Modelling of Autoclave Curing of a Porous Polymer

Paper Number : 1382

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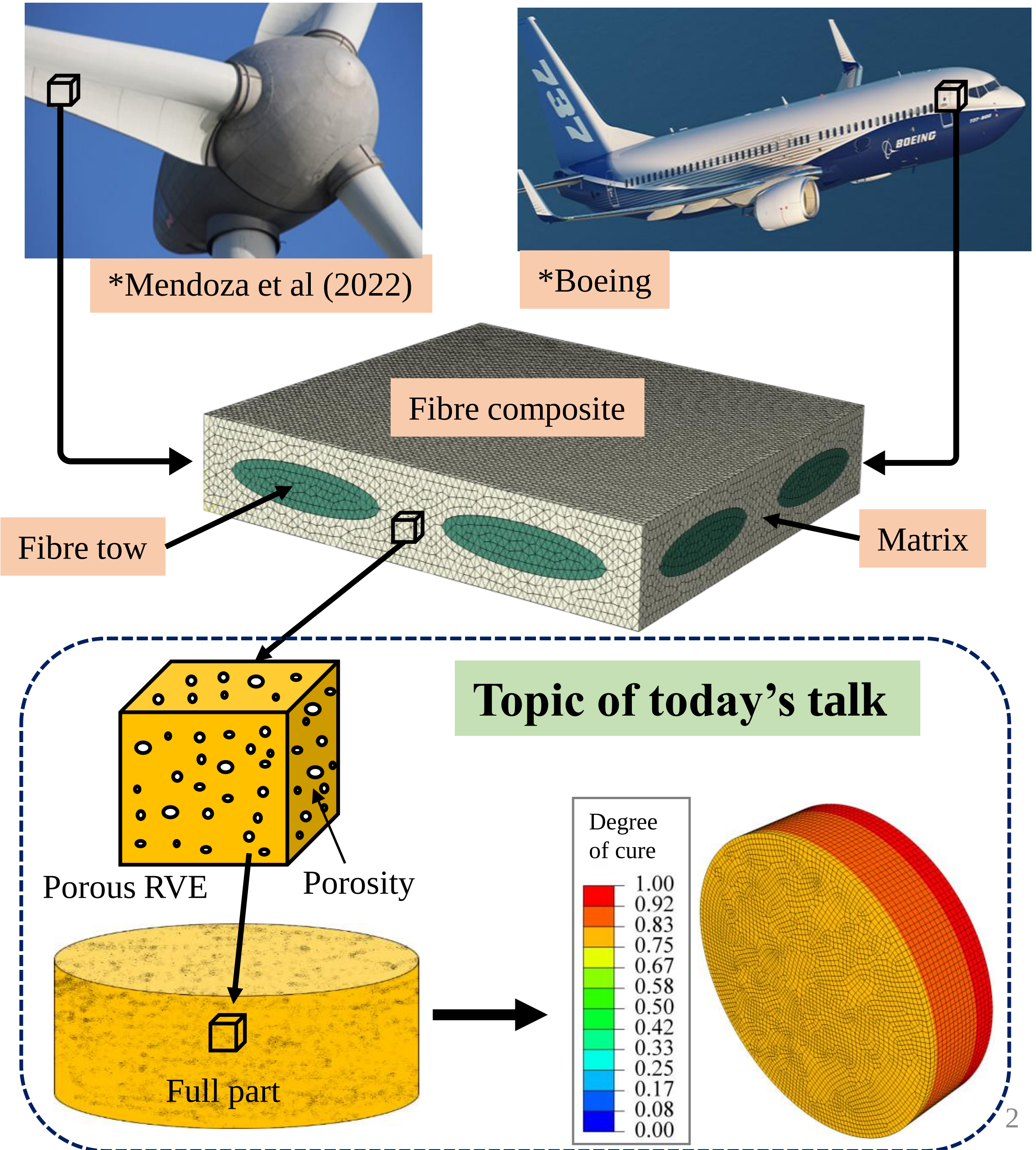
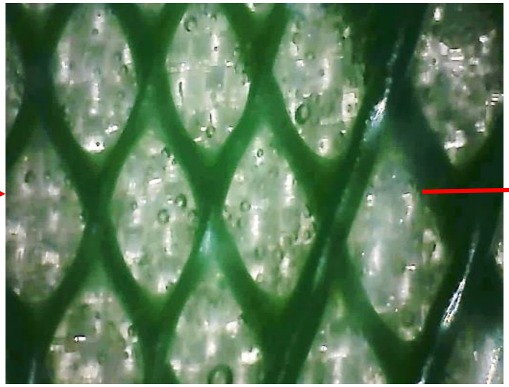
❑ Outline of presentation

- Introduction
- Literature Review
- Flowchart
- Materials
- Methodology
- Periodic Boundary and RVE Modelling
- Concept of Dynamic RVE
- Autoclave Curing
- Conclusion and Future Work
- Selected References



Introduction

➢ High demand of defect-free advanced fibre polymer composites



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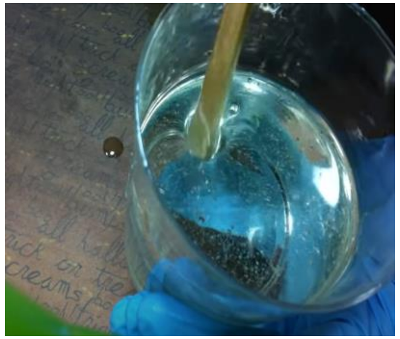

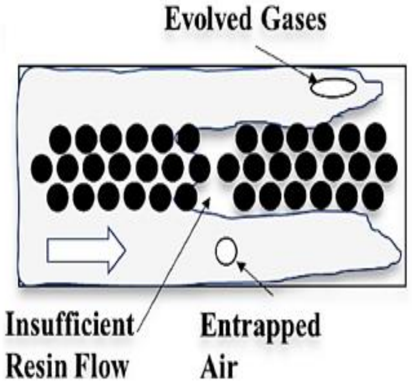

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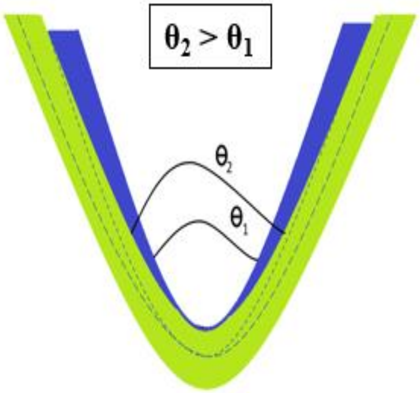
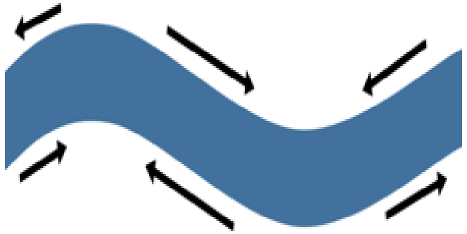
Others curing Defects:



