



Multi-scale computational homogenisation to predict the long-term durability of composite structures



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ABSTRACT

A coupled hygro-thermo-mechanical computational model is proposed for fibre reinforced polymers, formulated within the framework of Computational Homogenisation (CH). At each macrostructure Gauss point, constitutive matrices for thermal, moisture transport and mechanical responses are calculated from CH of the underlying representative volume element (RVE). A degradation model, developed from experimental data relating evolution of mechanical properties over time for a given exposure temperature and moisture concentration is also developed and incorporated in the proposed computational model. A unified approach is used to impose the RVE boundary conditions, which allows convenient switching between linear Dirichlet, uniform Neumann and periodic boundary conditions. A plain weave textile composite RVE consisting of yarns embedded in a matrix is considered in this case. Matrix and yarns are considered as isotropic and transversely isotropic materials respectively. Furthermore, the computational framework utilises hierarchic basis functions and designed to take advantage of distributed memory high performance computing.

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1. Introduction

Fibre reinforced polymer (FRP) composites have exceptional mechanical and chemical properties, including light weight, high specific strength, fatigue and corrosion resistance, low thermal expansion and high dimensional stability. They are commonly used in engineering application including aerospace, ships, offshore platforms, automotive industry, prosthetics and civil structures [1,2]. Textile or woven composites is a class of FRP composites, in which interlaced fibres are used as reinforcement, which provides full flexibility of design and functionality due to the mature textile manufacturing industry [3]. A detailed review, explaining the design and fabrication of textile preforms including weaving, knitting, stitching and braiding with their potential advantages and limitations is given in [4]. As compared to the standard laminated composites, textile composites have better damage and impact resistance, better through-thickness properties and reduced manufacturing cost. However, waviness of the yarns in the textile composites reduces the tensile and compressive strengths [5].

Due to their complicated and heterogeneous microstructure, Computational Homogenisation (CH) provides an accurate modelling framework to simulate the behaviour of FRP composites and determine the macro-scale homogenised (or effective) properties, including mechanical stiffness, thermal conductivity and moisture diffusivity, based on the physics of an underlying, microscopically heterogeneous, representative volume element (RVE) [6–10]. The homogenised properties calculated from the multi-scale CH are subsequently used in the numerical analysis of the macro-level structure. A variety of analytical and numerical homogenisation schemes have been developed for textile based FRP composites, which are normally based on the existence of an RVE and focus attention on the mechanical behaviour. Analytical methods are quick and easy to use but generally give poor estimates of the homogenised properties and are normally based on oversimplified assumptions of the microstructure and states of stress and strain. In the literature, some of the analytical homogenisation schemes, with their potential applications and limitations highlighted, are given in [10–14]. Numerical techniques, on the other hand, can accurately estimate the homogenised properties by capturing accurately the intricate micro-structure exactly but are computationally expensive. Examples of numerical homogenisation schemes applied to FRP composites can be found in [15–20]. A

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review article, summarising some of the analytical and numerical homogenisation techniques for the mechanical properties of the textile composite is given in [21].

During their service lives, FRP structures can be exposed to harsh hygro-thermal environmental conditions in addition to mechanical loading, which can lead to matrix plasticisation, hydrolysis and degradation of fibres/matrix interfaces [22–24]. In the long-term, these processes significantly reduce the mechanical performance of these structures. Therefore, understanding heat and moisture transport mechanisms and their effect on the mechanical performance are fundamental for assessing the long-term use of FRP structures. Effective diffusivities of FRP composites with impermeable fibres were studied in [25] within the context of FEM, considering the variation in fibre volume within square and hexagonal unit cells. In [26], effective moisture diffusivity as a function of temperature and fibre volume fraction were investigated for FRP composites with permeable fibres using a unit cell approach. For textile composites, moisture transport was studied in [22,23] as a function of variation in tow architectural parameters, e.g. tow waviness, tow cross-section shape and wave pattern. Transient moisture transport in multilayer textile composites was investigated in [27]. An analogy between thermal and moisture transport analysis was used in [28] to study the moisture diffusion and corresponding weight gain for carbon braided composites. In [24,29], a multi-scale CH framework based on the hygro-mechanical analysis was proposed while using a two-dimensional RVE with randomly distributed fibres in 0° and 90° directions. A two way coupling was considered between the mechanical and moisture transport analysis and a model reduction scheme was used to reduce the computational cost. For the composite material, deformation dependent diffusion at finite strains was considered in [30]. Masonry wall reinforced with FRP reinforcement was studied in [31] while considering hygro-thermo-mechanical analysis. A recent review article [32], explains different degradation mechanism for FRP composites in connection with different environmental conditions.

In this paper, a coupled hygro-thermo-mechanical computational framework based on the multiscale CH is proposed for FRP composites. At each integration point, an RVE consisting of single plain weave textile composite is considered, consisting of yarns embedded in the matrix. Elliptical cross sections and cubic spline paths are used to model the geometry of these yarns. Separate RVEs are considered for the heat transfer, moisture transport and mechanical CH. One-way coupling is considered in this case, i.e. mechanical analysis is assumed to be dependent on both moisture transport and thermal analyses but any influence on the moisture or thermal behaviour due to the mechanical behaviour is ignored. A degradation model, developed from experimental data relating evolution of mechanical stiffness over time for given exposure temperatures and moisture concentration was also developed and incorporated in the proposed computational framework. A unified approach is used to impose the RVE boundary conditions, which allows convenient switching between the different RVEs boundary conditions (linear Dirichlet, uniform Neumann and periodic) [33]. For a given size of RVE the periodic boundary conditions gives a better estimation of the homogenised material properties as compared to linear Dirichlet and uniform Neumann boundary conditions, which give an upper and lower limit [33–35] respectively.

