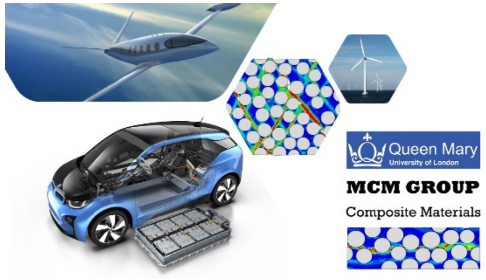

Hygroscopic Phase Field Failure Modelling of Composite Materials

ICCM23, Belfast, 30th July-4th August 2023

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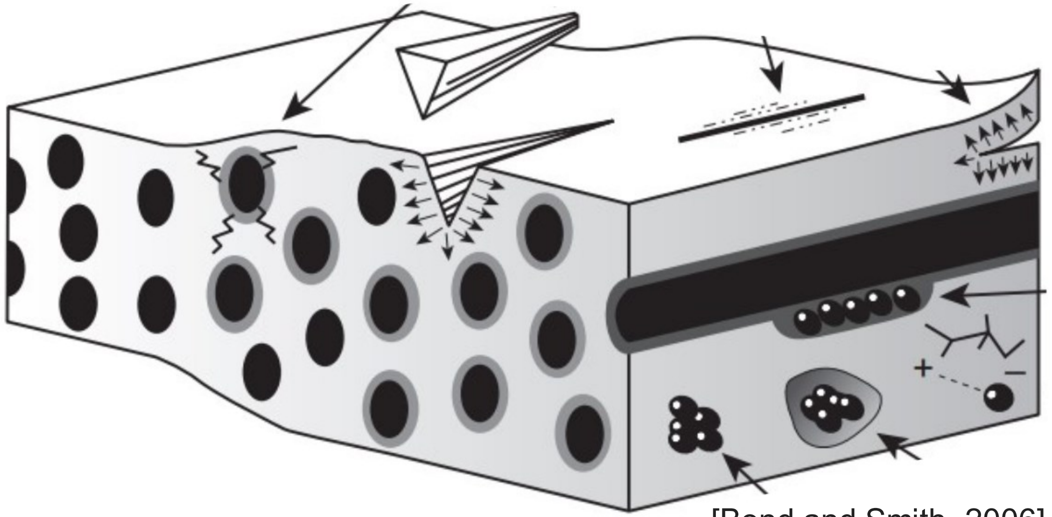
With excellent contributions from:

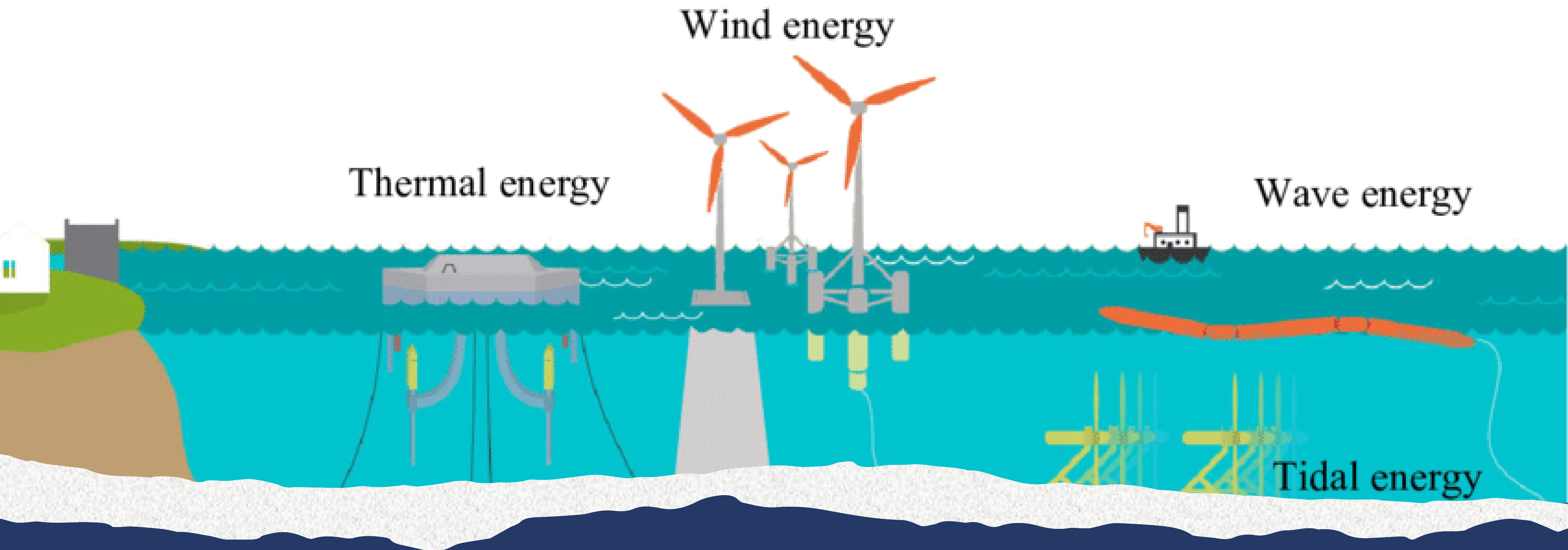
Kit Au-Yeung (QMUL), Emilio Martínez-Pañeda (Imperial), Adria Quintanas Corominas (Imperial, BSC), and many others.



[Bond and Smith, 2006]

Outline

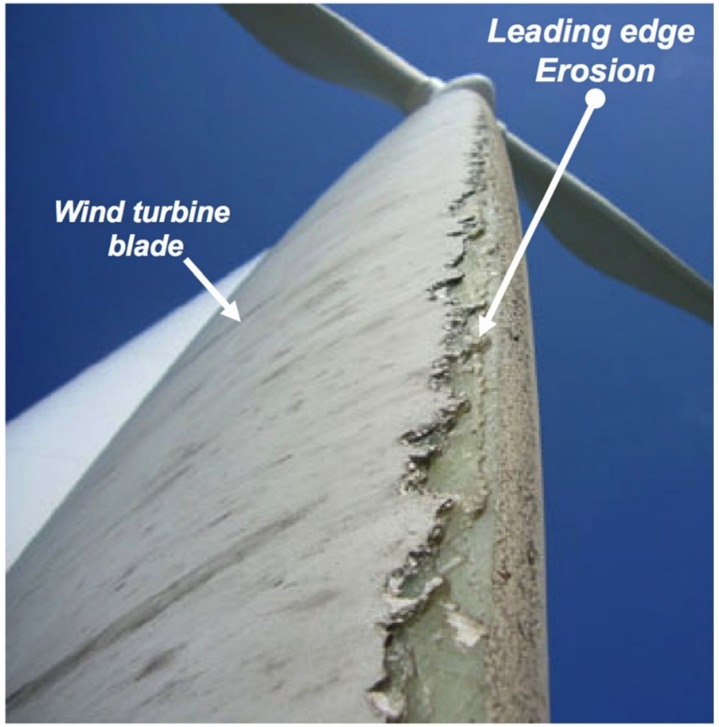
1. Motivation
2. Methods
3. Results

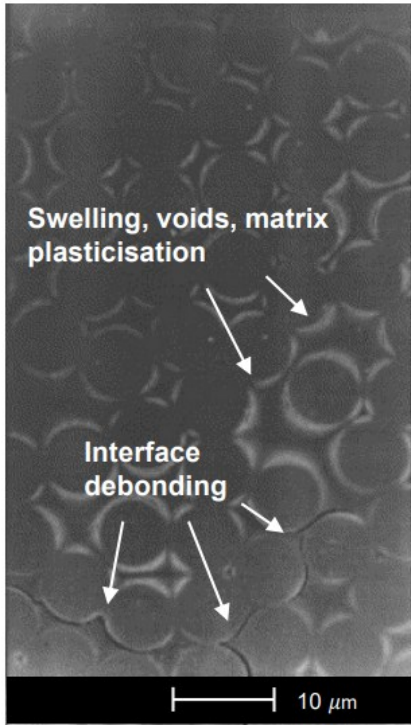


Background: Offshore energy

- Offshore energy is an effective solution to produce clean energy and mitigate global warming, including wind, wave, tidal and thermal, etc.
- Global offshore wind is expected to reach **2000 GW** by 2050. Wave and tidal energy would represent an additional **350 GW**.
- This can power **~ 2 billion** household, **~ 50%** of the population.
- This highlights the need for further investment and research in this area.

[1] Bastien Taormina, PhD thesis, 2019
[2] https://www.irena.org/publications/2021/Jul/Offshore-Renewables-An-Action-Agenda-for-Deployment





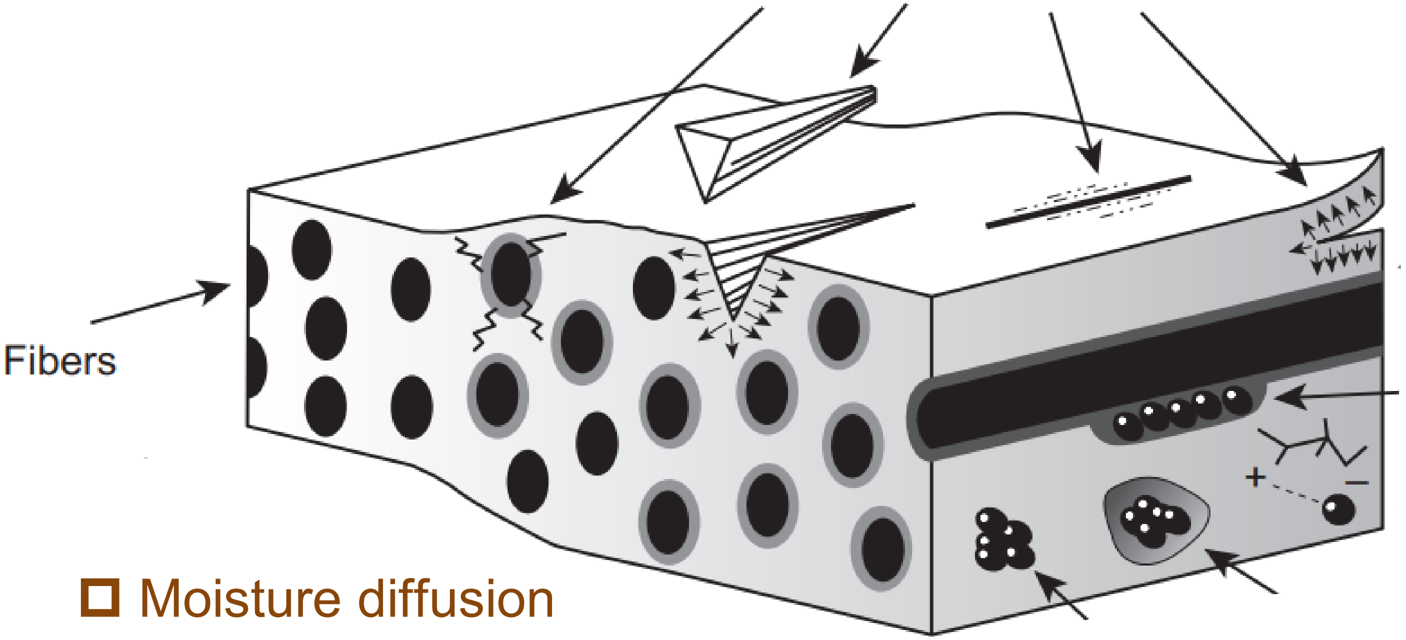
Problem:
Material degradations

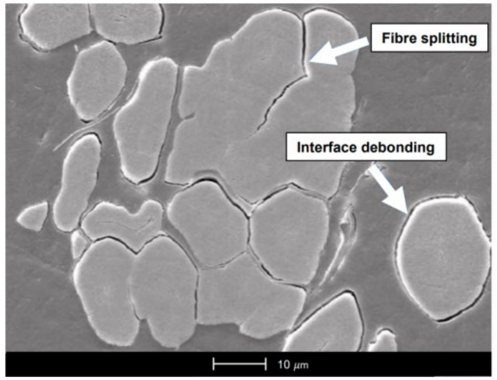
- Lightweight **composite materials** have been widely used in offshore energy (e.g. wind blades).
- In service, the offshore structures continuously experiences **extreme weather conditions.**
- Particularly the effect of **loading conditions**, **temperature, moisture** is detrimental.