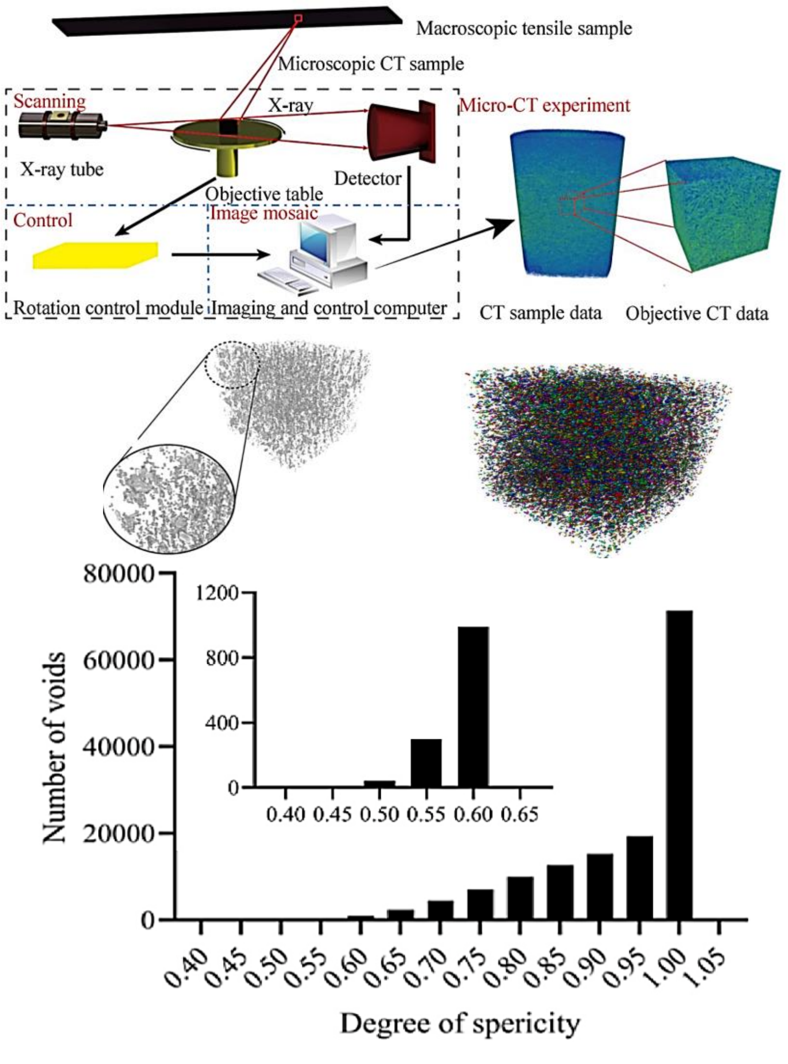
Spring back



Warpage

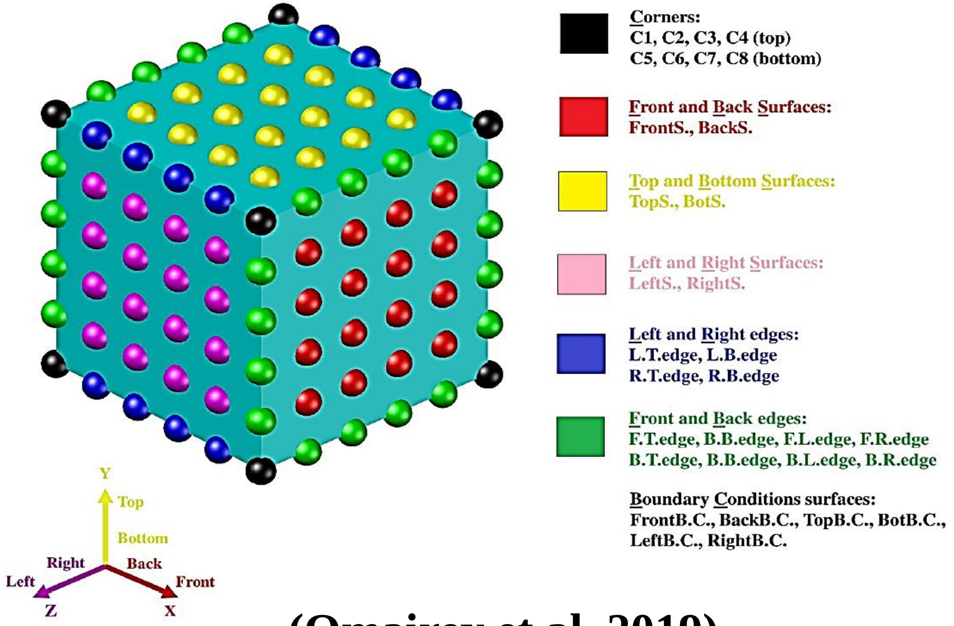
Literature review

RVE modelling



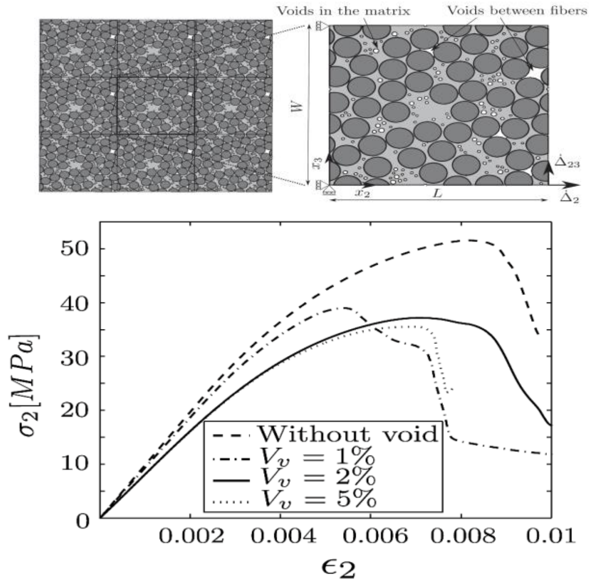
(Heng et al. 2022)

Periodic boundary condition



(Omairey et al. 2019)

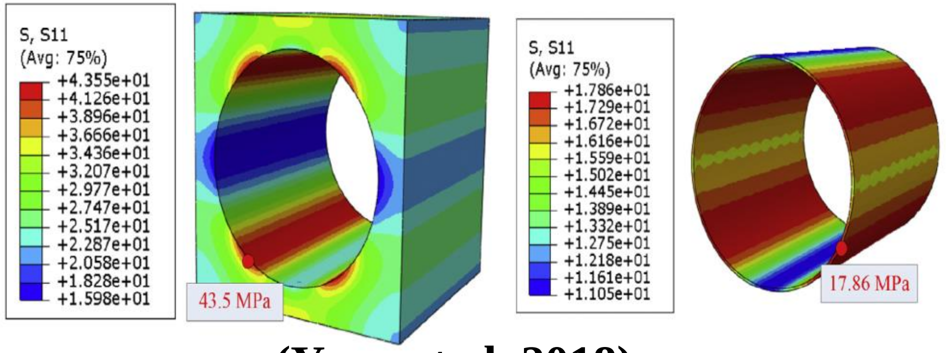
Porosity on composites



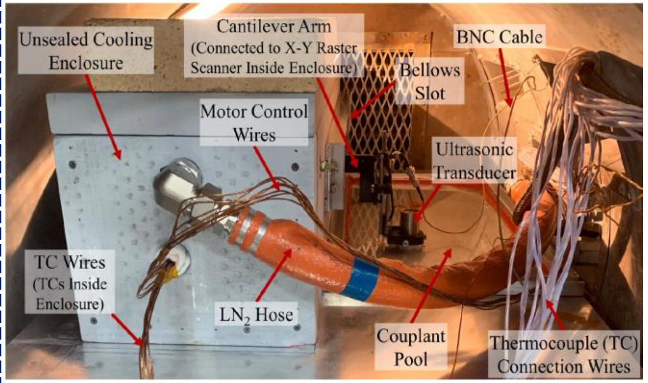
Transverse tension

(Vajari et al. 2014)

Residual stress on curing



(Yuan et al. 2018)



(Hudson et al 2021)

Flow chart of work

Modelling of Randomly Generated Pores Inside an RVE

Thermal Periodic Boundary Condition and RVE Homogenization

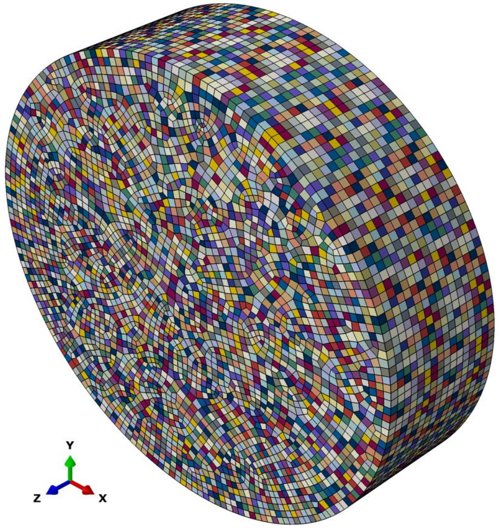
Structural Periodic Boundary Condition and RVE Homogenization

User Material (UMAT) with Multilinear Elastic Behavior

Single Element Verification Test

Sensitivity Analysis on Number of Division of Strain

Dynamic RVE



HETVAL Subroutine for Cure Kinetics

FE Modelling of Autoclave Curing

Temperature **Validation** of FE Curing Model

Autoclave Curing Experiment

Materials and materials models

Fourier heat conduction model:

$$K_{xx}\frac{\partial^2 T}{\partial x^2} + K_{yy}\frac{\partial^2 T}{\partial y^2} + K_{zz}\frac{\partial^2 T}{\partial z^2} + \dot{q} = \rho C_p \frac{\partial T}{\partial t}$$

$$\dot{q} = \rho_r H_r \frac{d\alpha}{dt}$$

Cure kinetics model (Zhang et al. 2009):

$$\frac{d\alpha}{dt} = (k_1 + k_2\,\alpha^m)(1-\alpha)^n$$

Arrhenius equation: $k_i = A_i\, e^{\left(-\frac{E_i}{RT}\right)}$

- K_{xx}, K_{yy} and K_{zz} = thermal conductivity (W/mK)
- k_i = cure rate constant (per second)
- A_i = pre exponential factor (per second)
- E_i = activation energy (J/mol)
- R = universal gas constant ($J{\cdot}mol^{-1}{\cdot}K^{-1}$)
- T = absolute temperature in kelvin
- $\dot{q}$ = internal heat generated flux (W/m^3)
- H_r = total heat reaction (J/Kg)
- α = degree of cure

Material :

Epoxy : Araldite LY1564
Hardener : Aradur 22962

Mixing ratio :

Epoxy: Hardener = 4:1

Properties of epoxy (*Zhang et al. (2009) and *Substech datasheet) :

Density (kg/m^3), ρ	1225
Elastic modulus (MPa), E	2500
Poisson's ratio, ν	0.3
Specific heat (J/kgK), C_p	967
Thermal conductivity (W/mK), $K_{xx} = K_{yy} = K_{zz}$	0.191
Coefficient of thermal expansion ($°C^{-1}$)	50×10^{-6}

Cure kinetics parameters of epoxy (Zhang et al. 2009):

A_1 (sec^{-1})	20.77
A_2 (sec^{-1})	0.821
E_1 (J·mol)	38330
E_2 (J·mol)	20000
m	0.786
n	3.207
R ($J{\cdot}mol^{-1}{\cdot}K^{-1}$)	8.314
H_r ($J.kg^{-1}$)	277000

