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Lattice Discrete Particle Model Tailored for Polymers

J. Vorel, J. Vozáb and J. Kruis

**Department of Mechanics, Faculty of Civil Engineering,
Czech Technical University in Prague, Prague, Czech Republic**

Abstract

Thermosetting polymers have many uses in numerous industries, including the building, automotive, aerospace, and marine sectors. They are frequently employed as adhesives or matrices in fibre-reinforced or particle-filled composites. Adhesives, repair, and rehabilitation of civil constructions are among the primary uses of particle-filled thermosets and thermoset-matrix composites in building and construction. Such applications necessitate novel strategies and dependable computational models that enable precise yet computationally effective structural or structural element prediction. This research will introduce a Lattice Discrete Particle Model (LDPM-P) that can simulate the failure behaviour of particle-filled polymers utilized in civil engineering. When considering the particles' size and distribution, LDPM-P may simulate the desired polymer composites at the particle scale. The phenomenological method serves as the foundation for constitutive relations. The suggested method aims to provide a trustworthy design for a large group of structural components, including rebar connections and adhesive anchors. The MARS software is used to incorporate the proposed model.

Keywords: polymers, lattice discrete particle model, volumetric-deviatoric split, viscoelasticity, tension, compression

1 Introduction

The architectural, automotive, aerospace, and marine sectors, among many others, all use thermosetting polymers extensively as adhesives or matrices in fibre-reinforced or particulate-filled composites. In civil engineering, thermosets and related fibre-reinforced composites have gradually replaced conventional building materials. Adhesives, repair, and rehabilitation of civil constructions are among the primary uses of particle-filled thermosets and thermoset-matrix composites in building and construction. Nowadays, particulate polymer behaviour is typically captured and predicted using continuum-based finite element computational models [1, 2, 3]. Scholars like Lieou [4] and Kothari [5] also suggested lower-scale models. However, the Lattice Discrete Particle Model (LDPM), typically used for concrete and similar quasi-brittle materials, is a promising choice to maintain a reasonable computational time and still consider the material's underlying structure. In order to meet the requirements of polymer-based composites, the paper modifies the standard LDPM [6, 7]. Furthermore, updating the current LDPM formulations for the Poisson ratio to be higher than the limiting value of 0.25 is necessary. Conventional polymers can encounter a value of between 0.3 and 0.4, depending on the type of material.

2 Lattice discrete particle model

The lattice discrete particle model is frequently used to simulate the behaviour of concrete [6] or rocks [8]. It is based on the idea that the material is a collection of rigid bodies (cells) interacting over the facets defined between them. These facets can be considered potential crack surfaces and are assumed to be located between the adjacent cells. First, spherical particles are introduced into the examined volume. The lattice system that depicts the mesostructure topology is defined by means of a Delaunay tetrahedralization of the particle centres and nodes used to characterize the external surface of the volume. The system of polyhedral cells is then created based on the 3D tessellation. Note that different options are utilized for the tessellation, e.g., described in [6] or [9]. The aggregate and surrounding matrix phase found between the particles create cells. In contrast to the original LDPM formulation, just the distribution of filler sizes needs to be prescribed.

The rigid body kinetics is utilized to describe the deformations associated with the facets [6]

$$\boldsymbol{u}\left(\boldsymbol{x}\right) = \boldsymbol{u}_i + \boldsymbol{\theta}_i \times \left(\boldsymbol{x} - \boldsymbol{x}_i\right), \tag{1}$$

where $\boldsymbol{u}_i$ and $\boldsymbol{\theta}_i$ are the translational and rotational degrees of freedom of node i. For the given displacements and rotations of the associated particles, the relative displacement at the centroid of facet k can be determined as

$$\boldsymbol{u}_{Ck} = \boldsymbol{u}_{Cj} - \boldsymbol{u}_{Ci}, \tag{2}$$

where $\boldsymbol{u}_{Ci}$ and $\boldsymbol{u}_{Cj}$ are the displacements at the facet centroid caused by the translations and rotations of the adjacent nodes i and j, respectively. Displacement vector

