MULTISCALE COMPUTATIONAL HOMOGENISATION TO PREDICT THE LONG-TERM DURABILITY OF COMPOSITE STRUCTURES

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Sequence of Presentation

Introduction (DURACOMP)

Multi-scale modelling

Model components (multiscale and multiphysics):
- Generalised RVE boundary conditions
- Transient field problems
- Degradation model
- Computational framework

Numerical example

Summary
Investigation of long-term degradation
an integrated program of computational modelling and physical testing

Objectives

Multi-scale analysis framework
confidence in durable composite structures

Reliability analysis for composites subject to epistemic and stochastic uncertainties

Structural-level characterisation tests properties required for the lifetime prediction analyses

New paradigm of testing and analysis methods
To assess composites over service lives

Involves six universities
Bath, Bristol, Glasgow, Leeds, Newcastle and Warwick
Investigation of long-term degradation
an integrated program of computational modelling and physical testing

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Multi-scale Modelling

- Predict and describe macroscopic material behaviour by considering the mechanics of the underlying microstructure.

FE\(^2\), because it requires the simultaneous computation of the mechanical (thermal or moisture transport) response at two different scale.

- Advantages:
  - No explicit assumptions for the macroscopic local constitutive equations.
  - Incorporation of detailed microstructural information, including physical and geometrical evolution of the microstructures.
  - Different modelling techniques can be used on both micro- and macro-level, e.g. FEM, BEM, meshless method.
Multi-scale Modelling
Basic Principles

- Definition of macrostructural B.V.P.
- Definition of a microstructural representative volume element (RVE).
  (with known constitutive behaviour of individual constituents)
- Formulation of the microstructural boundary conditions.
  (macro-to-micro transition or localization)
- Solution of microstructural B.V.P.
- Calculation of the macrostructural output variables.
  (micro-to-macro transition or homogenization)
- Generalised imposition of different RVE boundary conditions (displacement, traction and periodic) [1].
- Discretised system of equations

\[ K\mathbf{u} + C^T \lambda = 0 \]
\[ C\mathbf{u} = D\bar{\varepsilon} \]

where \( C = \int_{\Gamma} HN^T N d\Gamma \) and \( D = \int_{\Gamma} HN^T X d\Gamma \)

Homogenised stress \( \bar{\sigma} = \frac{1}{V} D^T \lambda \).

Model Components
RVE boundary conditions

Mechanical Problem

Moisture transport (diffusion)

[1] Ł. Kaczmarczyk, C. J. Pearce, and N. Bicanic. Scale transition and enforcement of RVE boundary conditions in second-order computational homogenization. *International Journal for Numerical Methods in Engineering*, 74(3):506–522, 2008.
Conduction and diffusion models are considered for thermal and moisture transport problems (conservation of mass or energy for moisture and thermal problem respectively).

\[
\rho C_p \frac{\partial \psi}{\partial t} - K_\psi \nabla^2 \psi = 0
\]

Where

\[
\psi = T, c \quad \text{(scalar fields)}
\]

\[
\nabla^2 \quad \text{Laplace operator}
\]

\[
t \quad \text{time}
\]

\[
\rho \quad \text{density}
\]

\[
C_p \quad \text{specific volume capacity}
\]

\[
K_\psi \quad \text{conductivity}
\]
Experiments involves accelerated ageing with exposure temperatures of 25°C, 40°C, 60°C and 80°C and recording time of 28, 56, 112 days.

An exponential trend is assumed for the degradation of shear modulus for all the exposure temperatures

\[ G|_T = G_0 e^{-\alpha t} \]

\[ G|_T = \begin{cases} 
G_0 e^{-0.0023t} & \text{for } T = 25°C \\
G_0 e^{-0.0027t} & \text{for } T = 60°C \\
G_0 e^{-0.0040t} & \text{for } T = 80°C 
\end{cases} \]
Generalised degradation model

\[ G(T, t) = G_0 e^{-\alpha(T)t} \text{, where } \alpha(T) = \beta \ln \left( 1 - \frac{T}{T_g} \right) \]

Using least square fitting, i.e. minimising the following eq w.r.t \( \beta \)

\[ F(\beta) = \sum_{i=1}^{3} \left( \alpha_i - \beta \ln \left( 1 - \frac{T_i}{T_g} \right) \right)^2 \]

\( \beta = 0.001682 \)

Including effect of moisture concentration

\[ G(T, c, t) = G_0 e^{-\gamma(c)\alpha(T)t} \]

\[ G(T, c, t) = G_0 e^{-c\beta \ln \left( 1 - \frac{T}{T_g} \right) t} \]
Constant temperature and moisture concentration are assumed in the derivation of degradation model. $G(T, c, t) = G_o e^{-c\beta\ln(\frac{1-T}{T_g})t}$

Assuming real scenarios of variable temperature and moisture concentration, degradation model is written in rate form as $G(T, c, t) = G_o e^{-c(t)\beta\ln(\frac{1-T(t)}{T_g})t}$

$\frac{d}{dt}G(T, c, t) = \frac{\partial G}{\partial T}T' + \frac{\partial G}{\partial c}c' + \frac{\partial G}{\partial t}$

Assuming chemical reaction leading to degradation of mechanical properties is very slow as compared to daily variation of temperature and moisture concentration $\frac{d}{dt}G(T, c, t) = \frac{\partial G}{\partial T}T' + \frac{\partial G}{\partial c}c' + \frac{\partial G}{\partial t}$

$\frac{d}{dt}G(T, c, t) = -c\beta\ln \left(1 - \frac{T}{T_g}\right)G$

Generalised degradation model $\frac{d}{dt} (1 - \omega) = -c\beta\ln \left(1 - \frac{T}{T_g}\right) (1 - \omega)$

$\omega = 0$ no degradation

$\omega = 1$ fully degradation
Macro transient thermal analysis

Homogenised $K_T$

Temperature field $T$

Degradation parameter $(1 - \omega)$ on macro mesh

$(1 - \omega)$ field

Macro transient diffusion analysis

Homogenised $K_c$

Moisture concentration field $c$

Macro mechanical analysis at selected time steps

$(1 - \omega)$ at each macro Gauss point

Homogenised $D$

Mechanical RVE

$D_{matrix} = (1 - \omega)D_{matrix}$
- Simulation time = 1000 days
- Number of time steps = 100
- Mechanical problem was run for every 10th step
- Matrix and yarns are assumed as isotropic materials

Macro structure geometry
(561 elements, 218 nodes)

Macro structure mesh
(10285 elements, 2364 nodes)

Representative volume element
(10285 elements, 2364 nodes)
Numerical Example

Results

Mesh partition (8 processors)

Moisture concentration

Temperature (°C)

(1 − ω) field

Vertical displacement (mm)

Moisture concentration

\( (1 − ω) \) field

Relative displacement (mm)
Numerical Example
Undeformed and deformed RVEs

Deformed RVEs at the end of simulation
A fully generalised mechanical degradation model has been developed for FRP composites subjected to hygro-thermal environmental conditions based on the experimental data (from our project partner).

A coupled hygro-thermo-mechanical (considering only one-way coupling) computational framework based on multiscale (FE²) computational homogenisation, incorporating degradation model is developed and implemented in our group’s FE software MoFEM.

The developed computational framework have the flexibility of
- Arbitrary order of approximation (hierarchic basis functions)
- Generalized boundary conditions
- PETSc and MOAB libraries
- Parallel processing.