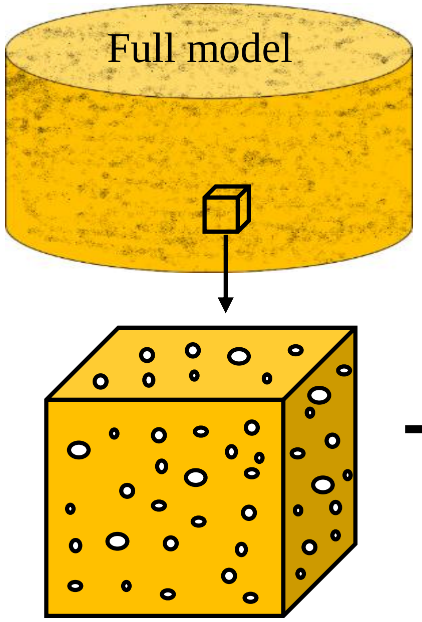
Methodology

Modelling of randomly distributed pores inside an RVE:

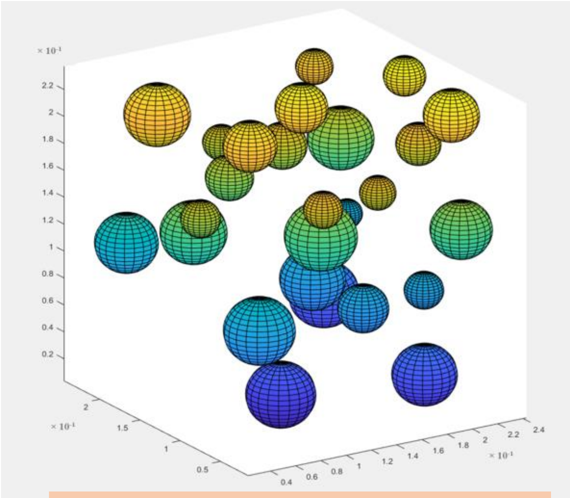
Assumptions:

- Spherical pores.
- Location and diameter of pores are random.
- Pores do not intersect each other
- Intersection of pores with RVE boundary is neglected

Diameter of spherical pores (Vajari et al. 2014) = 20 to 50 μm



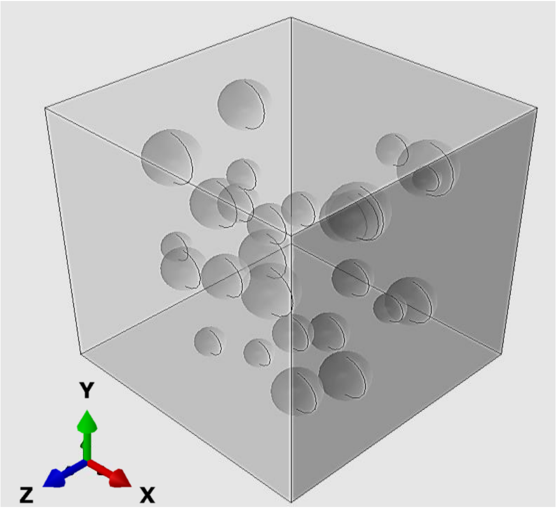
RVE contains pores



Generated on MATLAB

Export the information in .txt file

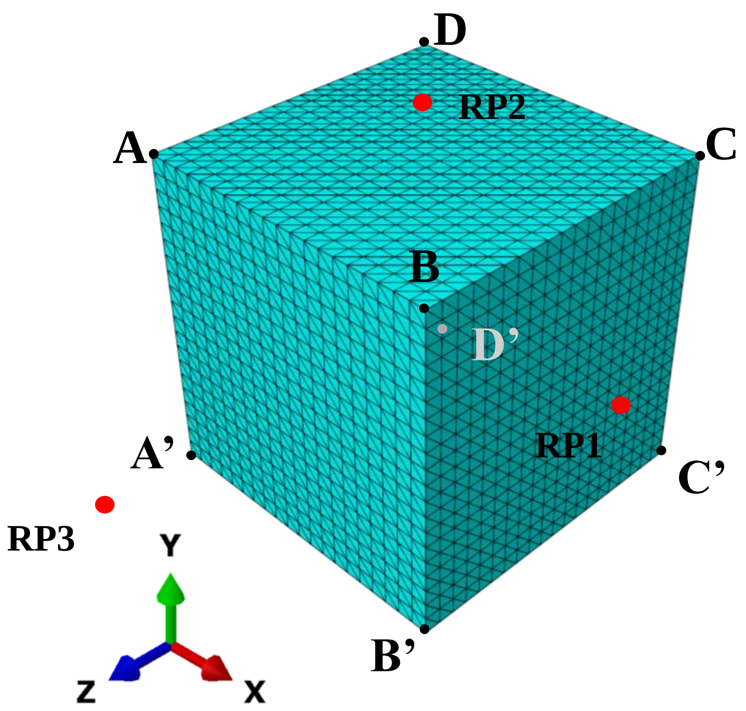
Generate the RVE with **Abaqus Python** scripting



Structural Periodic Boundary Condition (PBC)

Implementation of PBC (Tian et al 2019):

Mesh size 12.5 μm (C3D4)

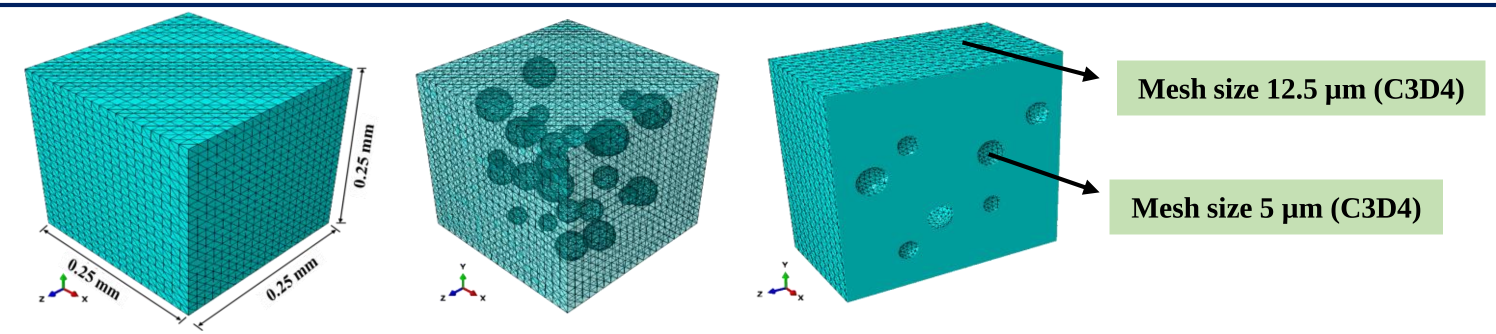


- **Step 1: Categorization of node**
  - Inner face (excluding node on common edges and corners)
  - Inner edge (excluding nodes of corners)
  - Corner
- **Step 2: Three reference points**
  - RP1 and RP2 for pure shear loading
  - RP3 for pure tensile loading
- **Step 3: linear multipoint constraint equation on each node of boundaries (*Abaqus manual)**

$$u_i^{k+} - u_i^{k-} - u_i^{RP} = 0$$

PBC constraint equations are **automated** in Abaqus via a **user-defined python script.**