$\boldsymbol{u}_{Ck}$ is then employed to define the strain measures and discrete compatibility equations as follows:

$$\varepsilon_{Nk} = \frac{\boldsymbol{n_k}^{\mathsf{T}} \boldsymbol{u}_{Ck}}{l_{ij}}, \quad \varepsilon_{Mk} = \frac{\boldsymbol{m_k}^{\mathsf{T}} \boldsymbol{u}_{Ck}}{l_{ij}}, \quad \varepsilon_{Lk} = \frac{\boldsymbol{l_k}^{\mathsf{T}} \boldsymbol{u}_{Ck}}{l_{ij}}, \tag{3}$$

where $\boldsymbol{n} = (\boldsymbol{x}_j - \boldsymbol{x}_i)/l_{ij}$, $\boldsymbol{m}$ and $\boldsymbol{l}$ are two mutually orthogonal vectors in the plane of the projected facet and $l_{ij} = \|\boldsymbol{x}_j - \boldsymbol{x}_i\| = [(\boldsymbol{x}_j - \boldsymbol{x}_i)^{\mathsf{T}}(\boldsymbol{x}_j - \boldsymbol{x}_i)]^{1/2}$. $\boldsymbol{x}_i$ and $\boldsymbol{x}_j$ stand for the positions of node i and j, respectively. Because of the restriction on Poisson's ratio ($-1 < \nu < 0.25$) caused by the aforementioned split into normal and shear components, the volumetric-deviatoric split introduced in the microplane models [10, 11] is considered. The volumetric-deviatoric split allows to recover the full Poisson ratio range ($-1 < \nu < 0.5$) needed for polymers. Because of the underlying tetrahedral mesh and corresponding facets Ω_e (see [6]) the volumetric (hydrostatic) strain is calculated as [12]

$$\varepsilon_{Vk} = \frac{1}{3\Omega_{e,0}} \sum_{k \in \mathcal{F}_e} \Gamma_k l_{ij} \varepsilon_{Nk}, \tag{4}$$

where $\Omega_{e,0}$ is the initial volume of the tetrahedral element, $\mathcal{F}_e$ is the set of facets belonging to one element and Γ and l_{ij} are the facet area and distance of the adjacent nodes corresponding to the facet, respectively. Note that this definition is different than in the original paper by [6] where the volumetric strain read $\varepsilon_{Vk} = (\Omega_e - \Omega_{e,0})/3\Omega_{e,0}$. Ω_e is the current tetrahedron volumes belonging to the facet k. The normal deviatoric strain takes the form

$$\varepsilon_{NDk} = \varepsilon_{Nk} - \varepsilon_{Vk}. \tag{5}$$

Moreover, the shear (tangential) strain in the plane of the facet is written as $\varepsilon_{Tk} = (\varepsilon_{Mk}^2 + \varepsilon_{Lk}^2)^{1/2}$ and deviatoric strain as $\varepsilon_{Dk} = (\varepsilon_{NDk}^2 + \varepsilon_{Tk}^2)^{1/2}$. The constitutive material law defined on the facets is described in the following section. By imposing the equilibrium through the principle of virtual work, the internal work and nodal forces associated with the facet can be calculated [6].

2.1 Formulation of generalized Leonov model (viscoelastic behaviour)

The stepping stone in the formulation of the Leonov model is the Eyring flow equation representing the plastic component of the shear strain rate in the form

$$\frac{\mathrm{d}\gamma^p}{\mathrm{d}t} = \frac{1}{2A} \sinh(\tau/\tau_0) \tag{6}$$

Note that subscript k is omitted in the following text for readability. The total shear strain rate combining the elastic and plastic strain rates then becomes

$$\frac{\mathrm{d}\gamma}{\mathrm{d}t} = \frac{\mathrm{d}\gamma^e}{\mathrm{d}t} + \frac{\mathrm{d}\gamma^p}{\mathrm{d}t} = \frac{\mathrm{d}\gamma^e}{\mathrm{d}t} + \frac{\tau}{\eta(\,\mathrm{d}\gamma^p/\,\mathrm{d}t)} \tag{7}$$

which is the one-dimensional Leonov constitutive [13] model with the shear-dependent viscosity η given by

$$\eta(\,\mathrm{d}\gamma^p/\,\mathrm{d}t) = \frac{\eta_0 \tau}{\tau_0 \mathrm{sinh}(\tau/\tau_0)} = \eta_0 a_\sigma(\tau) \tag{8}$$

where τ is the shear stress and A, τ_0 are the model parameters, η_0 is the viscosity corresponding to a linear viscoelastic response and a_σ is the stress dependent shift factor. Based on the approach defined in [14], the parameter $\tau_0 = \frac{kT}{V}$, where the temperature is denoted as T, k is the Boltzmann constant and V stands for the activation volume. Notice that Eq. (7) represents a single Maxwell unit with variable viscosity. To describe the material response sufficiently accurately, the generalized Maxwell chain model is typically used.

