being the HTC model originally formulated continuum-wise, in contrast with the discrete nature of LDPM, a relevant modelling issue has consisted of adapting the HTC numerical implementation to the LDPM solving system. The feasibility of this operation has been proved by the studies presented by several authors (Wan et al. 2016, Alnaggar et al. 2017, Abdellatef et al. 2019, Pathirage et al. 2018). The HTC-LDPM coupling relies on the definition of Flow Lattice Elements (FLEs): flow channels installed within the LDPM tetrahedra-based mesh, which together make up a 3D network, referred to as transport lattice system. This strategy allows for having two frameworks numerically aligned, anchored to each other, and easier to be connected. The model resulting from HTC and LDPM coupling is generally referred to as M-LDPM (Multiphysics-Lattice Discrete Particle Model) (Figure 2).

MARS includes all the capabilities and versatility of a general finite element (FE) code and the multiphysics modelling is available for the continuous approach too. The coupling between the original HTC continuum formulation and the mechanical model relies on two different FE solvers, which originally worked in series, since no mechanical effects were considered on hygro-thermal problem. Recently, in parallel with M-LDPM, also the multiphysics FE model was developed in order to have a numerical framework enabling both one- and two-way coupled simulations. The latter is referred to as M-FEM. In MARS the FE mechanical problem can be performed by considering several material models, such as elastic and elasto-plastic models, together with microplane models M4 and M7 (Caner and Bažant 2013).

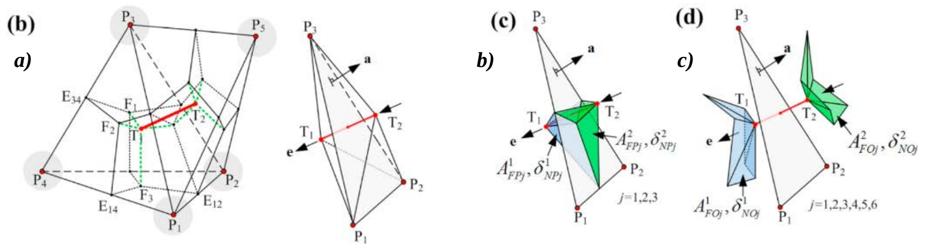

Figure 2. Flow Lattice Element (FLE) system geometry: (a) FLE in 3D, (b) LDPM facets related to mass transport, (c) LDPM facets related to heat transfer (Shen et al. 2020).

3 Applications

In the last decade the multiphysics modelling of cementitious materials in MARS environment has been matter of a prolific scientific production. Several research groups worldwide have coped with the simulation of concrete and mortar response by either using the available software features or developing dedicated modules. In this section some meaningful applications are showcased in order to provide an overview on the software capabilities in the field of multiphysics modelling for cement-based materials.

In (Wan et al. 2016) the authors adopted Multiphysics-LDPM to simulate the early age mechanical behaviour of a typical Ultra High Performance Concrete (UHPC) matrix. Both HTC and LDPM governing parameters were calibrated against data collected through an extensive experimental campaign on the material of interest. Afterwards, the calibrated parameters were validated by comparing experimental and numerical outcomes relevant to service scenarios unexploited during the calibration process (Wan-Wendner et al. 2018). It stood out that the proposed aging framework was capable of describing and predicting the main trends experimentally detected, such as the non-monotonous relationship between fracture energy and concrete aging, due to the different evolution rates that modulus, tensile characteristic length and tensile strength might experience (Figure 3).

The aging framework has been enriched over the years by accounting for the shear strength as an additional age-dependent parameter first (Pathirage et al. 2018), and later including the effect of slag on the material aging (Cibelli 2022). In both cases the calibration and validation were successfully carried out with respect to mortar and UHPC.

Structures in highly moist environments are prone to be endangered by ASR. The latter leads to the formation of an expansive gel that imbibes water over time, resulting in cracking and consequent reduction of concrete strength and stiffness. In MARS it is possible to simulate such phenomenon through the formulation presented by (Alnaggar et al. 2013). In addition, (Alnaggar et al. 2017) implemented the coupling between ASR and other time dependent behaviours, namely creep, shrinkage, and thermal strains (Figure 4). As a matter of fact, accurate simulations of long-term performance cannot disregard the cross effects induced by sustained loads and strains due to either moisture and/or heat transport processes. In the mentioned published works for concrete as well as in (Pathirage et al. 2018) for mortars, the model proved to have the potential of capturing the experimental trends and turning into a predictive tool once properly calibrated.