Structural RVE Homogenization + UMAT

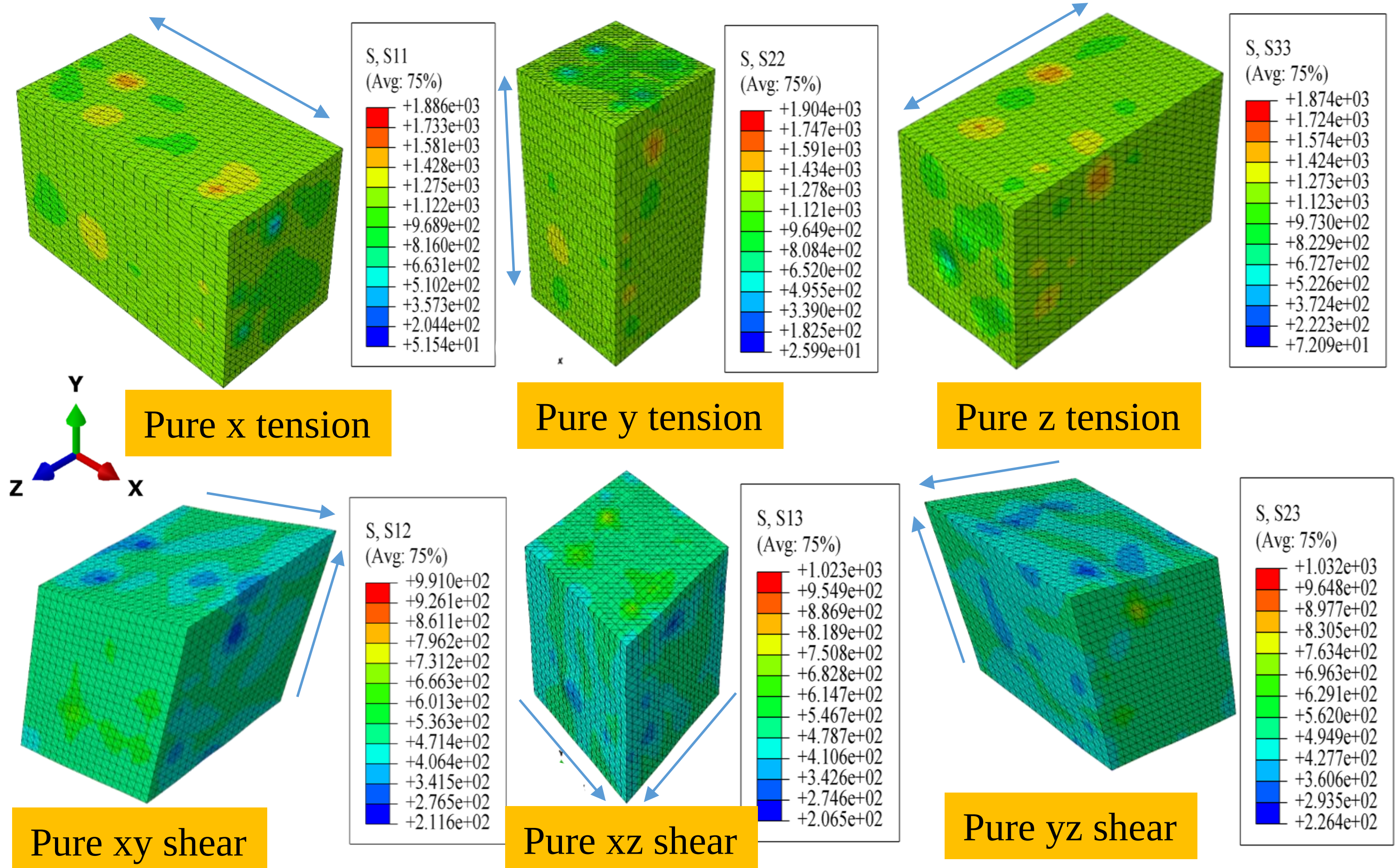


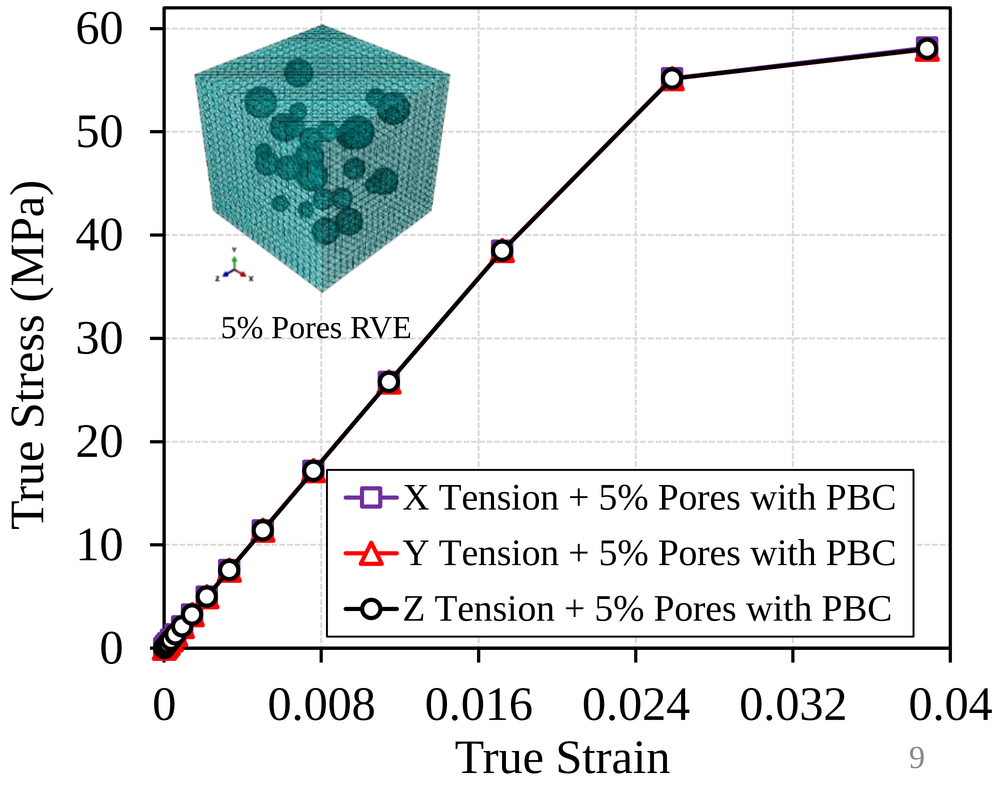
To determine the effective properties of RVE:

1) $\varepsilon_{kk} = \bar{\varepsilon}_{kk}$ and $\varepsilon_{ij} = 0$ for tensile deformation
2) $\varepsilon_{kk} = 0$ and $\varepsilon_{ij} = \bar{\varepsilon}_{ij}/2$ for shear deformation

here i, j, k = 1,2 and 3 and i ≠ j

Total no of mesh elements in RVE = 253,636
Total no of constraint equation (PBC) = 3,783





Structural RVE Homogenization + UMAT

Isotropic linear elastic model (assumed quasi-isotropy)

$$\begin{bmatrix}\sigma_{11}\\ \sigma_{22}\\ \sigma_{33}\\ \sigma_{23}\\ \sigma_{13}\\ \sigma_{12}\end{bmatrix} = \begin{bmatrix}\lambda+2\mu & \lambda & \lambda & 0 & 0 & 0\\ \lambda & \lambda+2\mu & \lambda & 0 & 0 & 0\\ \lambda & \lambda & \lambda+2\mu & 0 & 0 & 0\\ 0 & 0 & 0 & \mu & 0 & 0\\ 0 & 0 & 0 & 0 & \mu & 0\\ 0 & 0 & 0 & 0 & 0 & \mu\end{bmatrix} \begin{bmatrix}\epsilon_{11}\\ \epsilon_{22}\\ \epsilon_{33}\\ 2\epsilon_{23}\\ 2\epsilon_{13}\\ 2\epsilon_{12}\end{bmatrix}$$

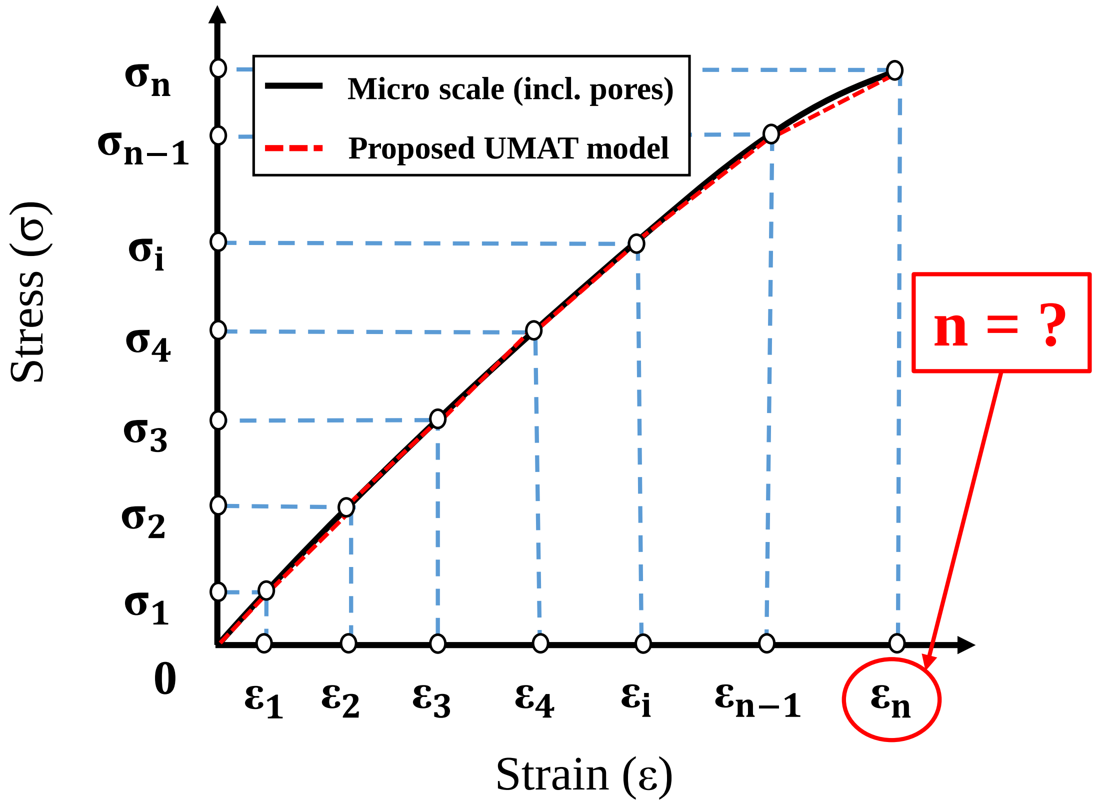
Where λ and μ are lame's parameters and given by:

$$\mu = G = \frac{E}{2(1+\nu)}$$

$$\lambda = \frac{E\nu}{(1+\nu)(1-2\nu)}$$

Where ν, E, G are Poisson's ratio, elastic modulus and shear modulus.