The extension of Leonov model to multidimensional behaviour introduces equivalent deviatoric stress and the interested reader is refered to [15]. Admitting the vectorial based formulation for the facets, material isotropy, small strain theory, and the bulk response to be linearly elastic we arrive at the complete set of constitutive equations defining the compressible generalized Leonov model in the form

$$\sigma_V = E_V^0 \varepsilon_V \tag{9}$$

$$\frac{\mathrm{d}\sigma_D}{\mathrm{d}t} = \sum_{\mu=1}^{M} E_{D,\mu} \left(\frac{\mathrm{d}\varepsilon_D}{\mathrm{d}t} - \frac{\mathrm{d}\varepsilon_D^p, \mu}{\mathrm{d}t} \right), \quad \sigma_D = \sum_{\mu=1}^{M} \sigma_{D,\mu} \tag{10}$$

$$\sigma_{D,\mu} = \eta_\mu \frac{\mathrm{d}\varepsilon_{D,\mu}^p}{\mathrm{d}t} = \eta_{0,\mu} a_\sigma(\sigma_D) \frac{\mathrm{d}\varepsilon_{D,\mu}^p}{\mathrm{d}t} \tag{11}$$

where σ_V and σ_D are volumetric and deviatoric stresses, respectively. $E_V^0 = E/(1 - 2\nu)$ is the material bulk modulus and $E_{D,\mu}$ stands for the deviatoric modulus, associated with the μ-th unit. Note that for elastic material $E_D^0 = E/(1 + \nu)$, where E represents Young's modulus and ν is Poisson's ratio. The stress shift factor reads

$$a_\sigma(\sigma_D) = \frac{\sigma_D}{\sigma_{D0} \mathrm{sinh}(\sigma_D/\sigma_{D0})}, \tag{12}$$

where σ_{D0} is the characteristic deviatoric stress (the model parameter). Note that the dependance of the viscosity on evolution, e.g., temperature, humidity, etc., can be taken into account by multiplication of initial characteristic viscosity $\eta_{0,\mu}$ by additional shift factors in Eq. (11). To integrate Eq. (10) in time we settle for the most simple, fully explicit forward Euler integration. Provided that the total strain rate is constant during integration, a new state of stress at the end of the current time step Δt assumes the form

$$\sigma_V(t_i) = \sigma_V(t_{i-1}) + E_V^0 \Delta\varepsilon_V \tag{13}$$

$$\sigma_D(t_i) = \sigma_D(t_{i-1}) + \widehat{E}_D(t_{i-1}) \Delta\varepsilon_D + \Delta\lambda(t_{i-1}) \tag{14}$$

where t_i is the current time at the end of the i-th time increment. In light of the assumed Dirichlet series expansion to represent the shear relaxation function, the in-

stantaneous deviatoric modulus $\widehat{E_D}$ and the increment of eigenstress $\Delta\lambda$ reads

$$\widehat{E}_D = \sum_{\mu=1}^{M} E_{D,\mu} \frac{\theta_\mu a_\sigma(t_{i-1})}{\Delta t} \left[1 - \exp\left(-\frac{\Delta t}{\theta_\mu a_\sigma(t_{i-1})}\right)\right] \tag{15}$$

$$\Delta\lambda_D = -\sum_{\mu=1}^{M} \left[1 - \exp\left(-\frac{\Delta t}{\theta_\mu a_\sigma(t_{i-1})}\right)\right] \sigma_{D,\mu}(t_{i-1}), \tag{16}$$

where θ_μ is the relaxation time of the μ_{th} unit. Thus the increment of eigenstrain reads

$$\Delta\widehat{\varepsilon}_D = \frac{\Delta\lambda_D}{\widehat{E}_D} \tag{17}$$

2.2 Inelastic behaviour

The nonlinear and inelastic behaviour is characterised by the lower-scale mechanisms: (a) fracture; (b) pore collapse and material compaction; (c) frictional behaviour.

