Thermal Equilibrium and Non-Equilibrium in Composite Materials: A Comparison between DNS and Analytical Homogenization

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Club Cast3M November 2025

- **Introduction**

Introduction: State of Art

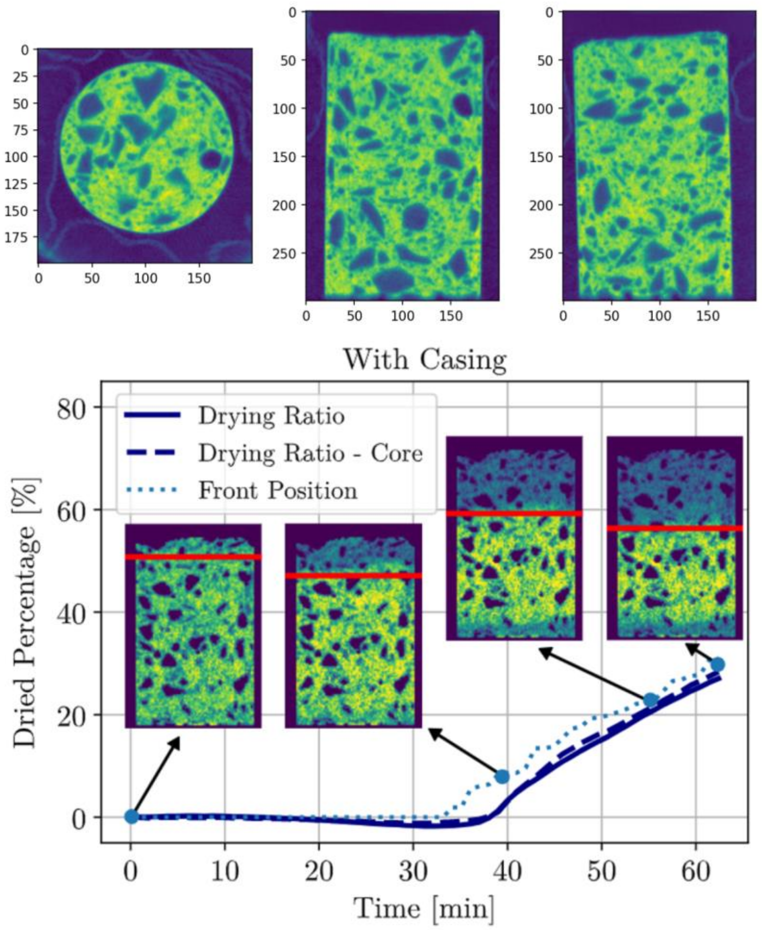
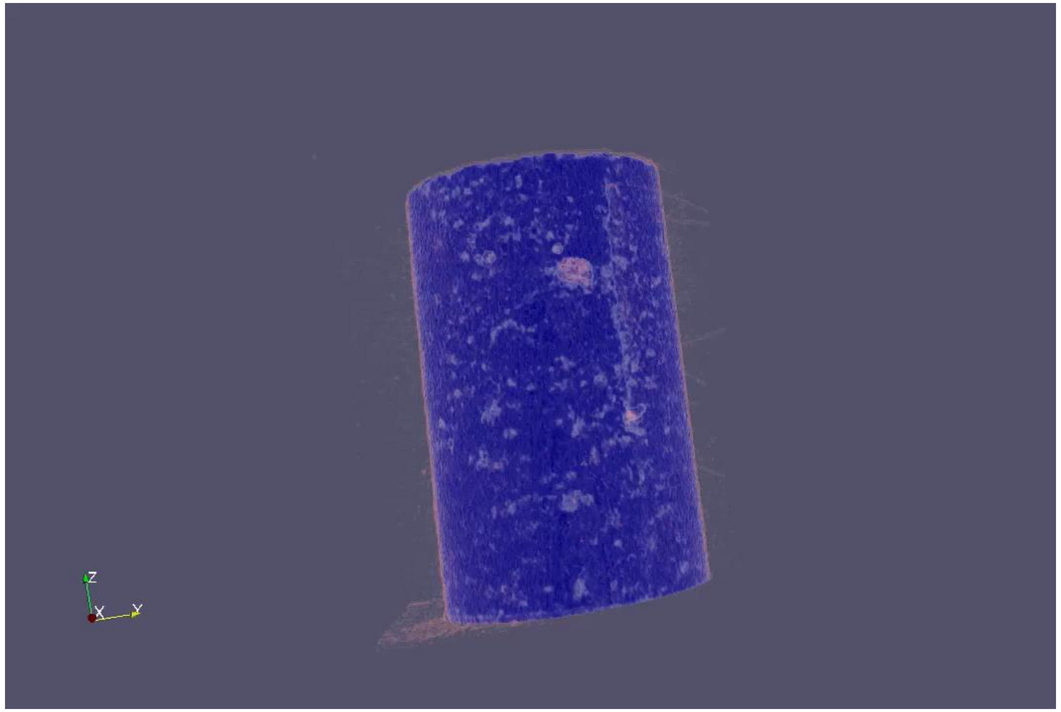
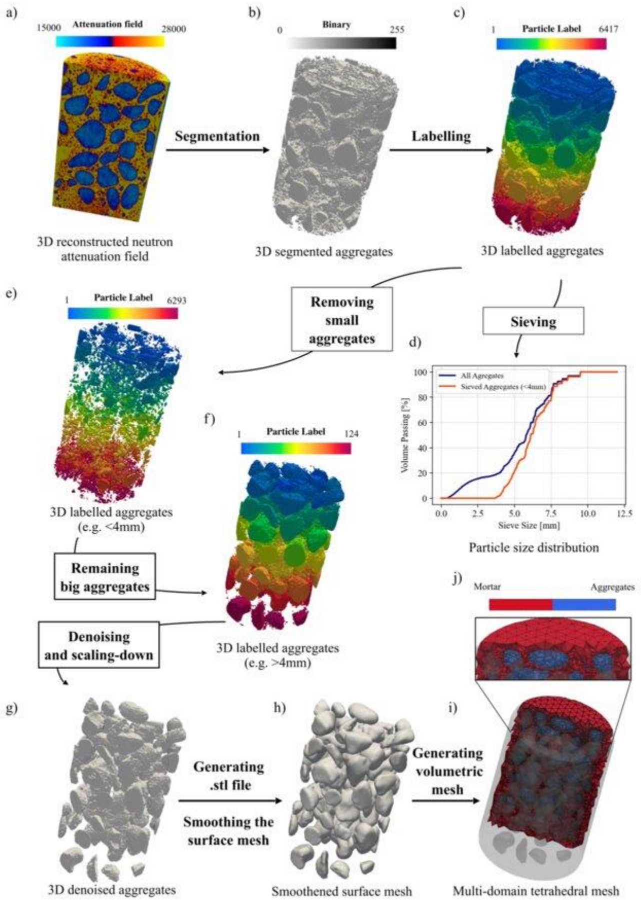