UMAT with proposed 'multilinear elasticity'

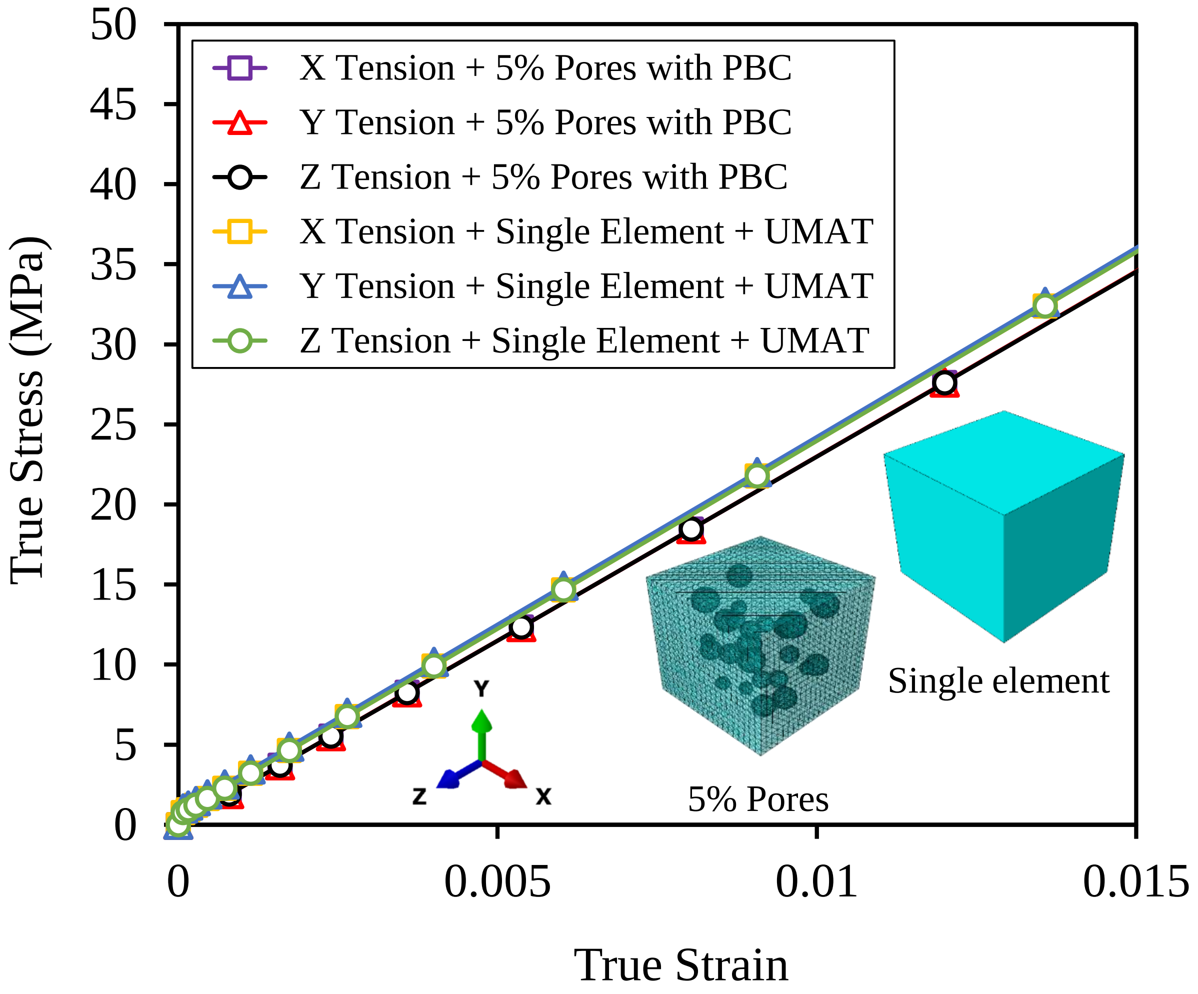


A python script is written to automate execution of proposed material model in abaqus

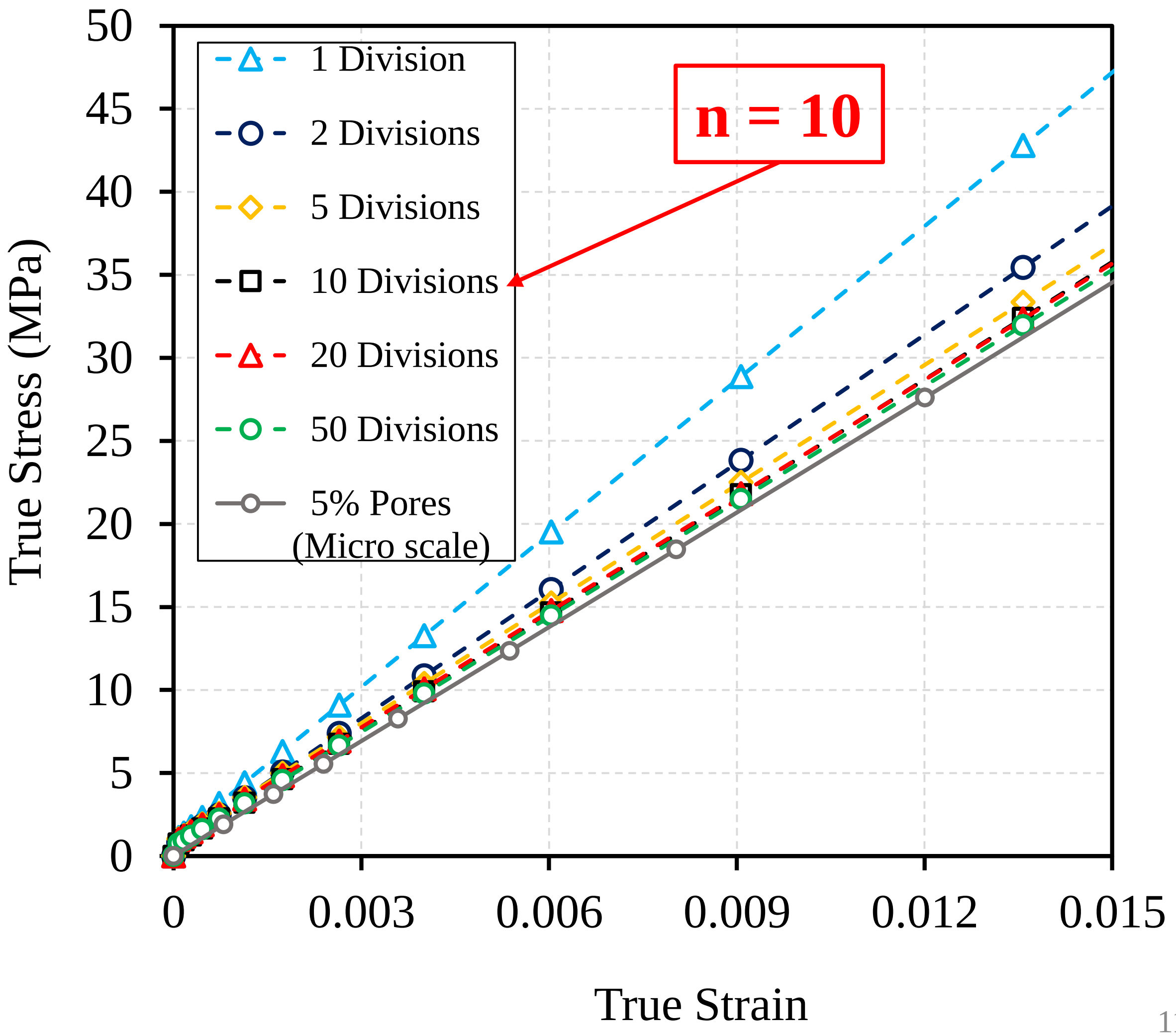
Structural RVE Homogenization + UMAT

Single element verification with UMAT

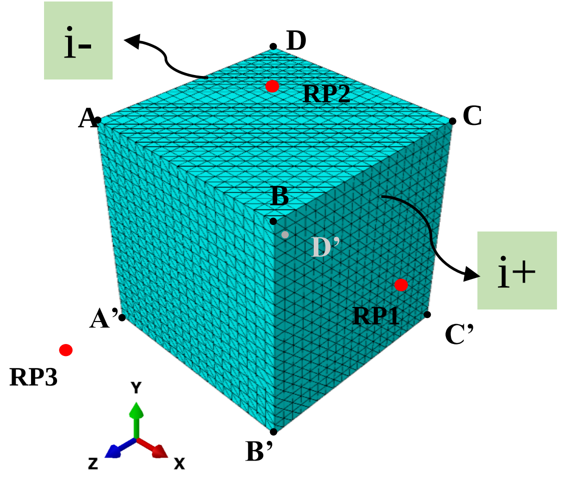
Single element mesh size = 0.25 mm (C3D8)
Total no of constraint equation (PBC) = 21



Mesh sensitivity parametric analysis for no of divisions in UMAT



Thermal PBC and Thermal RVE Homogenization



$$T^{i+} - T^{i-} - T^{RP} = 0$$

$$T^{RP} = \Delta\bar{T}$$

Effective thermal conductivity tensor $\langle k \rangle_{ij}$:

$$\langle k \rangle_{ij} = -\frac{\langle q \rangle_i}{\nabla T_j}$$

$$\nabla T_j = \frac{\Delta\bar{T}}{L_j}$$

$$\langle k \rangle_{ij} = \begin{bmatrix} k_{11} & k_{12} & k_{13} \\ k_{21} & k_{22} & k_{23} \\ k_{31} & k_{32} & k_{33} \end{bmatrix}$$