2.2.1 Fracture

It is known that the opening and sliding modes on the facets are inherently coupled together in fracture. Therefore, when the fracture on the facets is studied, it is beneficiary to define the fracture and damage evolution in terms of effective (equivalent) strain $\varepsilon^{\mathsf{eq}}$ and stress σ^{eq}, similar definitions can be found in [6, 16, 17] . However, because of the volumetric-deviatoric split, the equivalent normal strain is defined to characterise the material's fracture. The equivalent strain $\varepsilon_{\mathsf{eq}}$ takes the form

$$\varepsilon^{\mathsf{eq}} = \sqrt{(\varepsilon_V + \alpha\varepsilon_{ND})^2 + \alpha\left(\varepsilon_M^2 + \varepsilon_L^2\right)} = \sqrt{\left(\varepsilon_N^{\mathsf{eq}}\right)^2 + \alpha\varepsilon_T^2}, \tag{18}$$

where $\varepsilon_N^{\mathsf{eq}} = \varepsilon_V + \alpha\varepsilon_{ND}$, α stands for the interaction coefficient. This definition of equivalent normal strain originates from the assumption that $\sigma_N = E_V^0 \varepsilon_N^{\mathsf{eq}}$. The coupling strain ω is then defined as

$$\tan\omega = \frac{\varepsilon_N^{\mathsf{eq}}}{\sqrt{\alpha}\varepsilon_T}. \tag{19}$$

Based on the principle of virtual power, we relate the stress components to the equivalent stress as

$$\sigma_N = \sigma^{\mathsf{eq}} \frac{\varepsilon_N^{\mathsf{eq}}}{\varepsilon^{\mathsf{eq}}}, \quad \sigma_M = \sigma^{\mathsf{eq}} \frac{\alpha\varepsilon_M}{\varepsilon^{\mathsf{eq}}}, \quad \sigma_L = \sigma^{\mathsf{eq}} \frac{\alpha\varepsilon_L}{\varepsilon^{\mathsf{eq}}} \tag{20}$$

and

$$\sigma_V = \sigma^{\mathsf{eq}} \frac{\varepsilon_V}{\varepsilon^{\mathsf{eq}}}, \quad \sigma_{ND} = \sigma^{\mathsf{eq}} \frac{\alpha\varepsilon_{ND}}{\varepsilon^{\mathsf{eq}}}. \tag{21}$$

By substituting Eqs. (20) and (21) into Eq. (18) we obtain the effective stress in terms of normal and shear stress

$$\sigma^{\mathsf{eq}} = \sqrt{\sigma_N^2 + \frac{\sigma_T^2}{\alpha}}. \tag{22}$$

Note that based on the derivations in [17], the coupling strain ω can be also expressed as

$$\tan\omega = \frac{\sqrt{\alpha}\sigma_N}{\sigma_T}, \tag{23}$$

which can be utilised for the formulation of frictional behaviour. If the elastic behaviour is assumed and taking into account Eqs. (20), the stresses are written as

$$\sigma_V = E^{\mathsf{eq}}\varepsilon_V, \quad \sigma_{ND} = \alpha E^{\mathsf{eq}}\varepsilon_{ND}, \quad \sigma_M = \alpha E^{\mathsf{eq}}\varepsilon_M, \quad \sigma_L = \alpha E^{\mathsf{eq}}\varepsilon_L, \tag{24}$$

where $E^{\mathsf{eq}} = E_V^0$ and thus the physical meaning of $\alpha = E_D^0/E_V^0 = 1 - 2\nu/1 + \nu$ which also allows covering the whole physical range of the Poisson ratio, see [6] for the difference. Note that tensile behaviour is assumed if $\sigma_N > 0$, which can also be written as $\varepsilon_V + \alpha\varepsilon_{ND} > 0$.