Moisture: Multiphysics degradation mechanisms

➢ Exposure to moisture can degrade the mechanical properties of composite materials.

☐ Plastication or Hydrolysis





☐ Moisture diffusion

☐ Matrix swelling

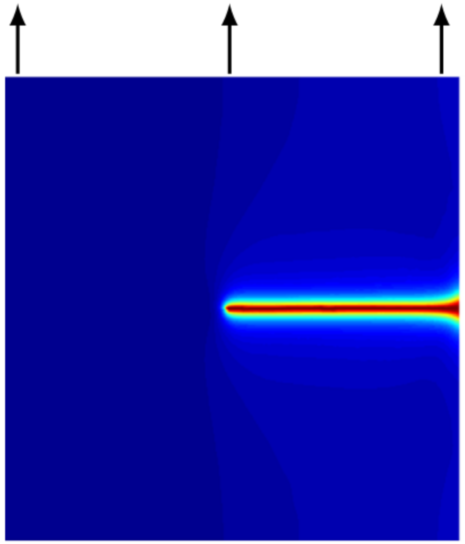
☐ Interface debonding

➢ **State-of-art: Modelling moisture-assisted degradation of composites remains relatively unexplored.**

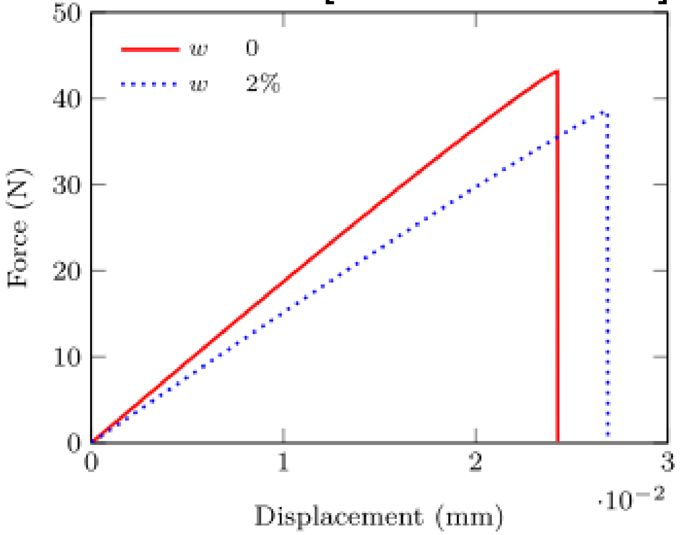
➢ Our aim: To develop **fully-coupled computational** models for moisture-assisted degradation.

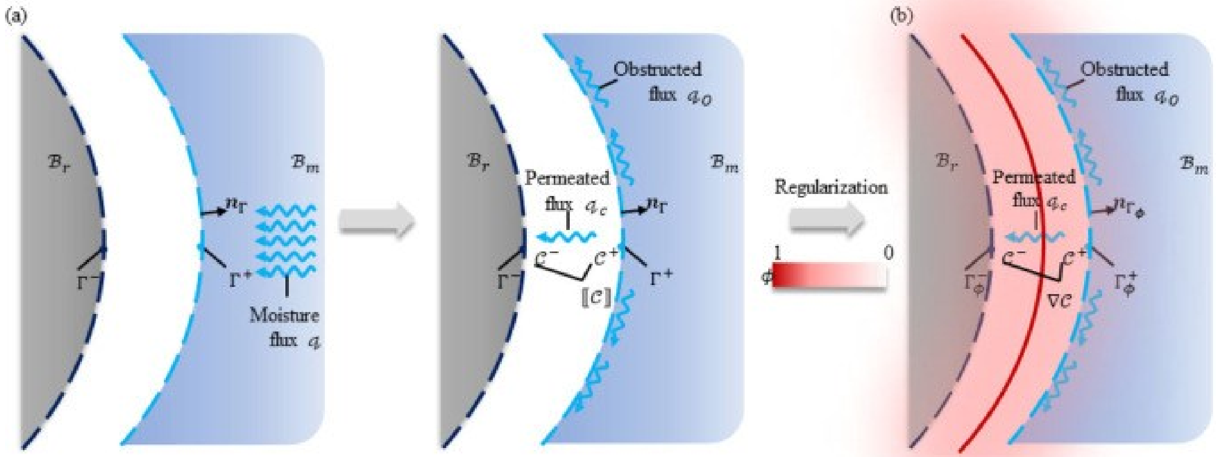
[1] David A., Bond and Paul A. Smith. (2006): 249-268.

State-of-art: Modelling moisture-assisted degradation in composites remains relatively unexplored



[Arash et al. 2022]





[Ye et al. 2022]

- The **moisture transport** problem was not explicitly resolved and, instead, a uniform moisture distribution was assumed.

- “**Crack filter theory**” is proposed to regularise the sharp fibre-matrix interface and controls the moisture fluxes.

- Finding the coefficients for the crack filter functions remains a challenge.

[1] Arash, B., Exner, W., Rolfes, R. Engineering with Computers (2022).
[2] Ye, J.-Y., Zhang, L.-W Computer Methods in Applied Mechanics and Engineering 388, 114213 (2022).

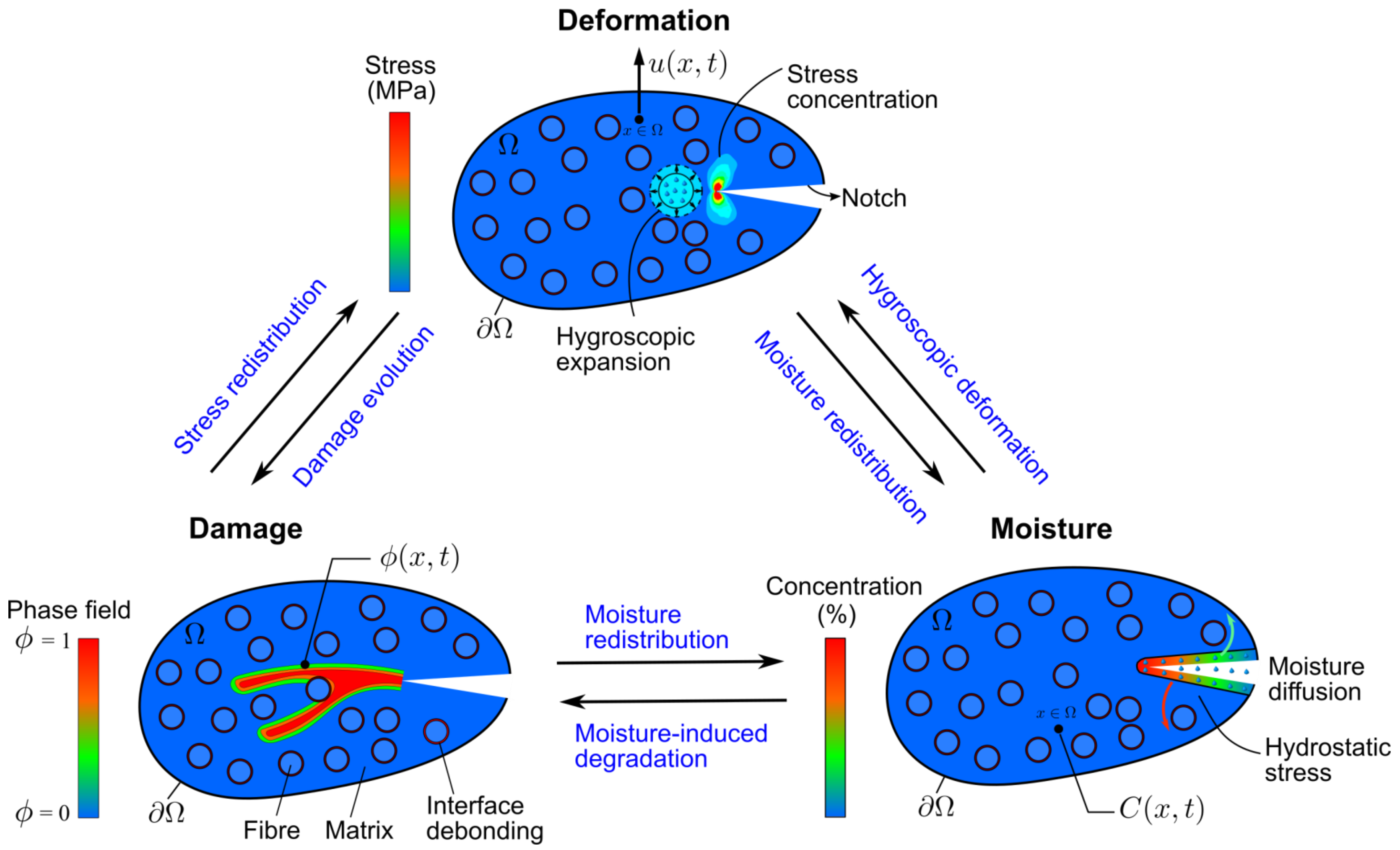
Outline

1. Motivation

2. Methods

3. Results

Fully coupled multiphysics phase field model



- The interplay between **moisture diffusion**, **hygroscopic expansion**, **crack evolution** and **stress redistribution**.

[1] Au-Yeung K, Quintanas-Corominas A, Martínez-Pañeda E., Tan W, *Engineering with Computer* (2023)

Mass transport: Moisture diffusion

- **Fick's law**

$$\frac{\partial C}{\partial t} = D\nabla^2 C$$

C - moisture concentration
D - Diffusion coefficient
t - time

- **Chemical potential of moisture**

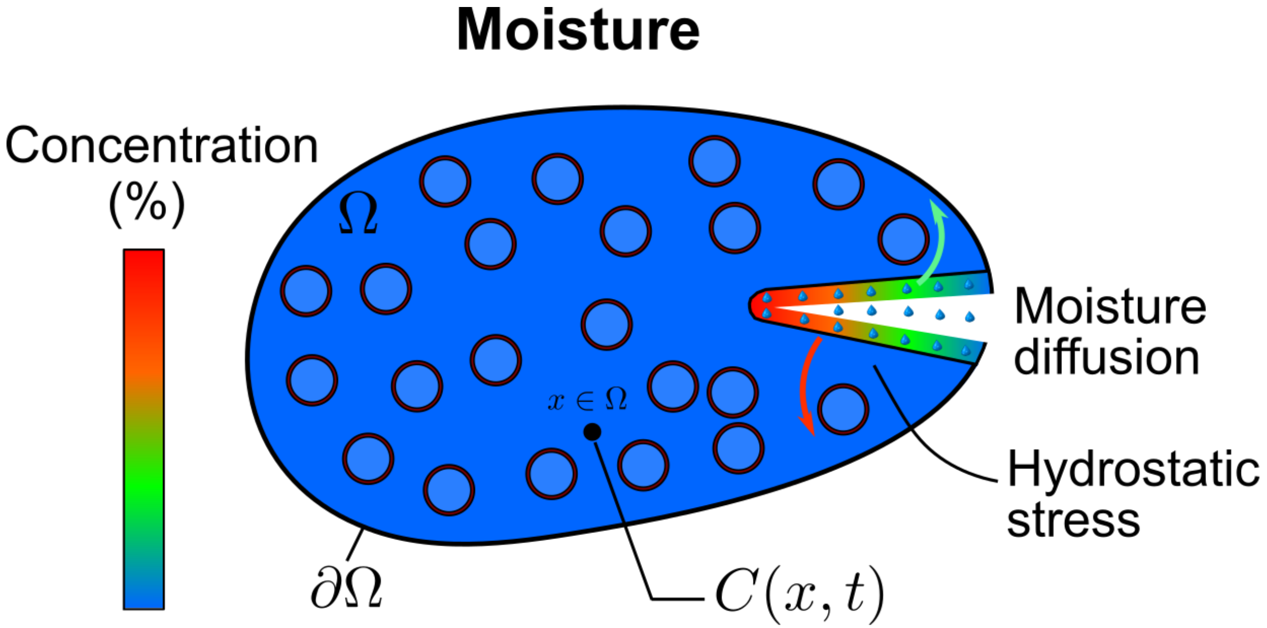
$$\mu = \mu^0 + RT\ln C - \bar{V}_H\sigma_H$$