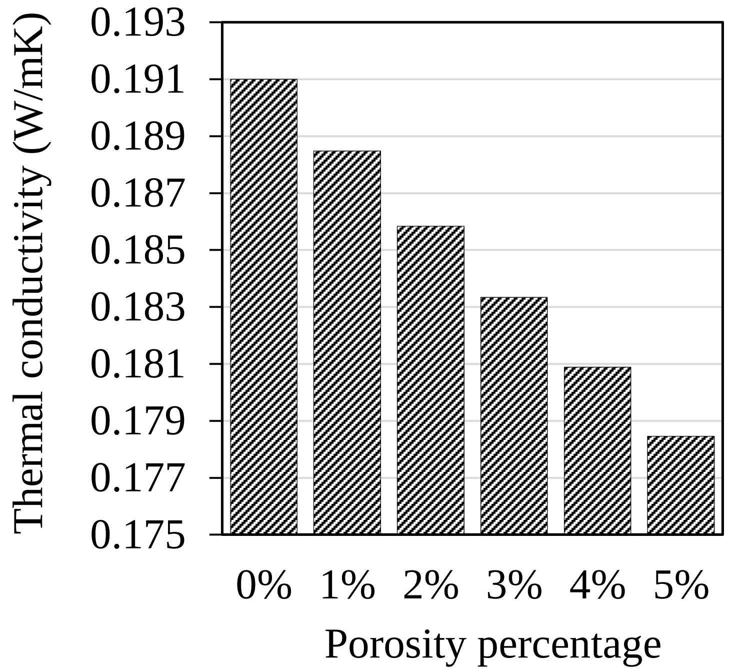
Where,

$\langle q \rangle_i$ = Effective heat flux vector

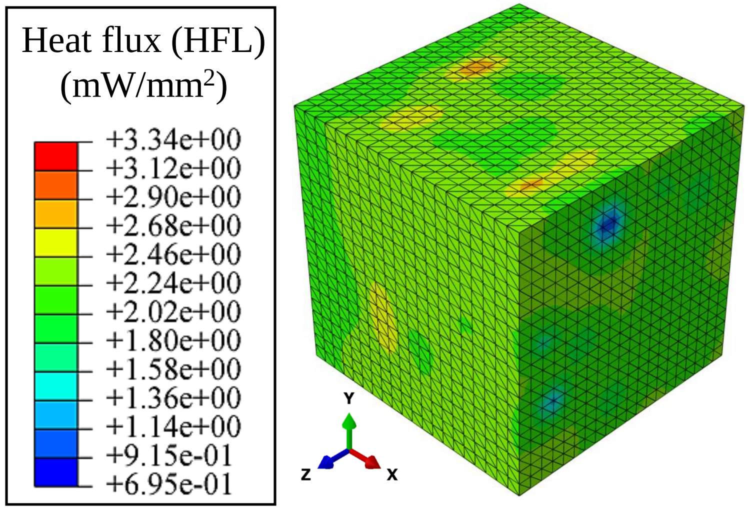
∇T_j = Temperature gradient vector

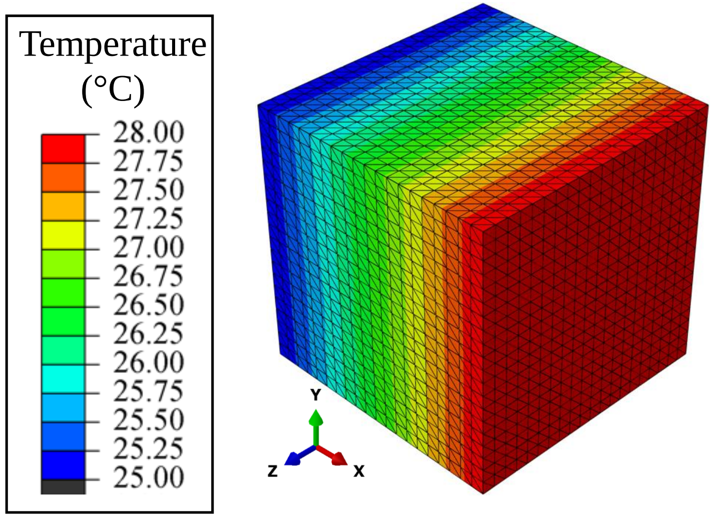
$\Delta\bar{T}$ = Imposed temperature boundary condition

L_j = Side length of the RVE the x_j direction

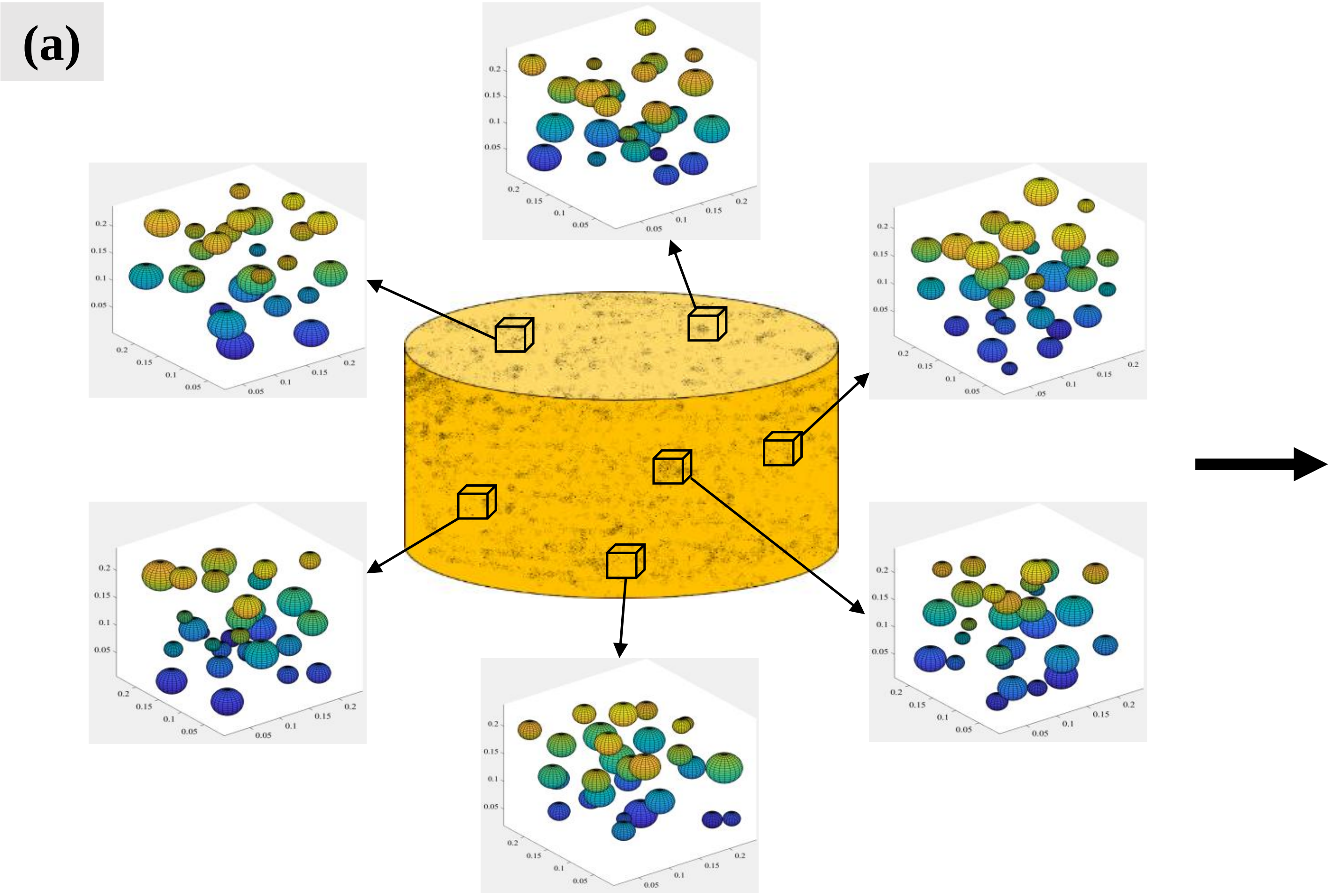


PBC constraint equations are **automated** in Abaqus via a **user-defined python script.**