Figure 1: Sample tomography and drying Evolution.
(M.H. Moreira et al. 2022, C.S. Hani et al. 2024)

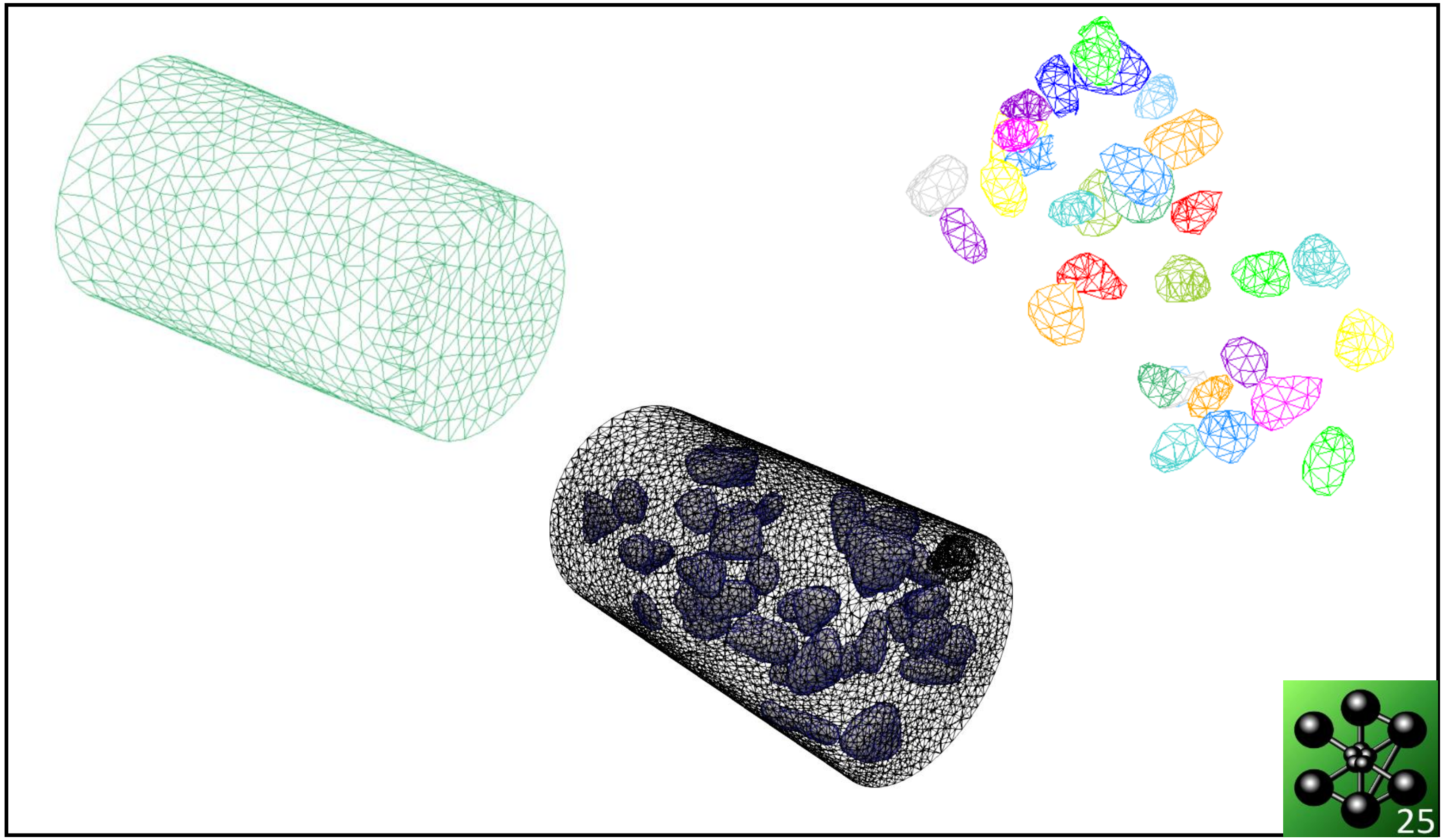


Video 1: X- ray/Neutron images of a drying concrete sample. (*S. Dal Pont 3SR*)

Introduction: Research Motivation



(A)



(B)

Figure 2: (A) *TomoToFE* Python pipeline: https://github.com/ANR-MultiFIRE/TomoToFE,
(*C.S. Hani et al. 2024, 10.21809/rilemtechlett.2023.184*). (B) Imported mesh on CAST3M .