The strain-dependent boundary $\sigma_{bt}(\varepsilon^{\mathsf{eq}}, \omega)$ is defined in [6, 17] int the form of equivalent strain. However, the improved formulation is utilized in this paper and takes the form

$$\sigma_{bt}\left(w^{\mathsf{eq}}, \omega\right) = \sigma_{t0}\left(\omega\right) \exp\left[-\frac{w_{\max}^{\mathsf{eq}}\left(\omega\right)}{w_f\left(\omega\right)}\right], \tag{25}$$

where $w_f\left(\omega\right)$ is the parameter controlling the material's ductility. The utilised coupling strain is calculated based on the maximum reached values of equivalent normal and shear strains as

$$\tan\omega = \varepsilon_{N,\max}^{\mathsf{eq}}/\sqrt{\alpha}\varepsilon_{T,\max}. \tag{26}$$

The coupling strain is written as

$$w_f\left(\omega\right) = w_{ft} + \left(w_{fs} - w_{ft}\right)\left(\frac{\pi/2 - \omega}{\pi/2 + \omega}\right)^{n_t}, \tag{27}$$

where $w_{ft} = G_{ft}/f_t$ and $w_{fs} = G_{fs}/f_s$ are the parameters controlling the ductility of the material and are calculated as the ratio of the fracture energy (G_{ft} - tension, G_{fs} - shear) and the tensile (f_t) or shear (f_s) strength. n_t is the material coefficient controling the transition from the brittle behaviour to perfectly plastic material. The equivalent maximum crack opening ever reached is defined as

$$w_{\max}^{\mathsf{eq}} = \sqrt{\left(w_V + w_{ND}\right)_{\max}^2 + w_{T,\max}^2} = \sqrt{\left(w_{N,\max}^{\mathsf{eq}}\right)^2 + w_{T,\max}^2}, \tag{28}$$

where the increments of the crack opening for a given time step can be expressed as

$$\begin{aligned}
\dot{w}_V\left(\omega\right) &= \left(\dot{\varepsilon}_{V,\mathsf{cr}}\right) l = \left(\dot{\varepsilon}_V - \dot{\sigma}_V/E_V^0\right) l, \\
\dot{w}_{ND}\left(\omega\right) &= \left(\dot{\varepsilon}_{ND,\mathsf{cr}}\right) l = \left(\dot{\varepsilon}_{ND} - \dot{\sigma}_{ND}/E_D^0 - \dot{\varepsilon}_{ND,\mathsf{creep}}\right) l, \\
\dot{w}_M\left(\omega\right) &= \left(\dot{\varepsilon}_{M,\mathsf{cr}}\right) l = \left(\dot{\varepsilon}_M - \dot{\sigma}_M/E_D^0 - \dot{\varepsilon}_{M,\mathsf{creep}}\right) l, \\
\dot{w}_L\left(\omega\right) &= \left(\dot{\varepsilon}_{L,\mathsf{cr}}\right) l = \left(\dot{\varepsilon}_L - \dot{\sigma}_L/E_D^0 - \dot{\varepsilon}_{L,\mathsf{creep}}\right) l,
\end{aligned} \tag{29}$$

where $\varepsilon_{\cdot,\mathsf{cr}}$ and $\dot{\varepsilon}_{\cdot,\mathsf{creep}}$ stand for cracking and creep strains, respectively. l is the lattice edge length. The strength limit $\sigma_t(\omega)$ in Eq. (25) is defined as

$$\sigma_{t0}(\omega) = f_t \frac{\sqrt{\alpha} f_t \xi_2 c + \xi_3 s + \sqrt{2\xi_1^2 \left[\left(\xi_2 s + \sqrt{\alpha} f_t c\right)^2 + \alpha f_t^2 c^2 - \xi_3 s^2 \right]}}{\left(\xi_2 s + \sqrt{\alpha} f_t c\right)^2}, \tag{30}$$

where $c = \cos\omega$, $s = \sin\omega$ and $\xi_1 = \mu_0 f_t - f_s$, $\xi_2 = 2\mu_0 f_t - f_s$ and $\xi_3 = 2\mu_0^2 f_t^2 - f_s^2$. The denominator in Eq. (30) is equal to zero if

$$\tan\omega = \frac{\sin\omega}{\cos\omega} = -\frac{\sqrt{\alpha} f_t}{\xi_2} = \frac{\sqrt{\alpha}\sigma_N}{\sigma_T}, \tag{31}$$

therefore

$$\sigma_{t0} = f_t \left[1 - \left(\frac{\xi_2}{2\xi_1}\right)^2\right] \sqrt{1 + \left(\frac{\xi_2}{\sqrt{\alpha} f_t}\right)^2}, \tag{32}$$