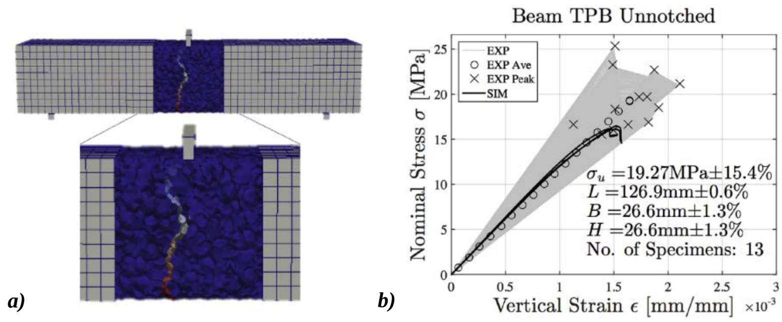

Figure 3. M-LDPM ageing model validation: (a) setup and crack opening, (b) experimental and simulated stress-strain curves (Wan et al. 2016).

Whereas phenomena such as aging and time-dependent response (e.g., ASR, creep, shrinkage) can be modelled through one-way HTC-LDPM coupling satisfactorily, there are several others requiring a two-way pairing approach. The latter include conditions where it is necessary to simulate the effect of damage on the hygro-thermo-chemical processes.

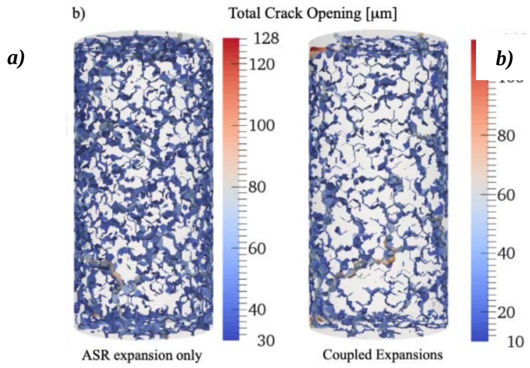

Figure 4. M-LDPM simulation for ASR-induced cracks: (a) ASR expansion only, (b) ASR coupled with creep and shrinkage (Alnaggar et al. 2017).

In (Cibelli et al. 2022, Cibelli 2022) the two-way coupling has been used as basis for the implementation of the crack self-healing for ordinary and fibre-reinforced concrete. The healing process is simulated through an improved version of the Hygro-Thermo-Chemical (HTC) model, whereas the mechanical effect of cracks repair is implemented into the LDPM to capture the recovery in mechanical performance that the healed material might experience. The healing implementation relies on the assumption that the phenomenon develops at two different scales:

at meso-scale, where the matrix cracks are responsible of permeability increasing and mechanical softening response, and at micro-scale, where the tunnel cracks at matrix-fibre interface determine the reduction in the load carried by the reinforcement (Figure 5).

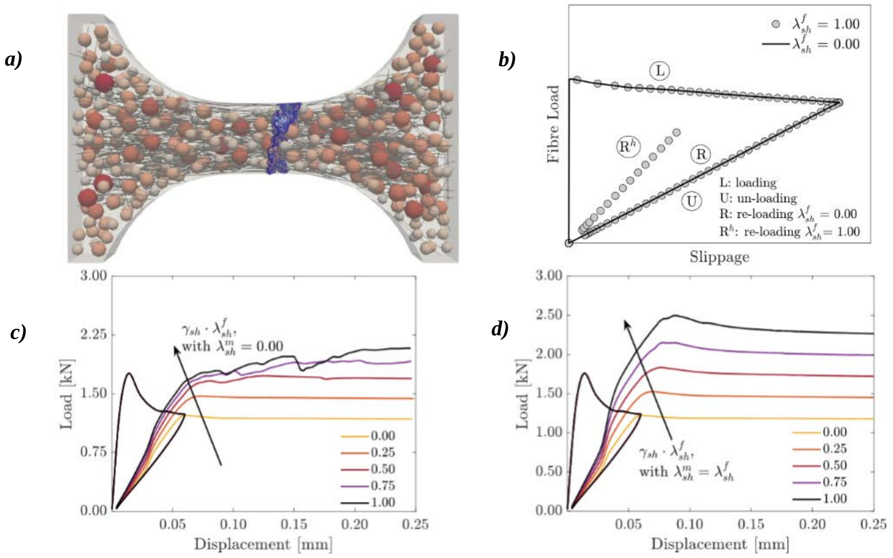

Figure 5. M-LDPM simulation for self-healing: (a) cracked FRC sample, (b) fibre load-slip curve along a damaged facet, (c) only tunnel cracks healing, (d) both matrix and tunnel cracks healing (Cibelli et al. 2022).