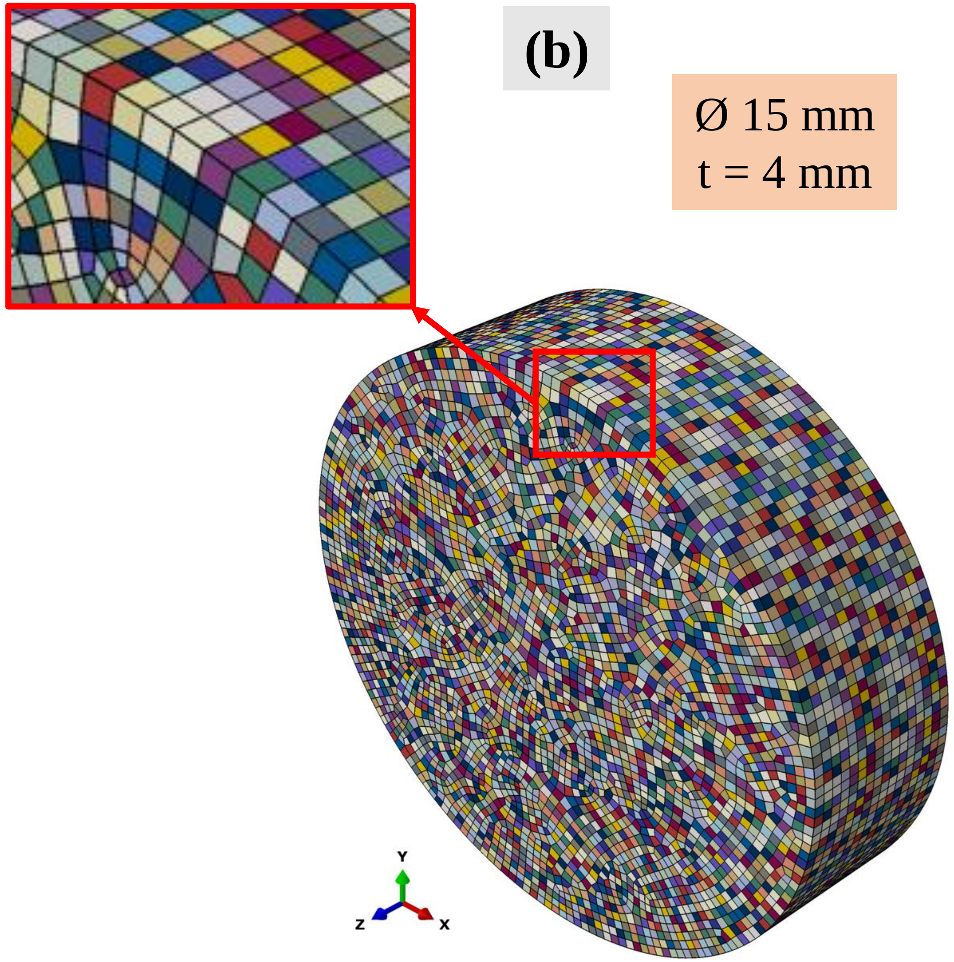




Concept of Dynamic RVE



Porosity at different location have different distribution represented in 6 RVEs

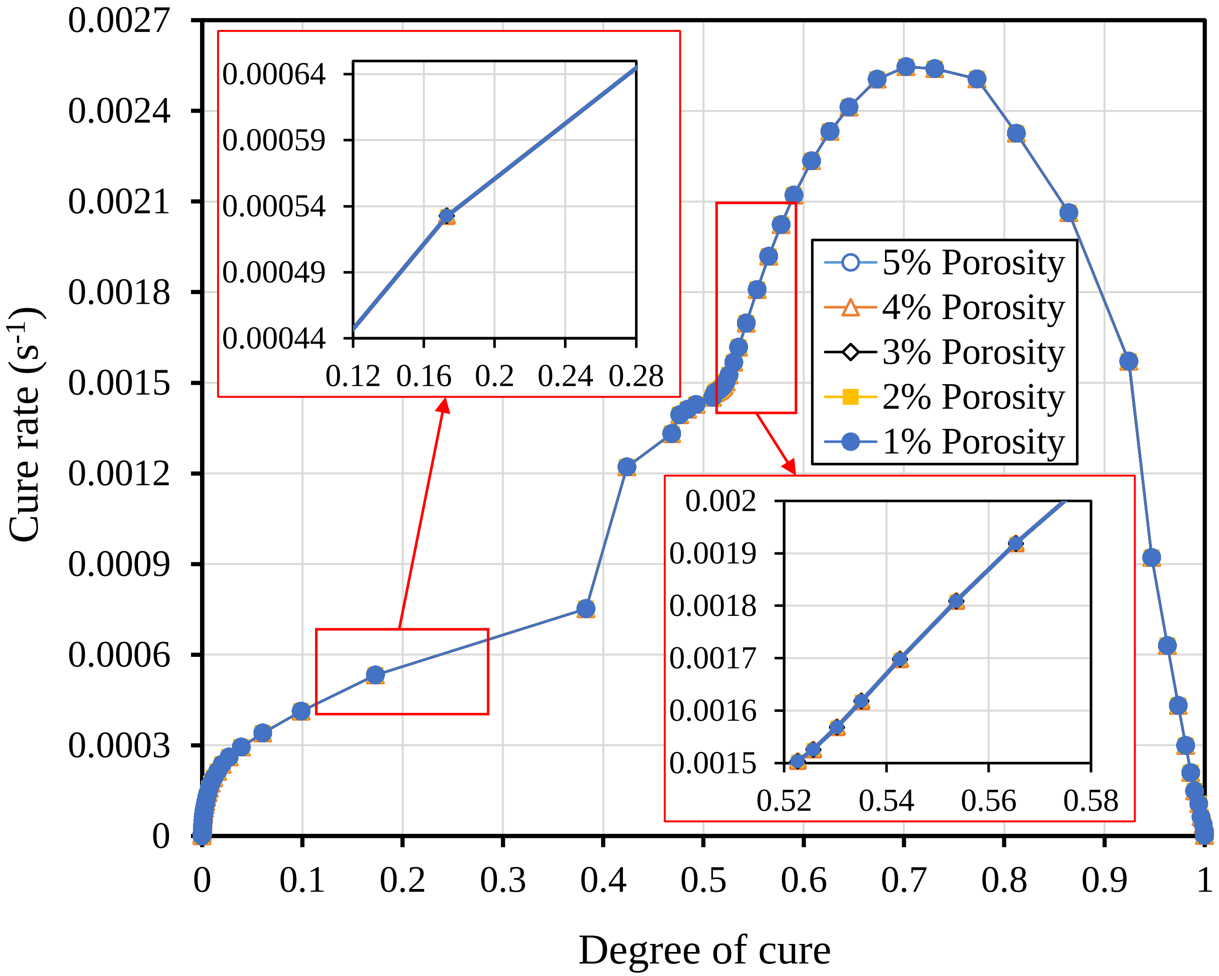


Macro scale domain with Dynamic RVE

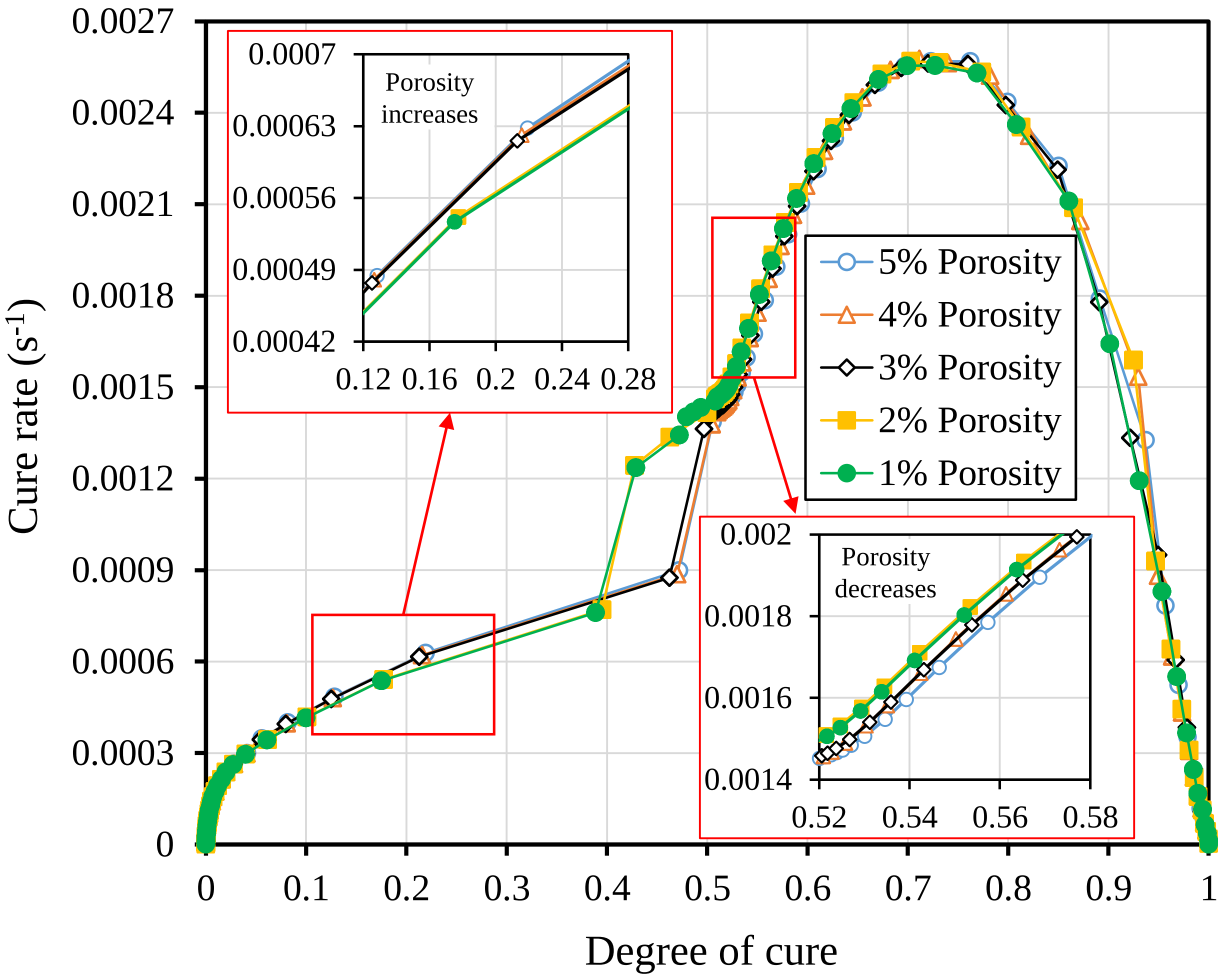
Dynamic RVE is generated in the **Abaqus** by **python scripting** to **automate preprocessing**.