- **Mass flux (Linear Onsager)**

$$\mathbf{J} = -\frac{DC}{RT}\nabla\mu = -D\nabla \mathrm{C} + \frac{D}{RT}C\bar{V}_H\nabla\sigma_H$$

- **Balance equation (mass conservation)**

$$\frac{\mathrm{d}C}{\mathrm{d}t} + \nabla\cdot\mathbf{J} = 0$$



- **The weak form of moisture diffusion:**

$$\int_\Omega \left[\delta C\left(\frac{1}{D}\frac{\mathrm{d}C}{\mathrm{d}t}\right) + \nabla \mathrm{C}\nabla\delta \mathrm{C} - \nabla\delta C\left(\frac{\bar{V}_H C}{RT}\nabla\sigma_H\right)\right]\mathrm{d}V = -\frac{1}{D}\int_{\partial\Omega_q}\delta C q\,\mathrm{d}S$$

[1] Au-Yeung K, Quintanas-Corominas A, Martínez-Pañeda E., Tan W, *Engineering with Computer* (2023)

Deformation: The effect of moisture

Moisture concentration leads to the presence of hygroscopic strains:

- **Hygroscopic strain**

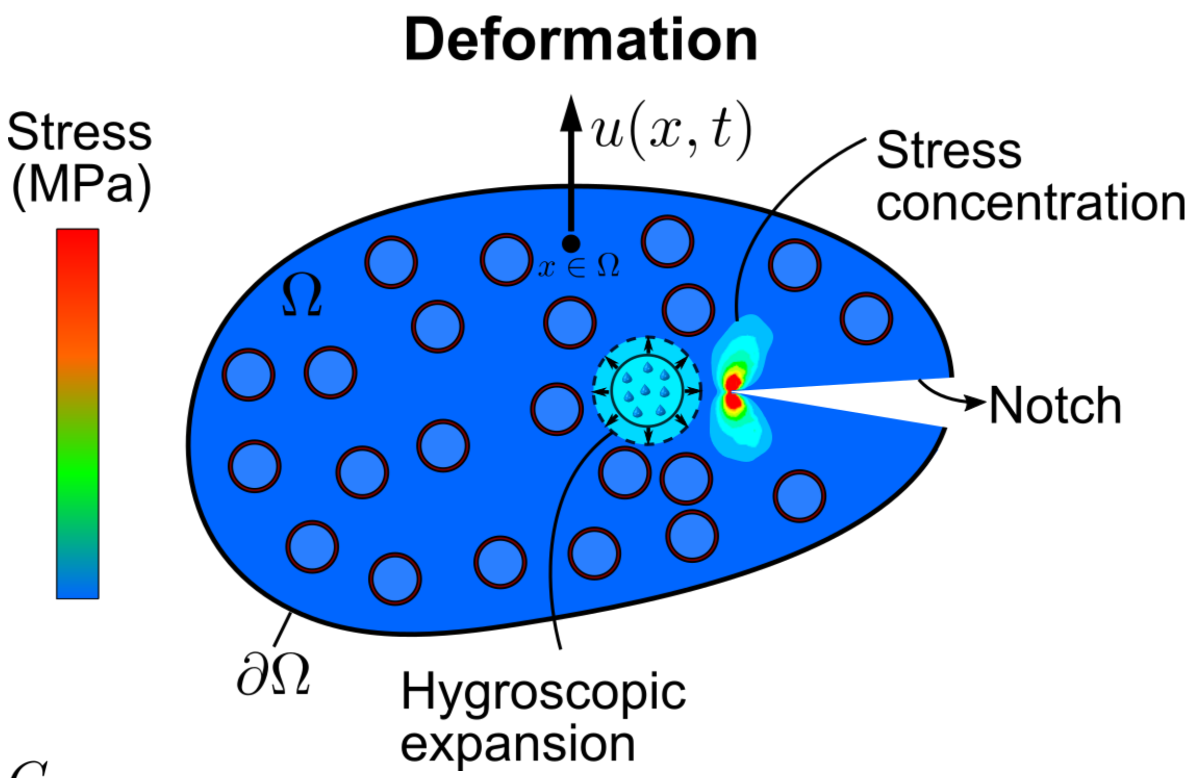
$$\boldsymbol{\varepsilon}^m = \alpha\left(C - C_0\right)$$

- **Cauchy stress**

$$\boldsymbol{\sigma}_0 = \mathcal{C}\boldsymbol{\varepsilon}^e = \mathcal{C}\left(\boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}^m\right)$$

- **Moisture-dependent fracture toughness:**

$$G_c^I = \begin{cases} a_1 \exp(a_2 C) + a_1 \exp(a_2 C) & C < C_0 \\ G_{c0} & C \geq C_0 \end{cases}$$

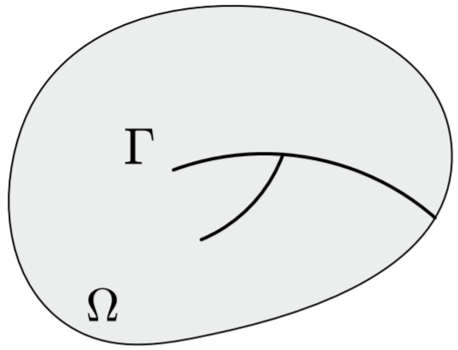


Damage: Phase field fracture model

- **Griffith's energy balance [Griffith, 1920]**

$$\frac{d\Pi}{dA} = \frac{d\psi}{dA} + G_c = 0$$

Π - total potential energy
A - crack area
Ψ - strain energy density
G_c - critical energy release rate



- **Variational approach to fracture [Francfort and Marigo, 1998]**

$$\min \ \Pi = \int_\Omega \psi\left(\boldsymbol{\varepsilon}\right)\, \mathrm{d}V + \underline{\int_\Gamma G_c \, \mathrm{d}S} - \int_\Omega b \cdot \delta u \, \mathrm{d}V - \int_{\partial\Omega_h} h \cdot \delta u \, \mathrm{d}S$$

- **Phase field fracture [Bourdin et al., 2008, Miehe et al., 2010]**

$$\min \ \Pi_\ell = \int_\Omega (1-\phi)^2 \, \psi\left(\boldsymbol{\varepsilon}\right)\, \mathrm{d}V + \underline{\int_\Omega G_c \left(\frac{\phi^2}{2\ell} + \frac{\ell}{2}|\nabla\phi|^2\right)} \, \mathrm{d}V - \int_\Omega b \cdot \delta u \, \mathrm{d}V - \int_{\partial\Omega_h} h \cdot \delta u \, \mathrm{d}S$$

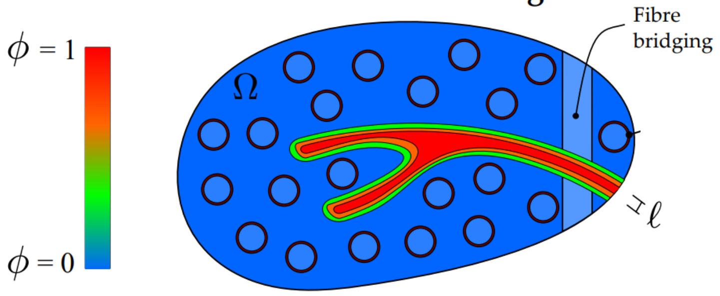
- **Coupled field equations:**

$$(1-\phi)^2 \, \nabla \cdot \boldsymbol{\sigma} = \mathbf{0} \quad \text{in} \quad \Omega$$

$$G_c \left(\frac{\phi}{\ell} - \ell \Delta\phi\right) - 2(1-\phi)\,\psi = 0 \quad \text{in} \quad \Omega$$

ϕ - damage variable
ℓ - length scale

Phase field: matrix and fibre cracking

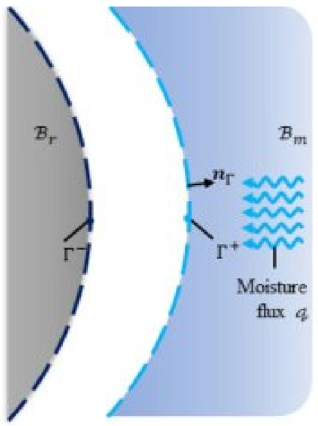


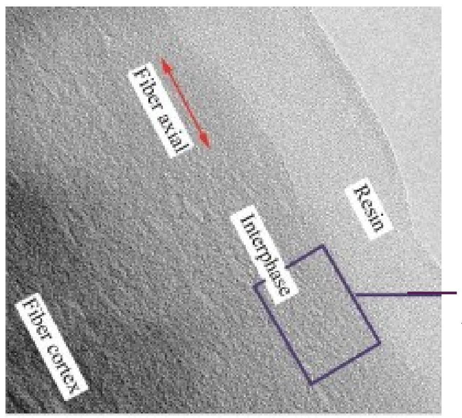
- **Crack increases the diffusion coefficient:**

$$D = D_0[1 + k_d \mathrm{H}(\phi)(\phi - \phi_{th})]$$

Diffuse interface (Phase field)

Challenge: **Sharp interfaces** can not model the moisture diffusion and represent the graded interface.





Graded structure

- A diffuse transition zone between the fibre and matrix:

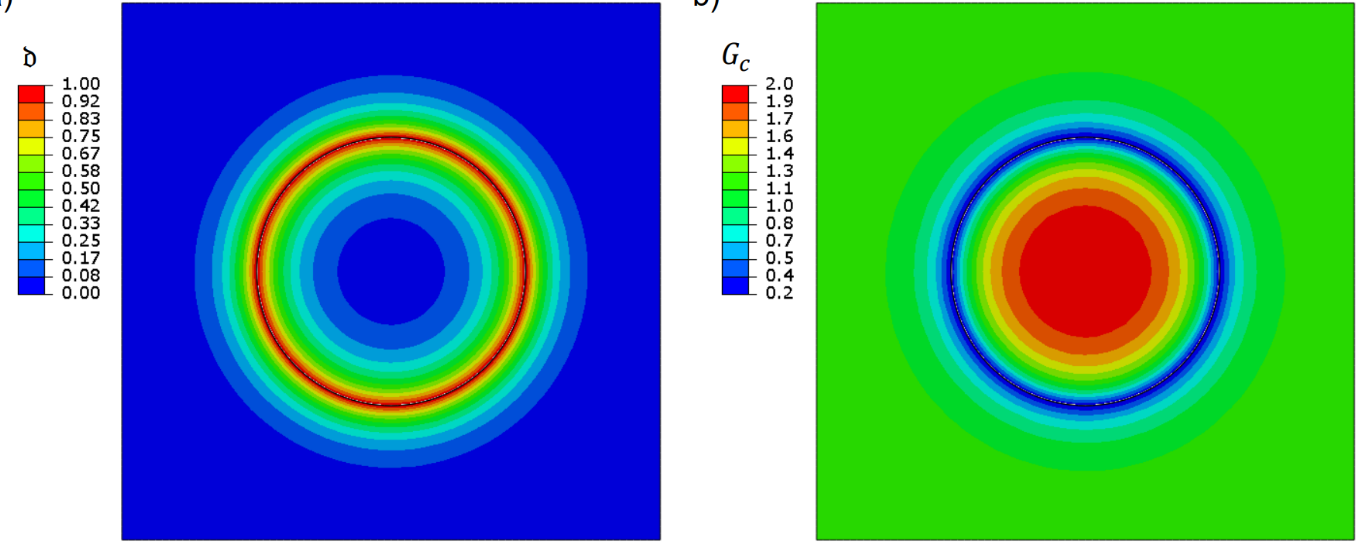
$$\begin{cases} \mathfrak{d} - \ell_{\mathfrak{d}}^2 \, \nabla^2 \mathfrak{d} = 0 & \text{in} \quad \Omega \\ \mathfrak{d}\,(0) = 1 & \text{on} \quad \Gamma \\ \nabla \mathfrak{d} \cdot \mathbf{n} = 0 & \text{on} \quad \partial\Omega \end{cases}$$