which is valid for the tensile behavior ($0 \leq \omega \leq \pi/2$). Therefore $\xi_2 \leq 0$ which leads to the conditions $f_s \geq 2\mu_0 f_t$ and also $\xi_1 \leq -\mu_0 f_t$. Note that if $\mu_0 = f_s/2f_t$, Eq. (30) reduced to the strength limit for effective stress presented in [17]

$$\sigma_{t0}(\omega) = f_t \frac{-\sin(\omega) + \sqrt{\sin^2(\omega) + 4\alpha\cos^2(\omega)/r_{st}^2}}{2\alpha\cos^2(\omega)/r_{st}^2}, \tag{33}$$

where $r_{st} = f_s/f_t$. However, in the current formulation, the friction coefficient μ_0 is ensured for pure shear ($\omega = 0$). In this case smooth transition between the compression and tension is thus ensured.

2.2.2 Pore collapse and material compaction

Pore collapse in compression follows the similar idea proposed in [6, 18]. However, it is simplified and the equivalent normal stress is related to the equivalent normal strain. The boundary in compaction then takes the form

$$\begin{aligned} \sigma_{bc} &= -f_{Nc0} + H_{c0}\left(\varepsilon_{Ncf} - \varepsilon_{Nc0}\right) \ln\left(1 + \frac{\varepsilon_N^{\mathsf{eq}} + \varepsilon_{Nc0}}{\varepsilon_{Ncf} - \varepsilon_{Nc0}}\right) \\ &= -f_{Nc0} + H_{c0}\left(\varepsilon_{Ncf} - \varepsilon_{Nc0}\right) \ln\left(\frac{\varepsilon_{Ncf} + \varepsilon_N^{\mathsf{eq}}}{\varepsilon_{Ncf} - \varepsilon_{Nc0}}\right), \quad \text{for } \varepsilon_N^{\mathsf{eq}} < 0 \end{aligned} \tag{34}$$

where stress f_{Nc0} denotes the material parameter limiting elastic part, $\varepsilon_{Nc0} = f_{Nc0}/E_V^0$ is thus the compaction strain and H_{c0} stands for the initial hardening modulus at the onset of pore collapse. ε_{Ncf} is the limit (asymptotic) strain. Note that parameters $f_{Nc0}, \varepsilon_{Nc0}, \varepsilon_{Ncf}, H_{c0}$ are assumed to be positive. The loading/unloading modulus is determined as $E_V = \max\left(E_V^0;\ \mathrm{d}\sigma_{bc}/\mathrm{d}\varepsilon_N^{\mathsf{eq}}\right)$, where $\mathrm{d}\sigma_{bc}/\mathrm{d}\varepsilon_N^{\mathsf{eq}} = H_c \frac{\varepsilon_{Ncf} - \varepsilon_{Nc0}}{\varepsilon_{Ncf} + \varepsilon_N^{\mathsf{eq}}}$.

2.2.3 Frictional behaviour

The shear strength increases due to the frictional effects in the presence of compressive forces ($\sigma_N < 0$). The frictional boundary is then defined similarly to Eq. (25) as

$$\sigma_{bs}\left(w_s, \omega, \sigma_N\right) = \sigma_{s0}\left(\sigma_N\right) \exp\left[-\frac{w_{\max}^{\mathsf{eq}}}{w_f\left(\omega\right)}\right], \tag{35}$$

where $w_f\left(\omega\right)$ is defined in Eq. (27) and $w_{\max}^{\mathsf{eq}}$ is defined in Eq. (28). The strength limit is rewritten in a similar form as in [6]

$$\sigma_{s0}\left(\sigma_N\right) \;\; = \;\; f_s + \mu_0 f_{Nc0}\left[1 - \exp\left(\frac{\sigma_N}{f_{Nc0}}\right)\right] \tag{36}$$

The simple friction slip boundary can be also assumed in the form

$$\sigma_{s0}\left(\sigma_N\right) = f_s - \sigma_N \mu_0. \tag{37}$$

3 Concluding remarks

The objective was to give an overview of the recently developed lattice discrete particle model for polymers. The current formulation combines viscoelasticity to capture the time-dependent behaviour, fracture and plasticity. Moreover, utilising LDPM allows the simple formulation of material law in the vectorial form on each facet. The presented formulation is implemented in MARS[1] software and will be tested against the experimental data obtained for different loading scenarios, e.g., tension, compression, and biaxial loading.

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