Structural vs coupled thermo-structural homogenized cure model

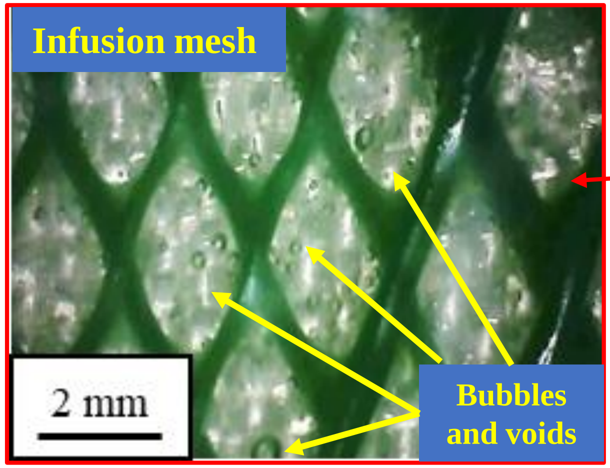
Only structural homogenized curing

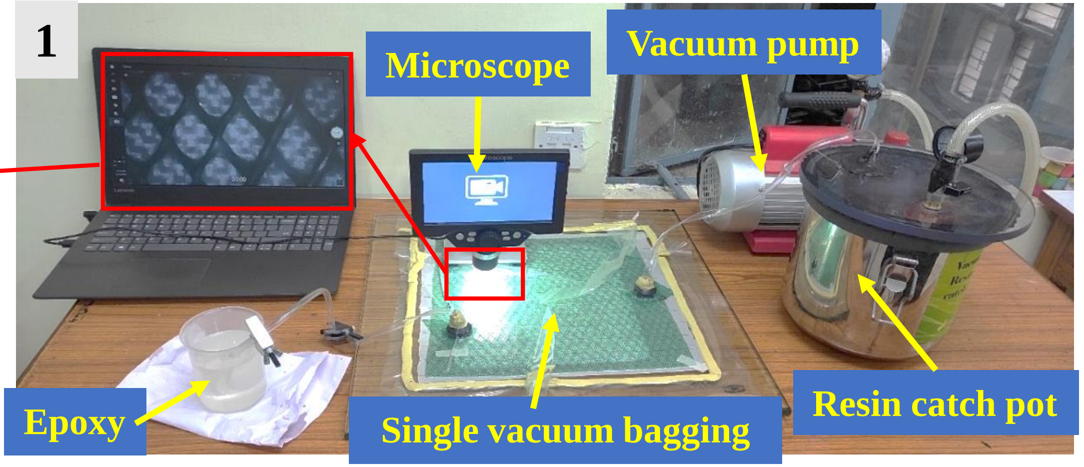


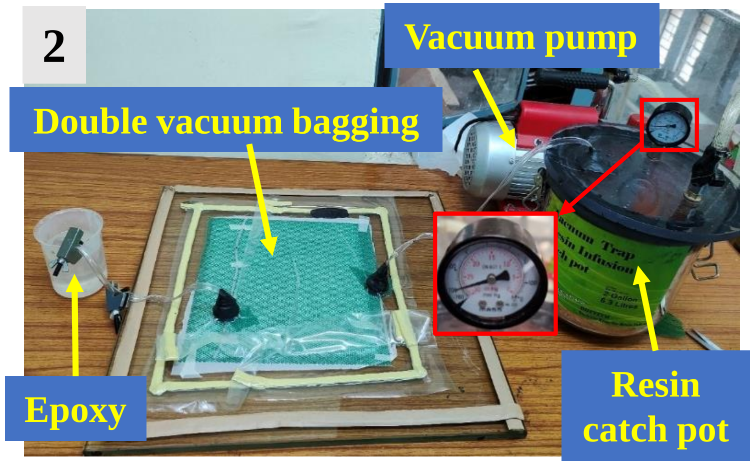
Coupled thermo-structural homogenized curing

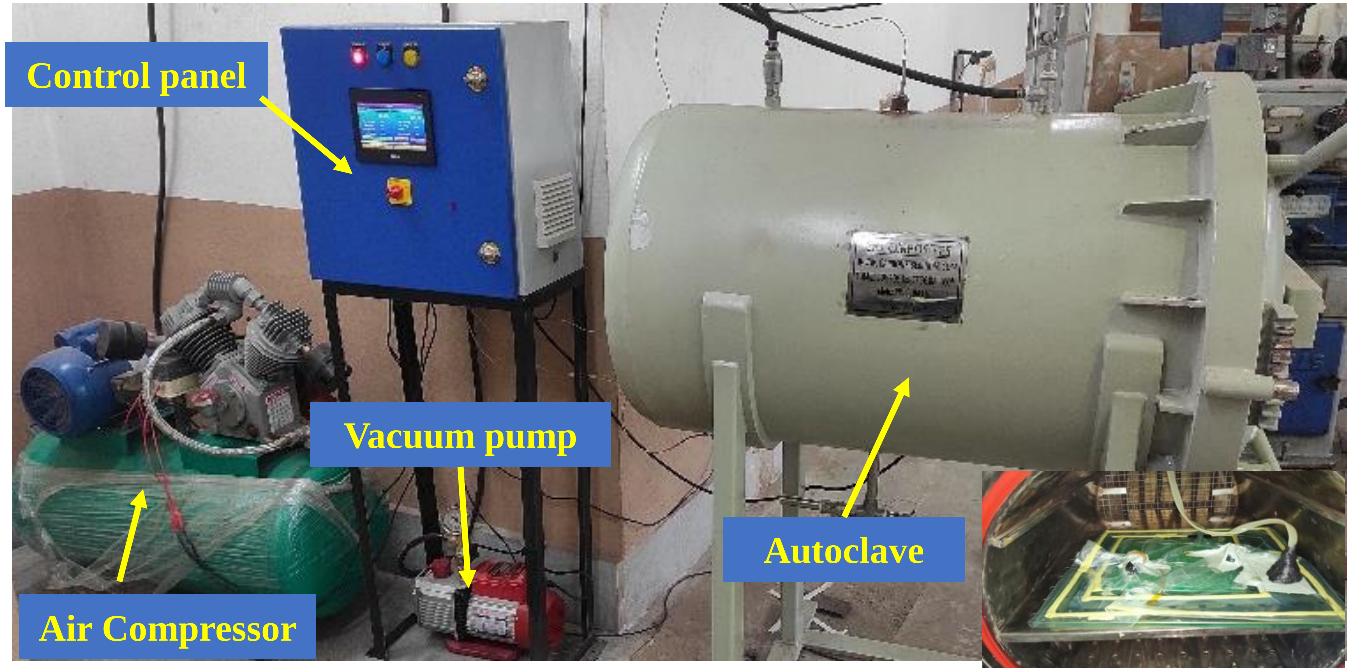


Autoclave curing

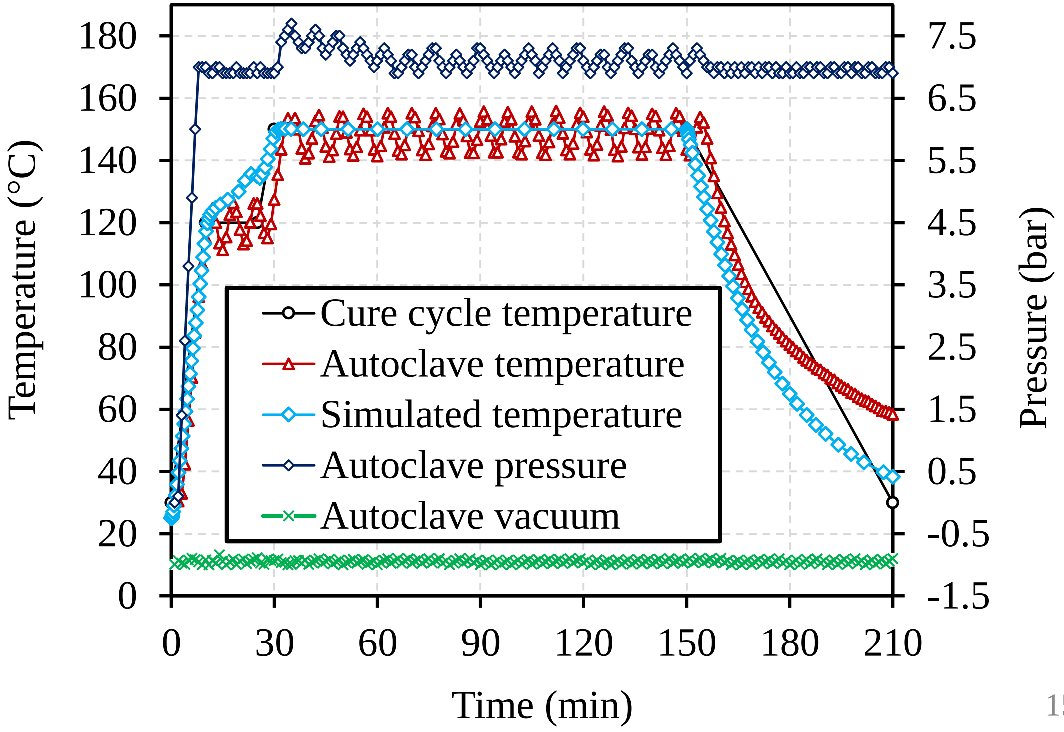








In-house built Autoclave (w/ CF Composites, India)



Conclusions

- Periodic boundary conditions with structural and thermal homogenization of RVE has been implemented.
- As number of multilinear divisions on UMAT increases, accuracy of results increases. For 10, 20, 50 divisions, accuracy of results is same, so based on CPU time 10 division is suitable for analysis.
- With an increase in porosity by 1% at micro scale, thermal conductivity of RVE decreases by 1.3%.
- A dynamic RVE approach is proposed and coupled with thermo-structural homogenized cure model.

Next plan of work:

- Incorporation of reinforcement to simulate curing of fibre reinforced polymer composite.
- Experimental validation of Macro scale FE model for tensile and flexural test will be performed.

Publication:

1) **B. Dewangan**, and N.D. Chakladar (2023). Effects of porosity on the cure kinetics and residual stress of a porous polymer. Materials Today Communications. Vol. 35, pp-105711.

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1) llT/SRIC/lSIRD/2019-2020/29 – IIT Kharagpur, ISIRD Scheme

2) IIT Kharagpur Doctoral Scheme

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