- An interpolation function:

$$G_c = h(\mathfrak{d}) \left(G_c^{(i)} - G_c^I \right) + G_c^I$$

$$D = h(\mathfrak{d}) \left(D^{(i)} - D_I \right) + D_I$$

a) b)



(a) phase field interface indicator
(b) interpolation of material toughness across the interface

[1] Ye, J.-Y., Zhang, L.-W Computer Methods in Applied Mechanics and Engineering 388, 114213 (2022).
[2] Au-Yeung K, Quintanas-Corominas A, Martínez-Pañeda E., Tan W, *Engineering with Computer* (2023)

Finite element discretisation

The weak form for the **coupled deformation-phase field fracture problem** is formulated as:

$$\int_\Omega \left[(1-\phi)^2 \boldsymbol{\sigma}_0 : \delta\boldsymbol{\varepsilon} - 2(1-\phi)\delta\phi\,\mathcal{H} + G_c \left(\frac{\phi}{\ell}\delta\phi + \ell\nabla\phi\cdot\nabla\delta\phi \right) \right] \mathrm{d}V = 0$$

The **deformation**, **diffusion** and **phase field** fracture problems are weakly coupled.

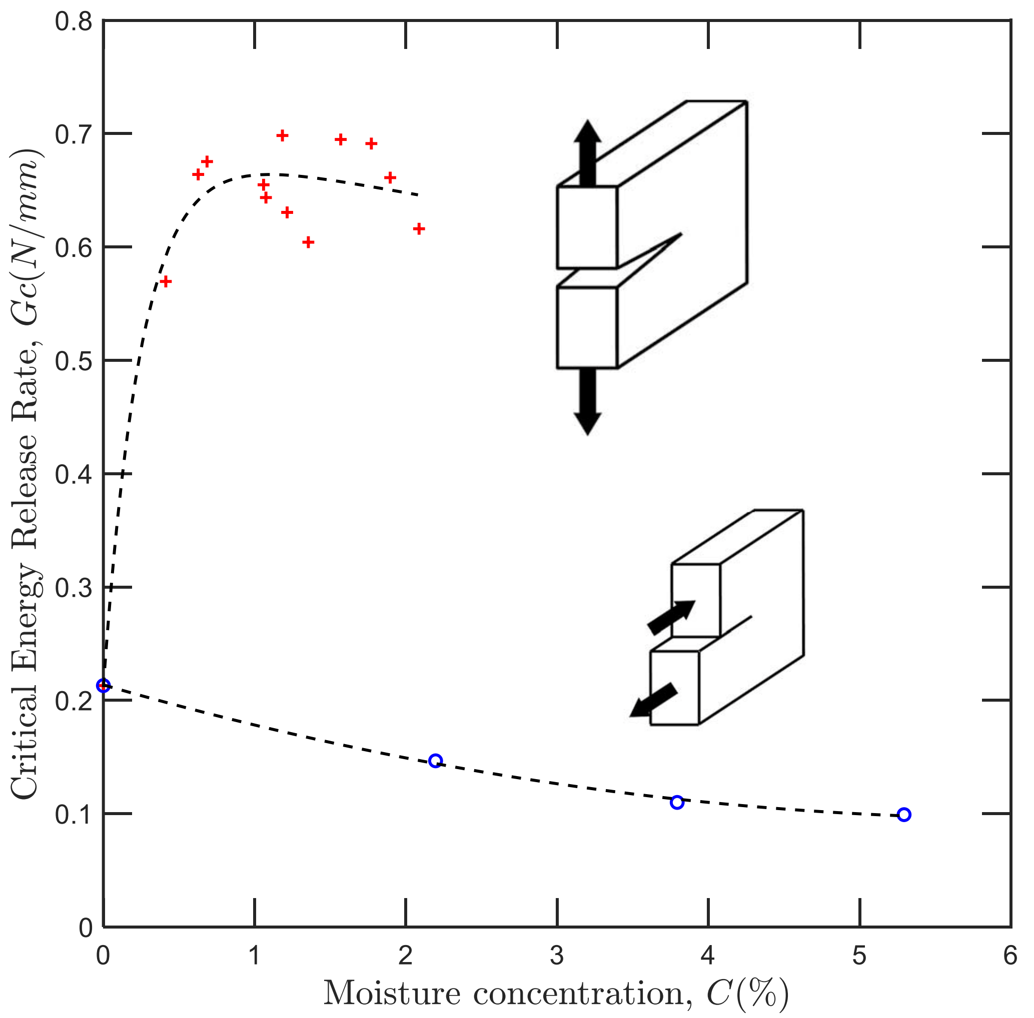
$$\begin{bmatrix} \boldsymbol{K}^{\mathbf{u}} & 0 & 0 \\ 0 & \boldsymbol{K}^{\phi} & 0 \\ 0 & 0 & \boldsymbol{K}^{C} \end{bmatrix} \begin{bmatrix} \mathbf{u} \\ \boldsymbol{\phi} \\ \boldsymbol{C} \end{bmatrix} + \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & \boldsymbol{M} \end{bmatrix} \begin{bmatrix} \dot{\mathbf{u}} \\ \dot{\boldsymbol{\phi}} \\ \dot{\boldsymbol{C}} \end{bmatrix} = \begin{bmatrix} \boldsymbol{r}^{\mathbf{u}} \\ \boldsymbol{r}^{\phi} \\ \boldsymbol{r}^{C} \end{bmatrix}$$

It is solved in an incremental manner, using the Newton-Raphson method. The solution scheme follows a so-called **staggered** approach.

Outline

1. Motivation
2. Methodologies
3. Results

The effect of moisture on fracture toughness: Mode I vs Mode II



Mode I: (Toughening)

$$G_c^I = \begin{cases} a_1 \exp(a_2 C) + a_1 \exp(a_2 C) & C < 2.09\% \\ 0.62 & C \geq 2.09\% \end{cases}$$

$$a_1 = 0.70\,,\ a_2 = -3.71,\ a_3 = -0.49,\ a_4 = -395.2$$

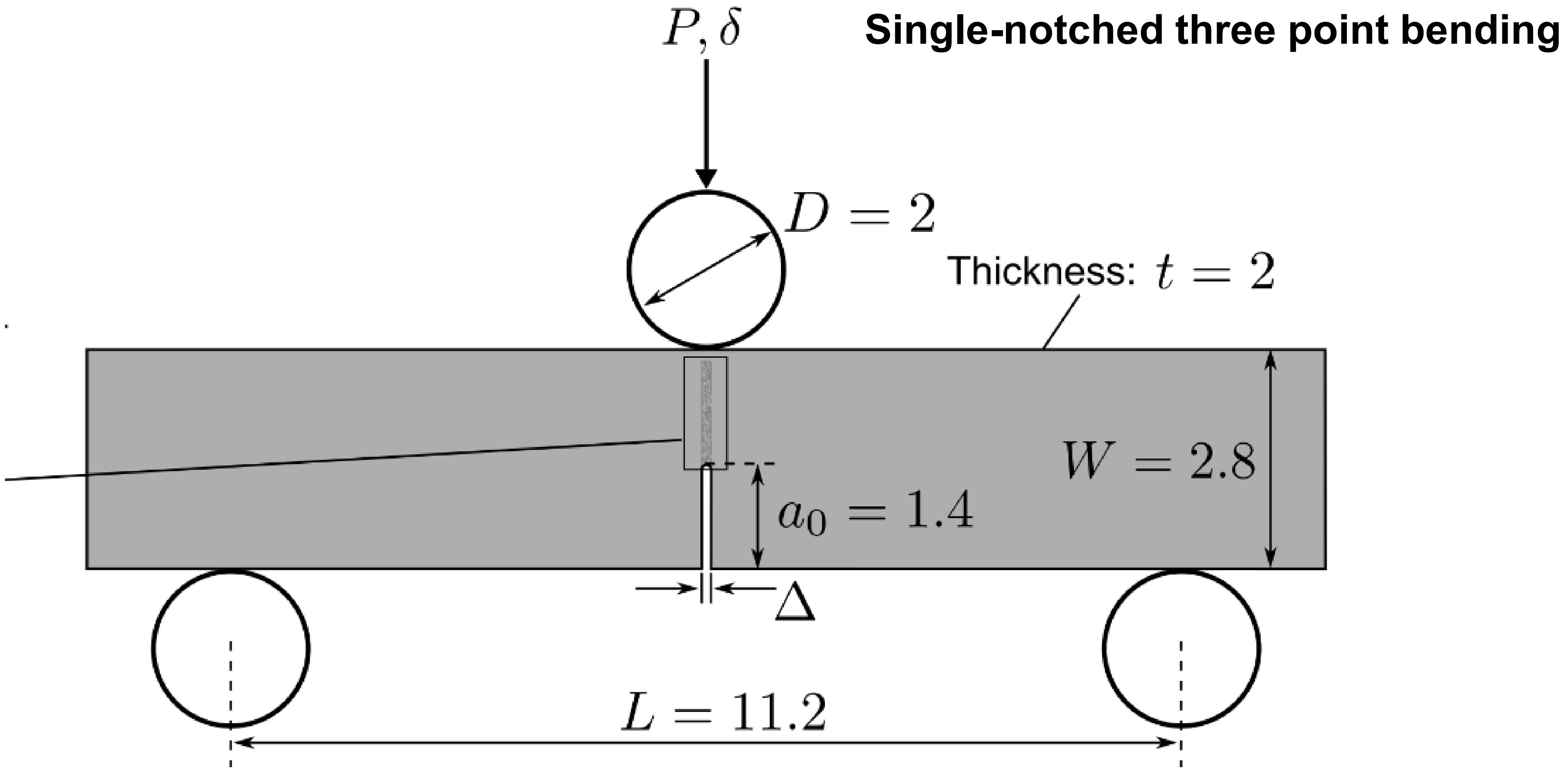
Mode II: (Embrittlement)

$$G_c^{II} = \begin{cases} b_1 C^2 + b_2 C + b_3 & C < 6.08\% \\ 0.096 & C \geq 6.08\% \end{cases}$$

$$b_1 = 31.58,\ b_2 = -3.85,\ b_3 = 0.21$$

[1] Sugiman, S., Putra, I.K.P. and Setyawan, P.D., *Polymer Degradation and Stability*, *134*, pp.311-321 (2016).
[2] Johar, M., Chong, W.W.F., Kang, H.S. and Wong, K.J., 2019. *Polymer degradation and stability*, *165*, pp.117-125.