The developed computational framework utilises the flexibility of hierarchic basis functions [36], which permits the use of arbitrary order of approximation, thereby improving accuracy for relatively coarse meshes. For the thermal and moisture transport analyses both matrix and yarns are assumed as isotropic materials, while for the mechanical analysis, the yarns are considered as transversely isotropic materials. The required principal directions of the yarns for the transversely isotropic material model are calculated from potential flow analysis along these yarns. Furthermore,

distributed memory high performance computing is used to reduce the computational cost associated with the current multi-scale and multi-physics computational framework.

This paper is organised as follows. The multi-scale CH framework and corresponding implementation of the RVE boundary conditions are described in Section 2. Transient heat and moisture transport analyses along with their FE implementation are discussed in Section 3. The derivation of the degradation model from the experimental data is next explained in Section 4. The overall multi-scale and multi-physics computational framework is described in detail in Section 5. Computation of yarns directions are explained in Section 6. A three-dimensional numerical example and concluding remarks are given in Sections 7 and 8 respectively.

2. Multi-scale computational homogenisation

In multi-scale CH, a heterogeneous RVE is associated with each Gauss point of the macro-homogeneous structure. Multi-scale CH gives us directly the macro-level constitutive relation, allows us to incorporate large deformation and rotation on both micro- and macro-level and both physical and geometric evolution can be included on both micro- and macro-level [34]. The multi-scale CH procedure and corresponding implementation of RVE boundary conditions is described initially for the mechanical case, which is subsequently extended to corresponding thermal and moisture transport cases. The first order multi-scale CH is used in the paper, the basic principle of which is shown in Fig. 1, where $\Omega \subset \mathbb{R}^3$ and $\Omega_\mu \subset \mathbb{R}^3$ are macro and micro domains respectively. Macro-strain $\bar{\boldsymbol{\varepsilon}} = [\bar{\varepsilon}_{11} \quad \bar{\varepsilon}_{22} \quad \bar{\varepsilon}_{33} \quad 2\bar{\varepsilon}_{12} \quad 2\bar{\varepsilon}_{23} \quad 2\bar{\varepsilon}_{31}]^T$ is first calculated at each Gauss point $\mathbf{x} = [x_1 \quad x_2 \quad x_3]^T$ of the macro-structure, which is then used to formulate the boundary value problem on the micro-level. After solution of the micro-level boundary value problem, homogenised stress $\bar{\boldsymbol{\sigma}} = [\bar{\sigma}_{11} \quad \bar{\sigma}_{22} \quad \bar{\sigma}_{33} \quad \bar{\sigma}_{12} \quad \bar{\sigma}_{23} \quad \bar{\sigma}_{31}]^T$ and stiffness matrix $\bar{\mathbf{C}}$ are calculated. Separation of scales is assumed in the first-order CH, i.e. the micro length scale is considered to be very small compared to the macro length scale and the macro-strain field attributed to each RVE is assumed to be uniform. Therefore, first-order CH is not suitable for problems with large strain gradient (but can be used for problems subjected to large strain) and cannot be used to take into account micro-level geometric size effects [7,34]. On the micro-level at any point $\mathbf{y} = [y_1 \quad y_2 \quad y_3]^T$ the displacement field is written as [37–39]

$$\mathbf{u}_\mu(\mathbf{y}) = \bar{\boldsymbol{\varepsilon}}(\mathbf{x})\mathbf{y} + \tilde{\mathbf{u}}_\mu(\mathbf{y}), \quad (1)$$

where $\bar{\boldsymbol{\varepsilon}}\mathbf{y}$ is a linear displacement field and $\tilde{\mathbf{u}}_\mu$ is a displacement fluctuation. The micro-strain associated with point \mathbf{y} is written as

$$\boldsymbol{\varepsilon}_\mu(\mathbf{y}) = \nabla^s \mathbf{u}_\mu = \bar{\boldsymbol{\varepsilon}}(\mathbf{x}) + \tilde{\boldsymbol{\varepsilon}}(\mathbf{y}), \quad (2)$$

where $\tilde{\boldsymbol{\varepsilon}}(\mathbf{y}) = \nabla^s \tilde{\mathbf{u}}_\mu$ is the strain fluctuation at the micro-level and ∇^s is the symmetric gradient operator. Furthermore, volume average of the micro-strain is equivalent to the macro-strain:

$$\bar{\boldsymbol{\varepsilon}}(\mathbf{x}) = \frac{1}{V} \int_{\Omega_\mu} \boldsymbol{\varepsilon}_\mu(\mathbf{y}) d\Omega_\mu = \bar{\boldsymbol{\varepsilon}}(\mathbf{x}) + \frac{1}{V} \int_{\Omega_\mu} \tilde{\boldsymbol{\varepsilon}}_\mu(\mathbf{y}) d\Omega_\mu, \quad (3)$$

where V is the volume of the RVE. It is clear from Eq. (3) that the volume average of the strain fluctuation is zero, i.e.

$$\frac{1}{V} \int_{\Omega_\mu} \tilde{\boldsymbol{\varepsilon}}_\mu(\mathbf{y}) d\Omega_\mu = 0. \quad (4)$$

The micro-equilibrium state in the absence of body force is written as

$$\text{div}(\boldsymbol{\sigma}_\mu) = \nabla \cdot \boldsymbol{\sigma}_\mu = \mathbf{0}, \quad (5)$$

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