HIERARCHICAL FINITE ELEMENT BASED MULTISCALE COMPUTATIONAL HOMOGENISATION OF COUPLED HYGRO-MECHANICAL ANALYSIS FOR FIBRE-REINFORCED POLYMERS

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Introduction (DURACOMP)

Multi-scale modelling

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

Numerical example

Summary
DURACOMP: Providing Confidence in Durable Composites

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

Involves six universities
Bath, Bristol, Glasgow, Leeds, Newcastle and Warwick

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

1. Journal
   • Perturbation based stochastic multiscale computational homogenization method for composites
   Formulaing perturbation based homogenization method
   Numerical comparison statistics of elasticity property by perturbation based SFEM with Monte Carlo simulation

2. Conference
   • 12th International Conference on Applications of Statistics and Probability in Civil Engineering, Vancouver, 2015
   [Deadline: June 2014 (Abstract); December 19 2014 (Full paper)]
   [Paper to be prepared]
   Sensitivity study for the homogenized elasticity properties of composites
   Uncertainty categorization and quantification analysis for stochastic reliability analysis of composites

WP3
Next stage plan (March 2014 – July 2014)…
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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.
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

\[
Ku + C^T \lambda = 0 \\
Cu = D\bar{\varepsilon}
\]

where

\[
C = \int_{\Gamma} HN^T N d\Gamma \quad \text{and} \quad D = \int_{\Gamma} HN^T \mathbf{X} d\Gamma
\]

Homogenised stress

\[
\bar{\sigma} = \frac{1}{V} D^T \lambda.
\]

Model Components

RVE boundary conditions

Conduction and diffusion models are considered for thermal and moisture transport problems (conservation of mass or energy for moisture and thermal problem respectively).

\[
\rho c_p \frac{\partial \psi}{\partial t} = K_x \frac{\partial^2 \psi}{\partial x^2} + K_y \frac{\partial^2 \psi}{\partial y^2} + K_z \frac{\partial^2 \psi}{\partial z^2},
\]

Where

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

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

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

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

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

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

Assuming real scenarios of variable temperature and moisture concentration, degradation model is written in rate form as

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

Assuming chemical reaction leading to degradation of mechanical properties is very slow as compared to daily variation of temperature and moisture concentration

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

Generalised degradation model

\[ \frac{d}{dt} (1 - \omega) = -c \beta \ln \left(1 - \frac{T}{T_g}\right) (1 - \omega) \]

\[ \omega = 0 \quad \text{no degradation} \]

\[ \omega = 1 \quad \text{fully degradation} \]
For the macro-level structure, a three-dimensional block of material is considered. The macro-structure and RVE are discretised with 10285 elements and 2364 nodes, which is the case of the RVE. For the macro-level thermal problem, the bottom surface is fixed while a constant traction of $1000 \text{ MPa}$ is applied to the top surface and constant heat flux is applied to the left side of the macro-block.

Thermal conductivity, density, and specific heat of the block are fully fixed, while a constant traction of $1000 \text{ MPa}$ is applied to the top surface and constant heat flux is applied to the left side of the macro-block. Due to its higher value of heat conductivity, moisture concentration of $7$ days for total of $110$ days. At the end of the simulation, temperature and vertical displacement are used, while the corresponding values used for the fibres are $1000$, $1.46$, and $2.8$ respectively.

Moreover, a Moisture transport analysis of degradation parameter $1/(1 - \omega)$ is calculated for each mechanical RVE and pass back on the macro-mesh. Temperature and moisture concentration fields are approximated as $T_0 + \omega T_1$ and $C_0 + \omega C_1$ respectively.

Homogenised value of $K_T$ for $\overline{K_T}$.

Homogenised value of $K_c$ for $\overline{K_c}$.

Macro transient thermal analysis

Macro transient diffusion analysis

Macro mechanical analysis at selected time steps

Mechanical RVE

$C_{\text{matrix}} = (1 - \omega)C_{\text{matrix}}$
Numerical Example
Geometries, meshes and BCs

- Simulation time = 1000 days
- Number of time steps = 100
- Mechanical problem was run for every 10\textsuperscript{th} step

Macro structure geometry
Macro structure mesh (780 elements)
Representative volume element (10285 elements)
Matrix as isotropic material

(2 elastic constants) $E$, $\nu$

Fibres as transversely isotropic material

(5 elastic constants) $E_p$, $\nu_p$, $E_z$, $\nu_{pz}$, $G_{pz}$

A potential flow problem is described by

$$\nabla^2 \varphi = \frac{\partial^2 \varphi}{\partial x^2} + \frac{\partial^2 \varphi}{\partial y^2} + \frac{\partial^2 \varphi}{\partial z^2} = 0$$

Velocity is a vector

$$\mathbf{v} = \nabla \varphi$$

Rotation of stiffness matrix

$$C^* = T_{\sigma} C T_{\epsilon}^{-1}$$
Numerical Example

RVE convergence studies

**Thermal & Moisture Transport RVEs**

<table>
<thead>
<tr>
<th>Order</th>
<th>DOFs</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>2,364</td>
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<tr>
<td>2</td>
<td>16,214</td>
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<td>3</td>
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**Mechanical RVE**

<table>
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<td>1</td>
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<tr>
<td>2</td>
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<tr>
<td>3</td>
<td>155,508</td>
</tr>
</tbody>
</table>
Numerical Example

Results

Moisture concentration
Temperature (°C)
(1 − ω) field
Vertical displacement (mm)

Moisture concentration vs. Time (days)

Temperature (°C) vs. Time (days)

(1 − ω) vs. Time (days)

Relative displacement (mm) vs. Time (days)
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 (FE\(^2\)) 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.