Case study 1: Moisture content on the fracture toughness (mode I)

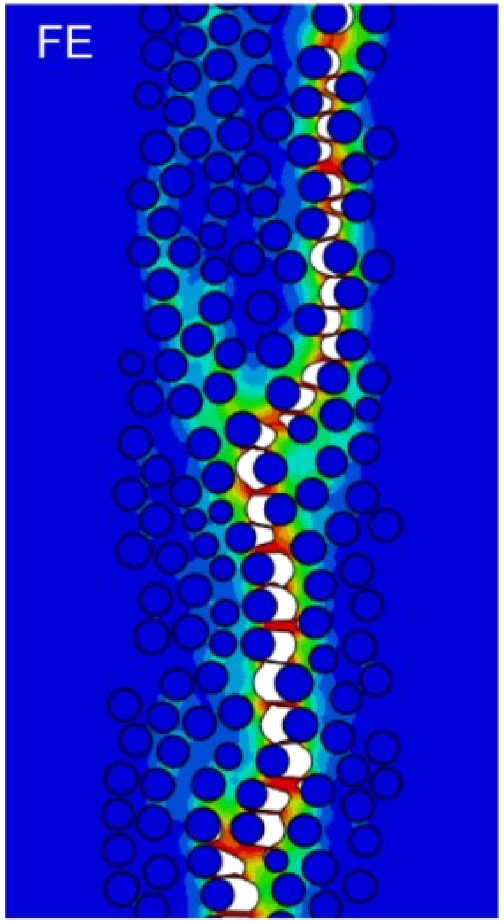


- The actual microstructure of the composite is simulated by an **embedded cell** in the fracture process zone, while the remaining area is homogenised to be an elastic anisotropic solid.

[1] Tan W, Martínez-Pañeda E., *Composites Science and Technology* (2021)
[2] Tan W, Martínez-Pañeda E., *Composites Structures* (2022), 115242

Microscopic crack growth and fracture toughness (Validation)

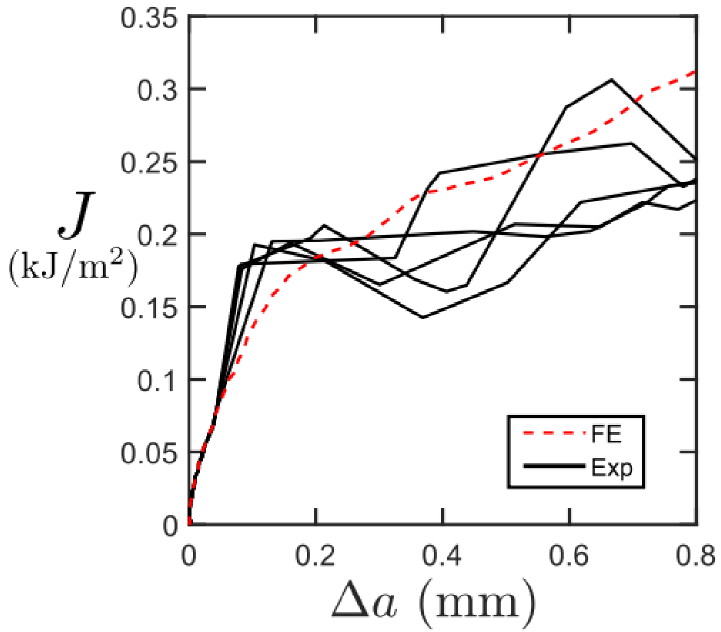
[Canal et al. 2012]



$\Delta = 53\mu m$

Cohesive zone (I) + PFM (M)

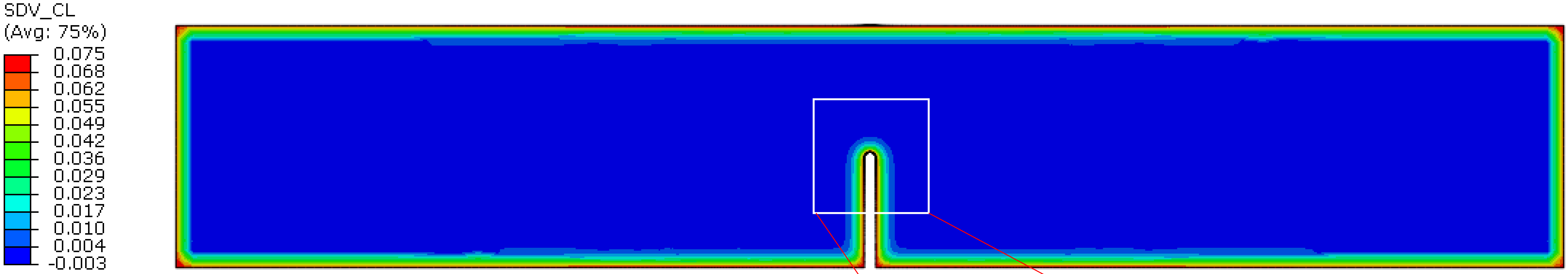
Constituents	E (GPa)	G_c (kJ/m^2)
Glass fibre	74	0.135
Epoxy matrix	3.5	0.010
Interface	5.0	0.005

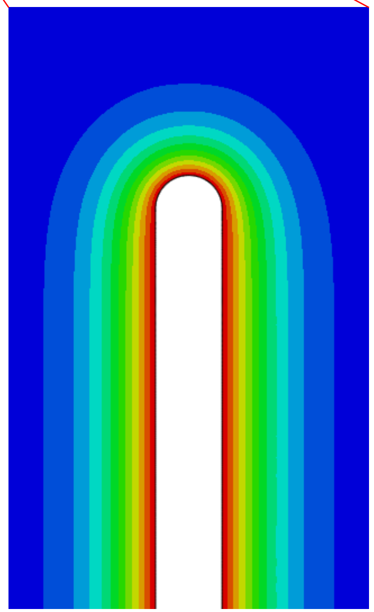


G_c^{22}: Transverse frature toughness

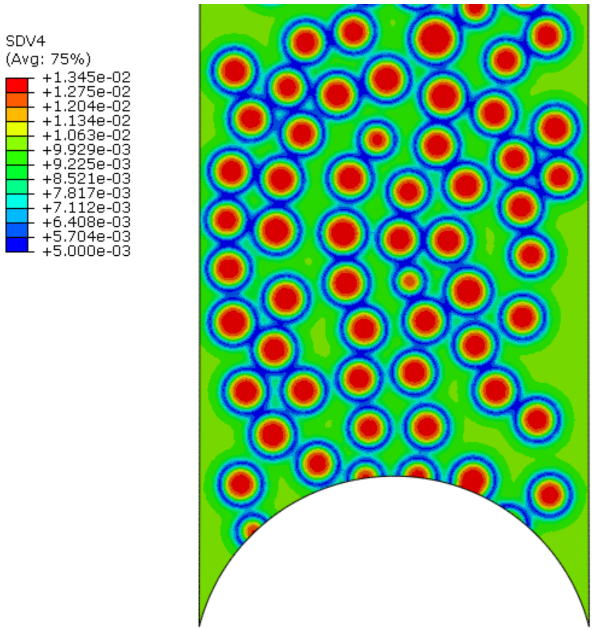
[1] Tan W, Martínez-Pañeda E., *Composites Science and Technology* (2021)

Now consider the moisture effect:





Diffused interface

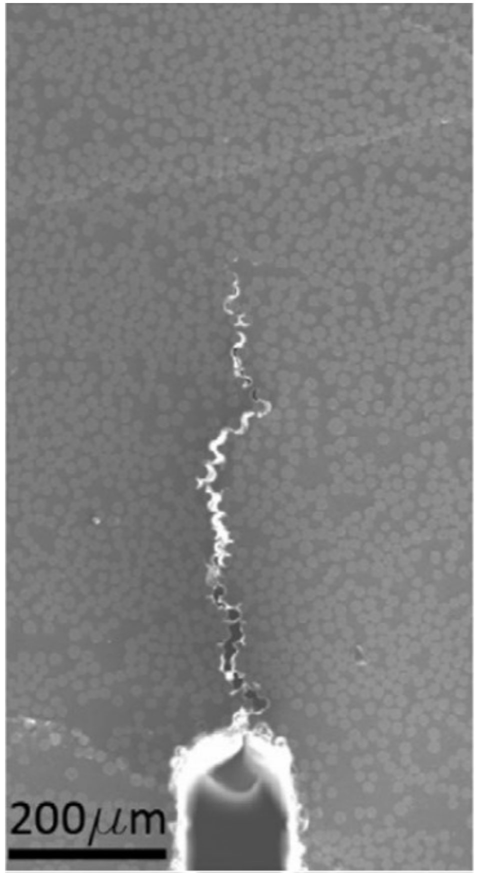


Graded material properties

Moisture diffusion

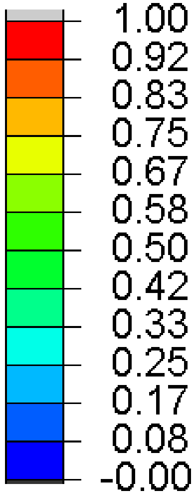
The effect of moisture on crack trajectories