In order to simulate the degradation of concrete elements, beyond the hygro-thermo-chemo-mechanical processes, it is necessary to include also a model able to capture the transport phenomena of aggressive agents through the cementitious matrix. An environment rich in chlorides (e.g., marine environments) is one of the most dangerous scenarios to which concrete structures might be exposed. Because of this, (Zhang et al. 2021) implemented the chloride diffusion mechanisms for saturated and non-saturated conditions into the discrete framework of M-LDPM (Figure 6). Recently, it has been coupled with the effect of crack on the permeability and the healing model. This has enabled the simulation of chlorides diffusion in cracked and healed concrete (Cibelli 2022).

Explosive thermal spalling behaviour during fire exposure is one of the major issues in the design of modern reinforced concrete structures. Past fire disasters have taught that concrete spalling might yield serious structural and economic consequences. For this reason, it must be taken into account in fire design approaches. However, spalling mechanisms and their interaction still represent an open issue for the scientific community. Aiming to shed some light on this phenomenon, (Shen et al. 2020) have proposed an M-LDPM-based model to simulate concrete at high temperature. The model proposed, resulting from the full coupling of DTemPor3 model with LDPM, features the effect of pore pressure and temperature on the mechanical response as well as the impact of cracking on moisture mass transport and heat transfer (Figure 7).

Despite a less prolific literature, in M-FEM the implementation of both microplane and HTC models allows to simulate the concrete behaviour discussed in (Di Luzio and Cusatis 2013, Di Luzio et al. 2018), and multiphysics concrete simulations dealing with complex phenomena, such as material ageing and time-dependent behaviour.

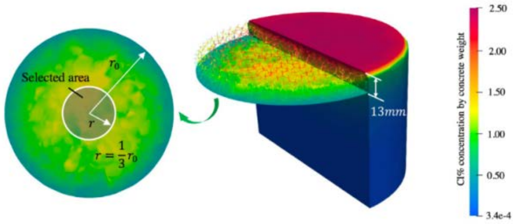

Figure 6. M-LDPM simulation of chloride distribution after 48-day ponding and cross section at depth=13 mm (Zhang et al. 2021).

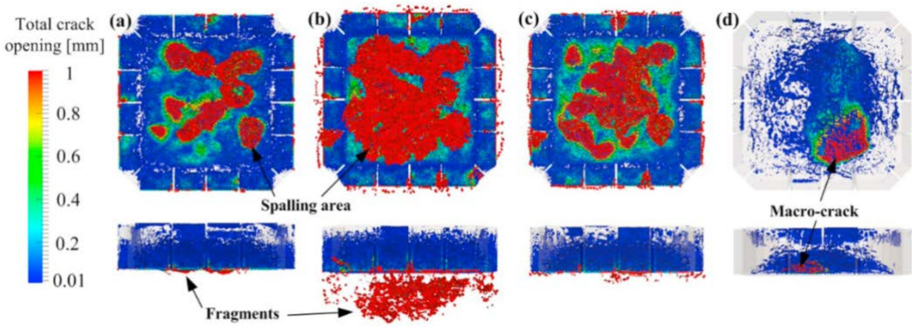

Figure 7. M-LDPM simulation for thermal spalling after different heating times: (a) after 15 min and (b) 30 min with all spalling factors included; (c) after 30 min with only thermal stresses effect; (d) after 30 min with only pore pressure effect (Shen et al. 2020).

4 Future Perspectives

Though the significant required effort and the number of tasks which are still open points, the modelling of concrete durability represents a key challenge for future generations of researchers. In this context, MARS developers and the research institutions collaborating with them are constantly focused on the software improvement. As a matter of fact, a relevant effort is being lately put on the simulation of printed concrete, in order to deliver a numerical tool able to effectively support the technological and technical progress in the civil engineering field.

As demonstrated by several applications available in the literature, the multiphysics framework today available in MARS already allows to simulate a wide range of complex phenomena, featuring the long-term performance of ordinary and advanced cementitious materials.

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