Experiment-Dry

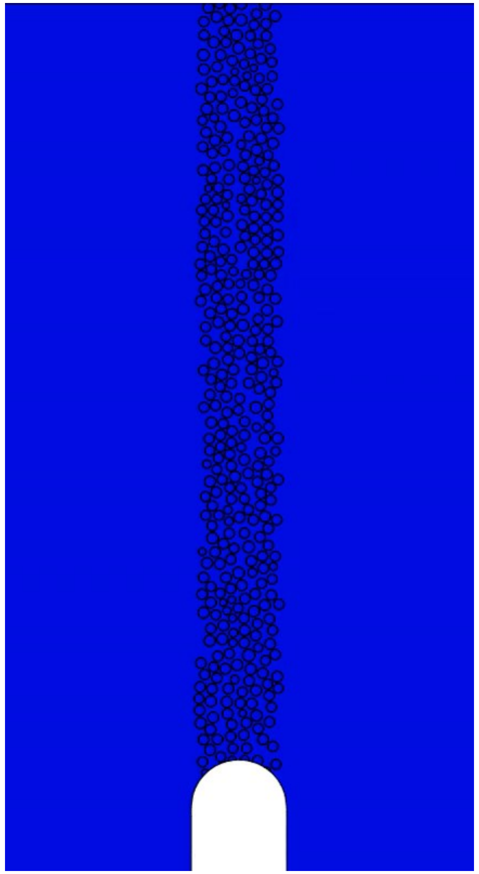


Phase field damage

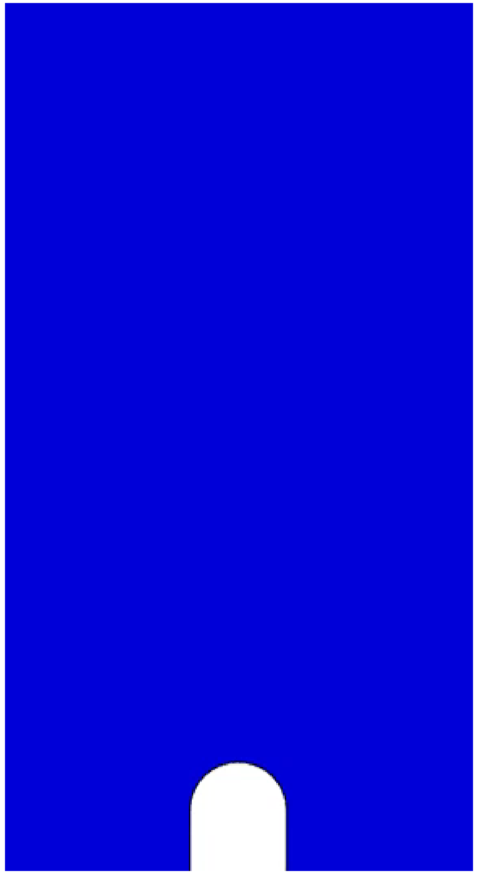
ϕ



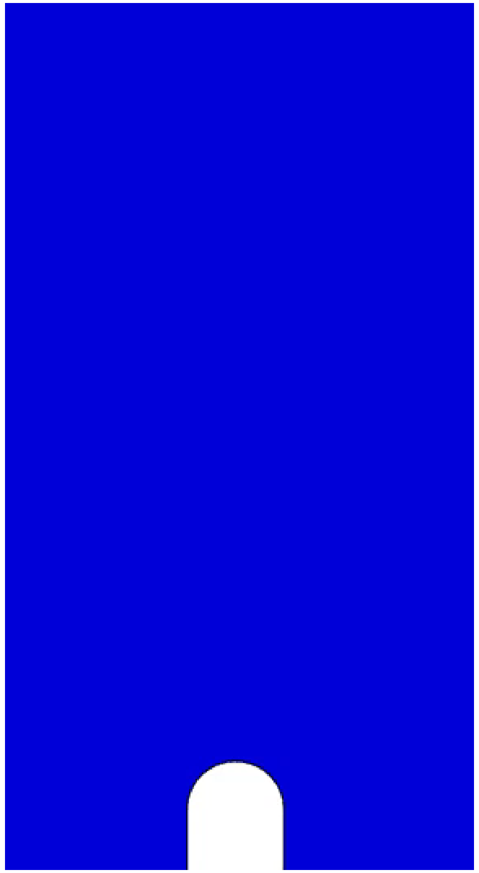
Cohesive zone-Dry



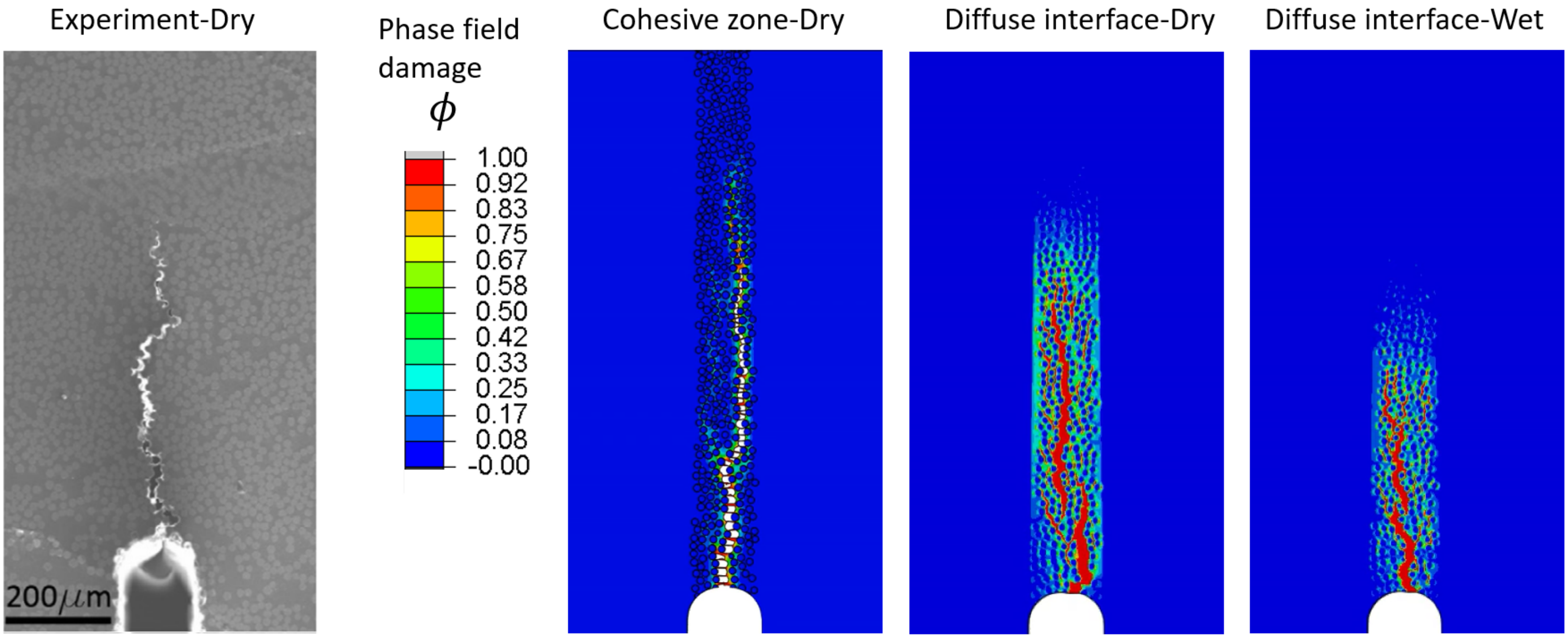
Diffuse interface-Dry



Diffuse interface-Wet



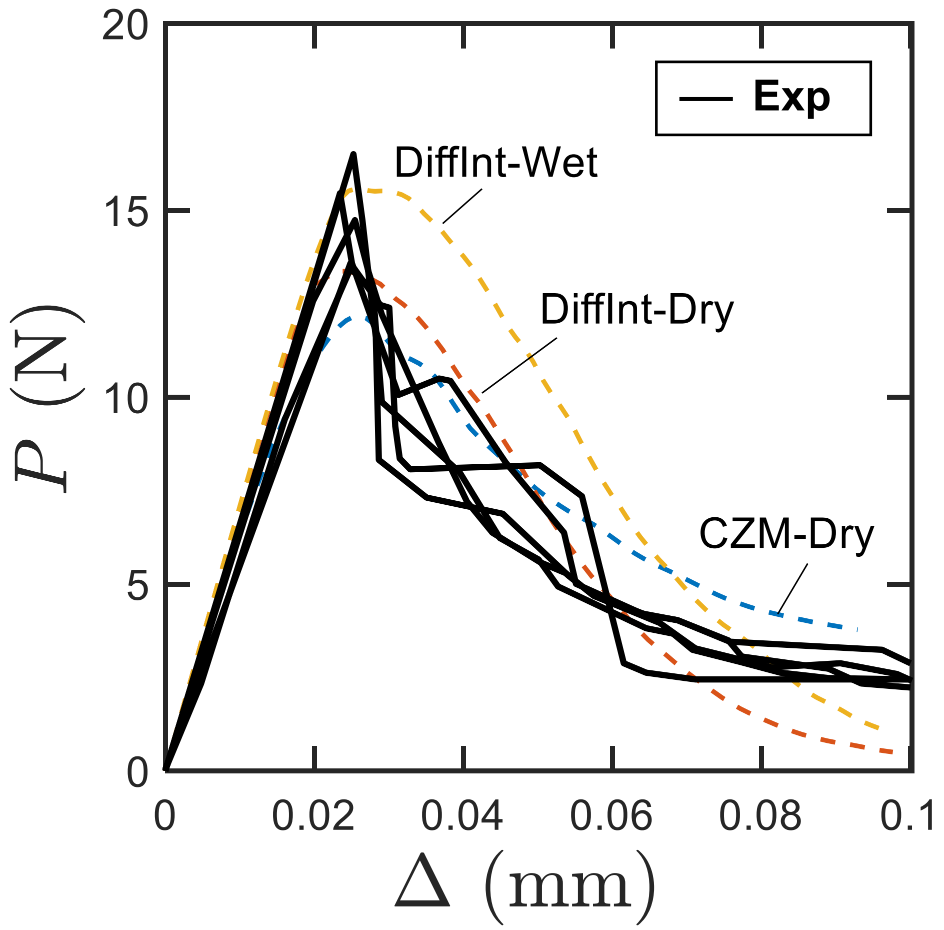
The effect of moisture on crack trajectories



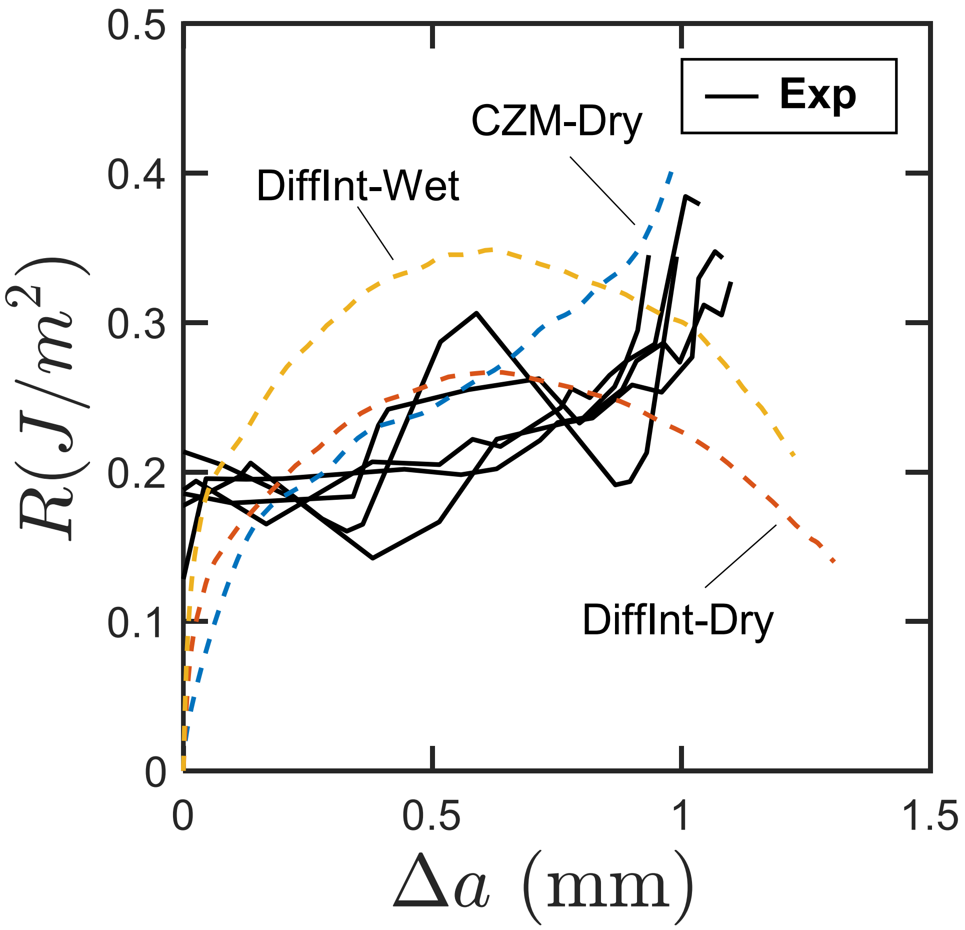
- Diffuse interface model shows a diffused crack propagation.
- The moisture content impedes the crack propagation under mode I loading.

The effect of moisture on fracture toughness

Load-displacement curves



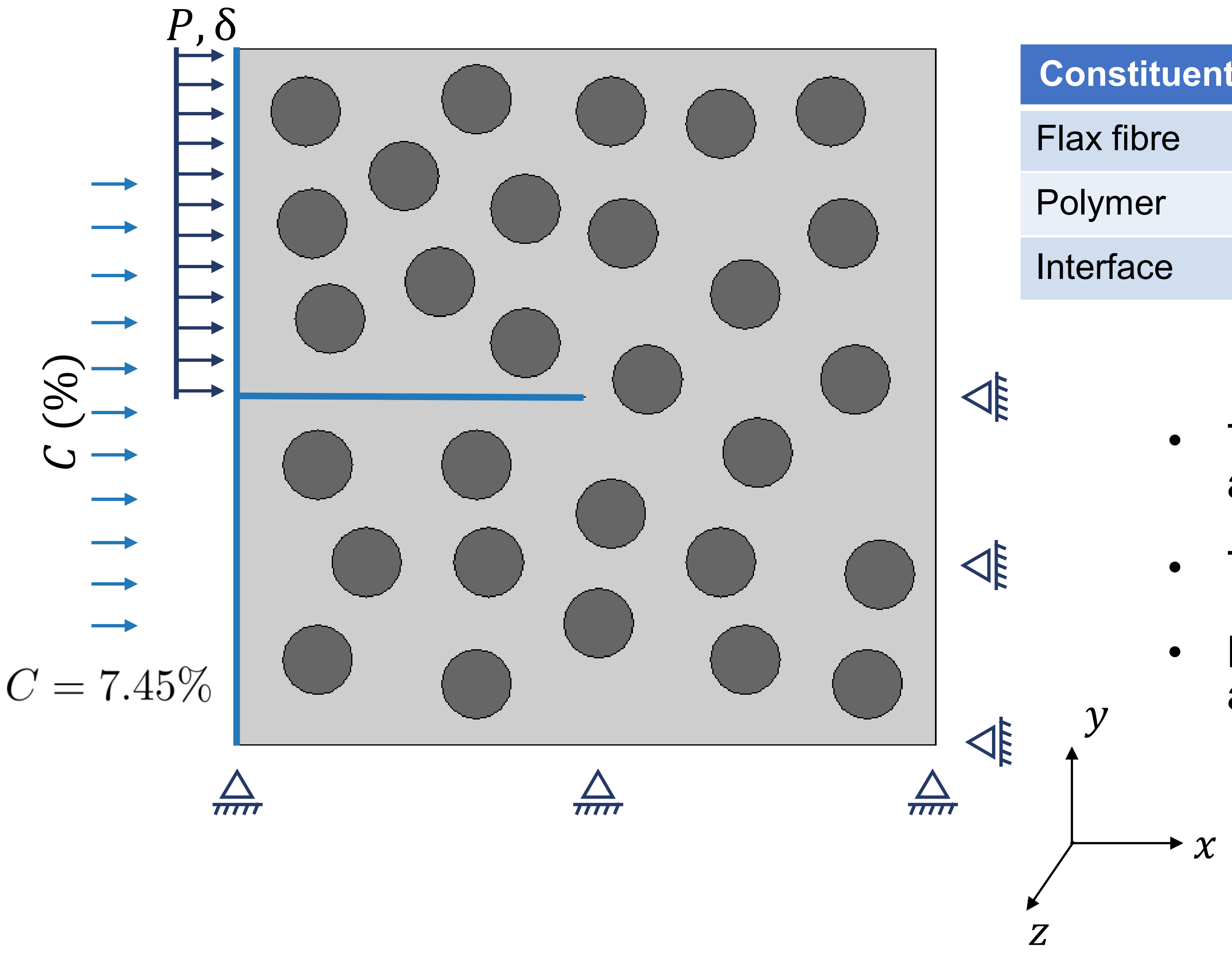
R-curves



- The fracture resistance increases with the increasing moisture contents.

Case study 2: A single notched sample under shear loading (mode II)

End-notch shear:



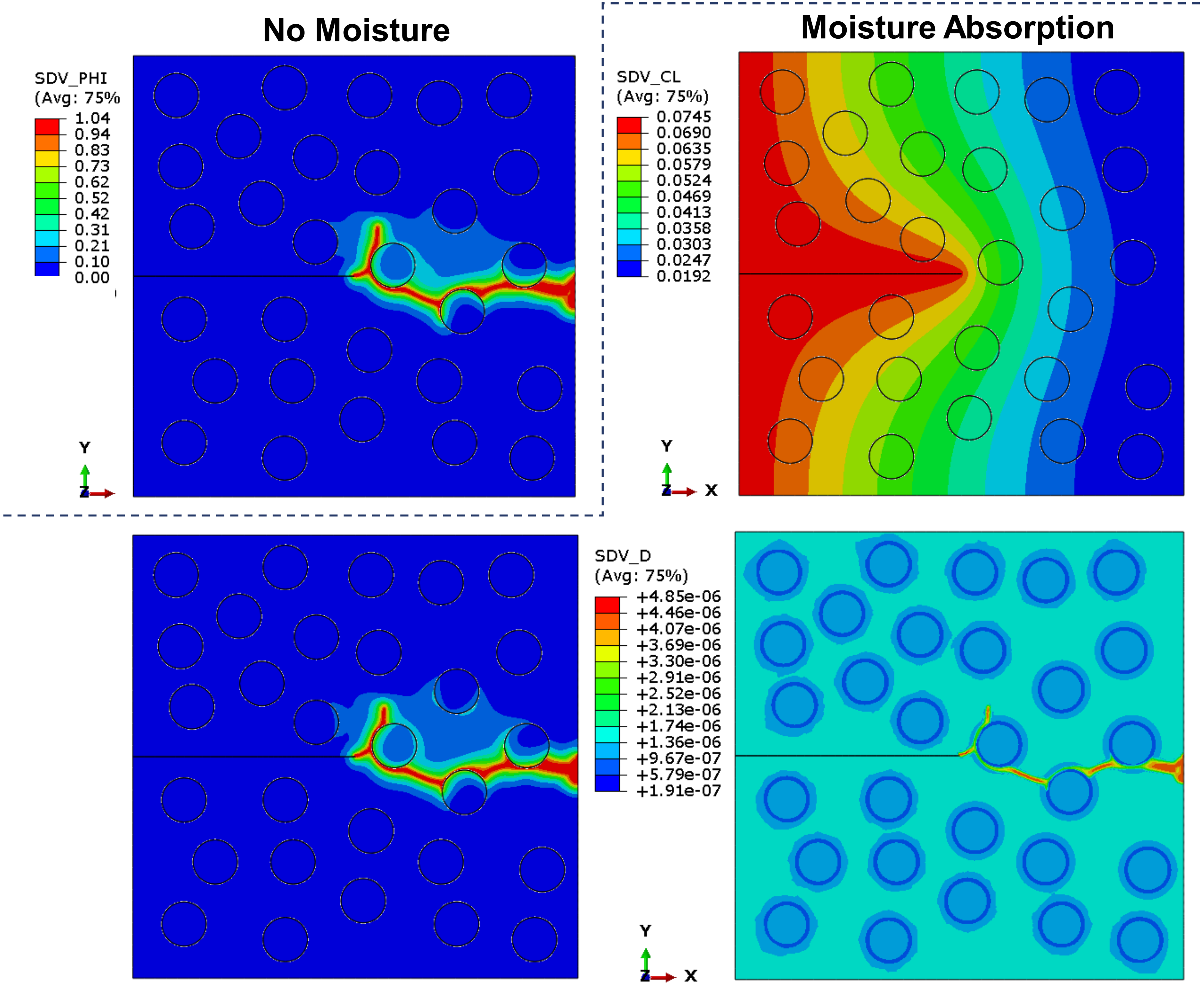
Material properties

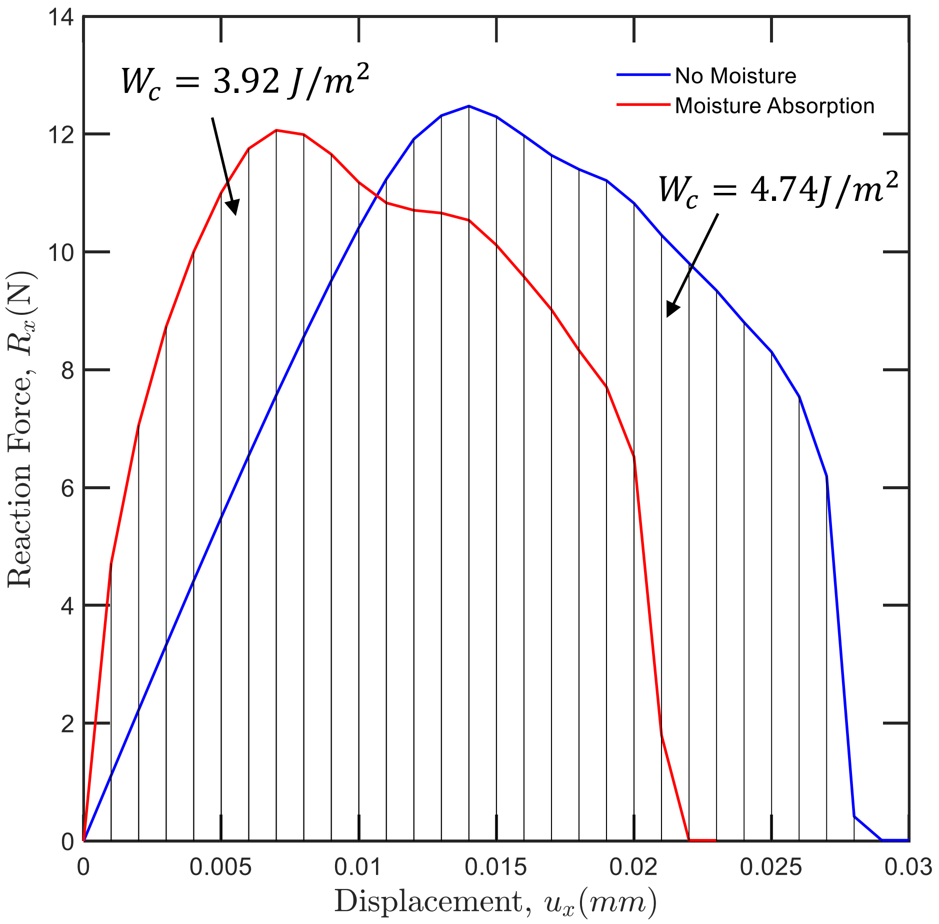
Constituents	E (GPa)	G_c (kJ/m²)	D (mm²/s)	α
Flax fibre	10.2	2.1	1.19×10^{-6}	1.06
Polymer	3.5	1.2	1.45×10^{-6}	0.6
Interface	4.0	0.213	0.8×10^{-6}	0.1

Boundary condition

- The moisture concentration 7.45% is applied at the left edge and notch area.
- The end-notch shear load is applied.
- **Moisture** and **mechanical** loading are applied concurrently.

Comparison of Composite Failure Under Moisture Absorption

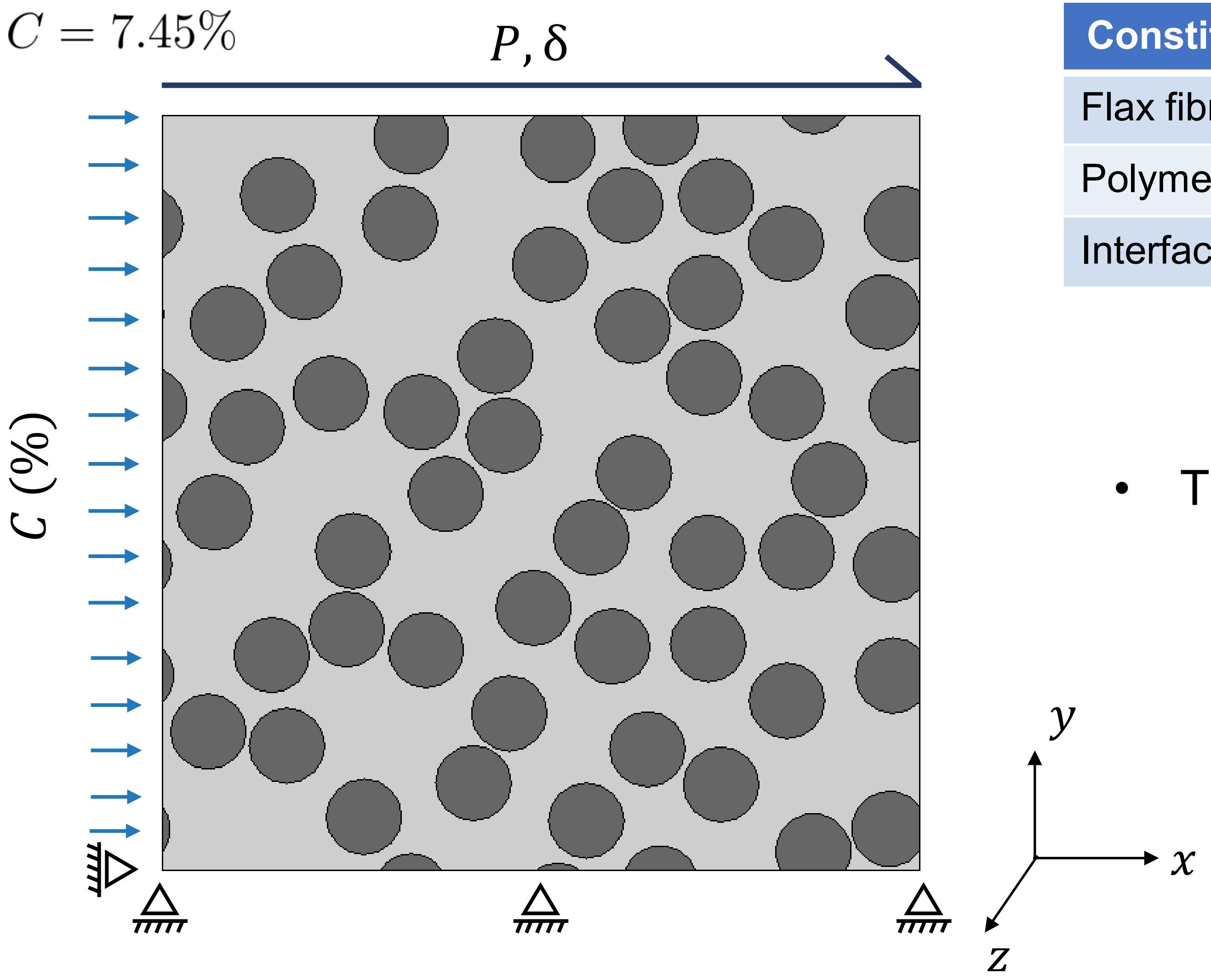




- The moisture degrades material toughness.

Case study 3: Representative volume element under shear loading (mode II)

Simple shear:



Material properties

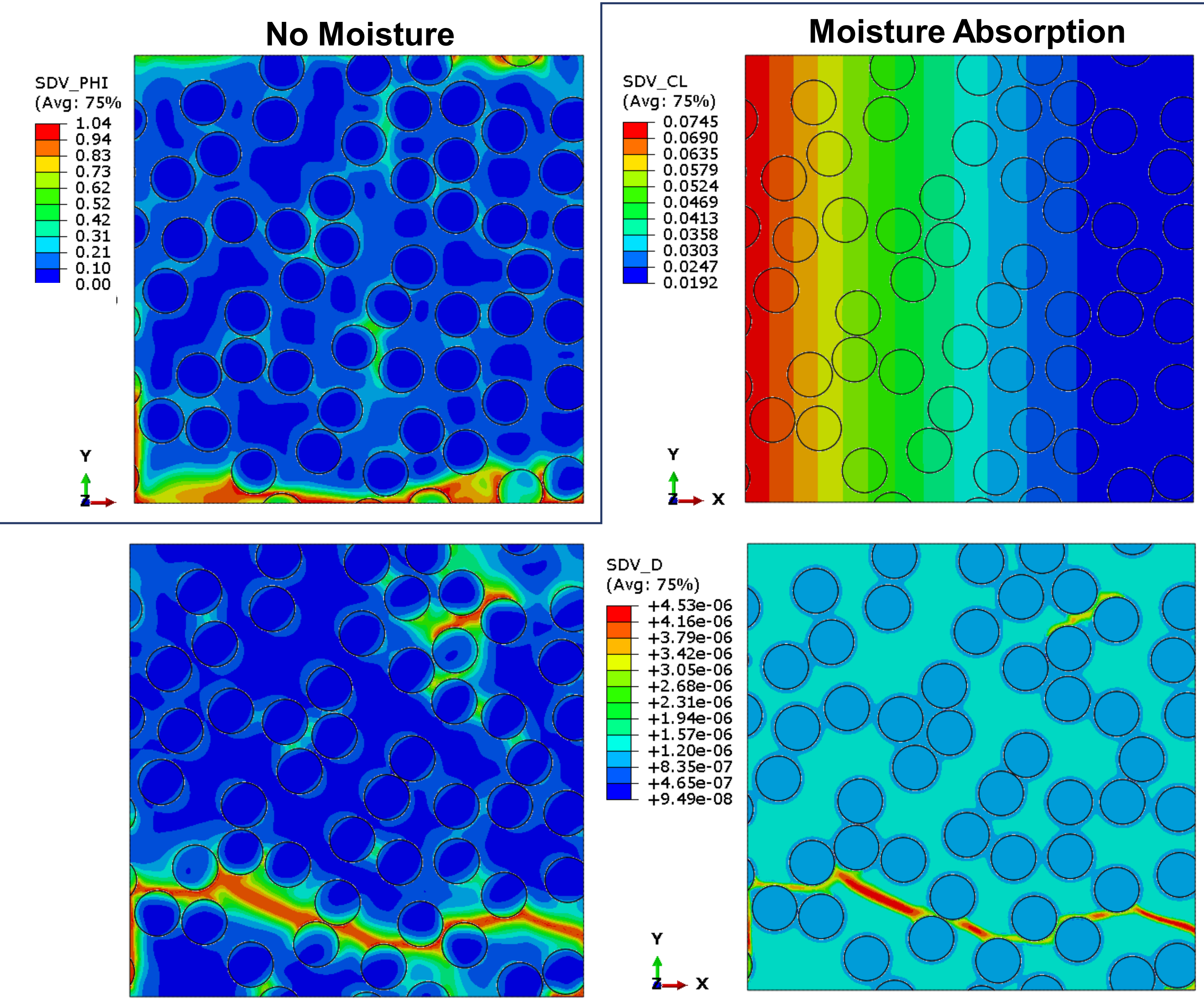
Constituents	E (GPa)	G_c (kJ/m²)	D (mm²/s)	α
Flax fibre	10.2	2.1	1.19×10^{-6}	1.06
Polymer	3.5	1.2	1.45×10^{-6}	0.6
Interface	4.0	0.213	0.8×10^{-6}	0.1

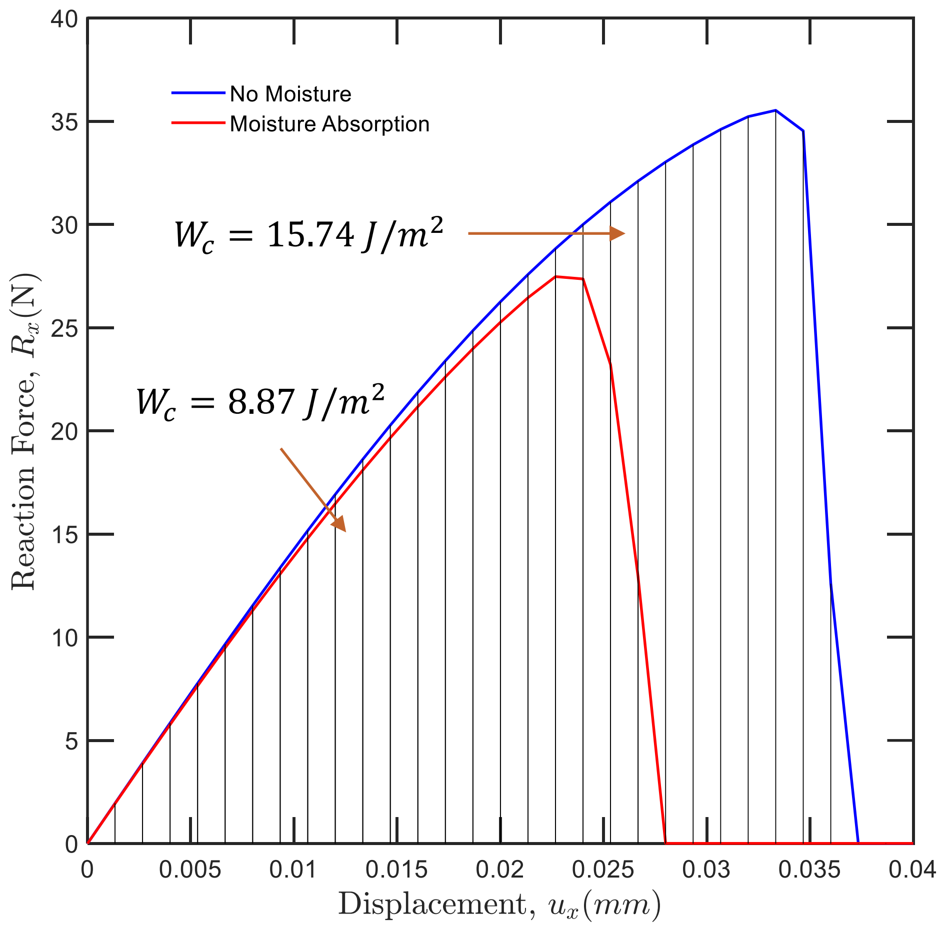
Periodic boundary condition

- The opposite faces should deform identically:

$$\begin{cases} u_R - u_L = u_x \\ u_T - u_B = u_y \\ u_F - u_B = u_z \end{cases}$$

Comparison of Composite Failure Under Moisture Absorption





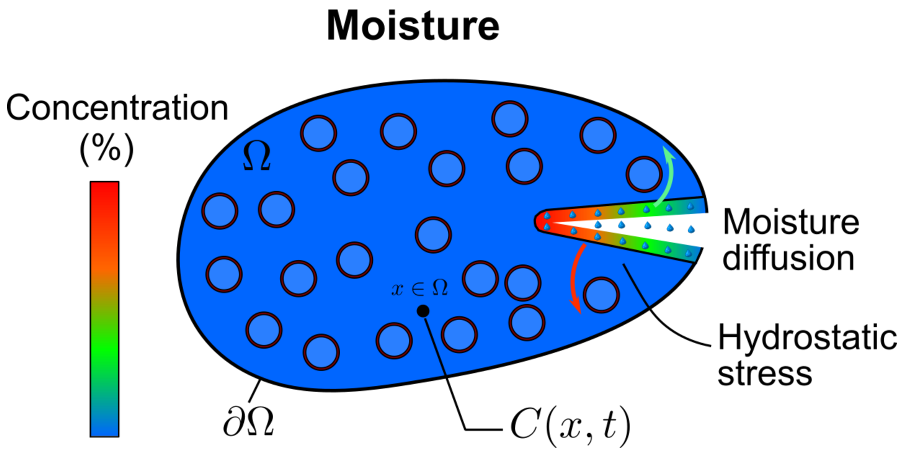
- The moisture degrades material toughness.

Summary

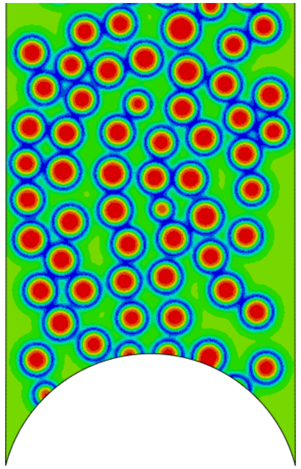
- We have presented a new **phase field-based multi-physics framework** to model **moisture-induced degradation** in composite materials.

- A novel **diffuse interface approach** is presented to interpolate relevant properties along the fibre-matrix interface.

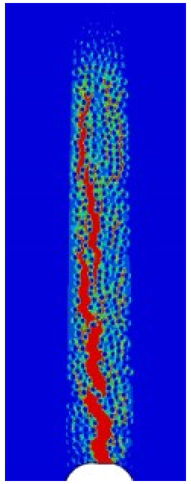
- The moisture contents promote the **mode I** fracture resistance and degrades the **mode II** fracture resistance.



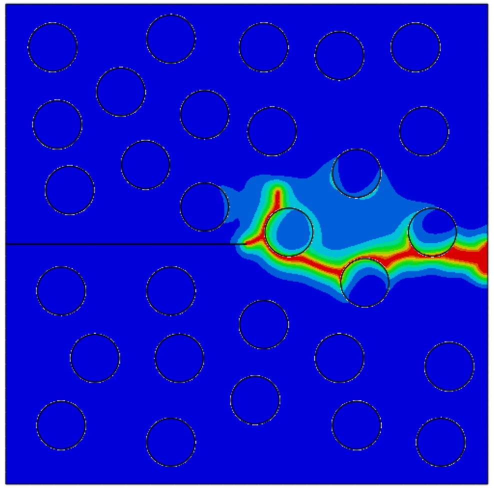
Diffused interface



Mode I



Mode II



Future work

- Conduct experiments under **environmental conditions** to further validate our model.
- Enhance the efficiency of the calculations by incorporating **adaptive** mesh refinement.

Thank you for your attention!

- Open-source research codes:
  - www.imperial.ac.uk/mechanics-materials/codes
  - wtanlab.com/codes/

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