Introduction: Research Motivation

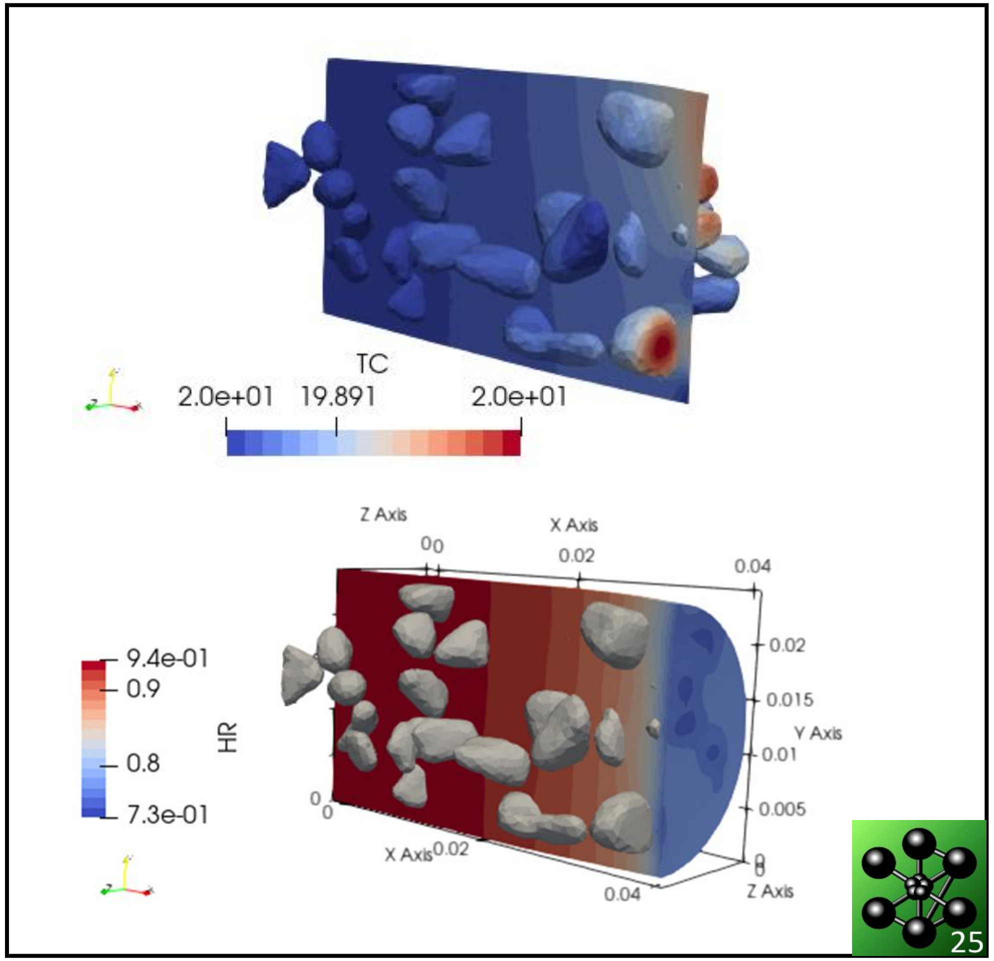
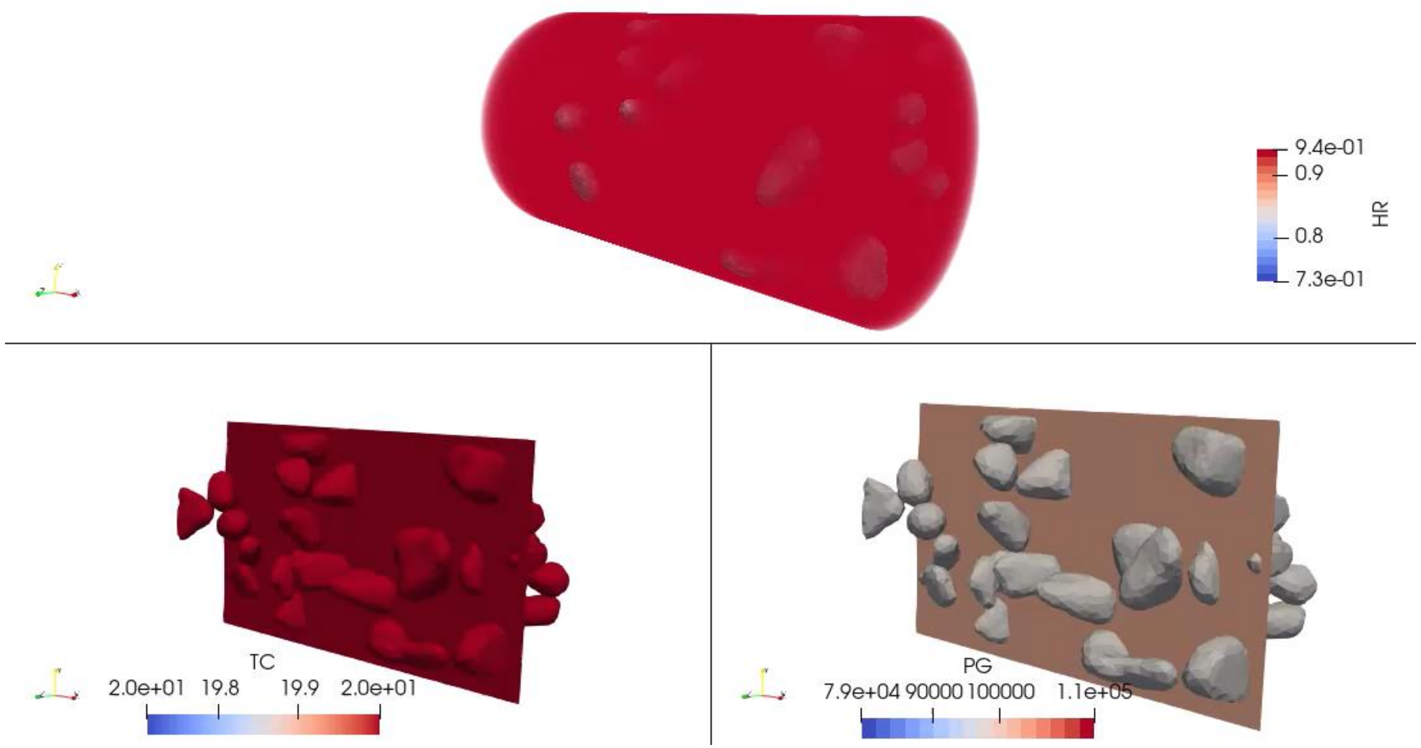


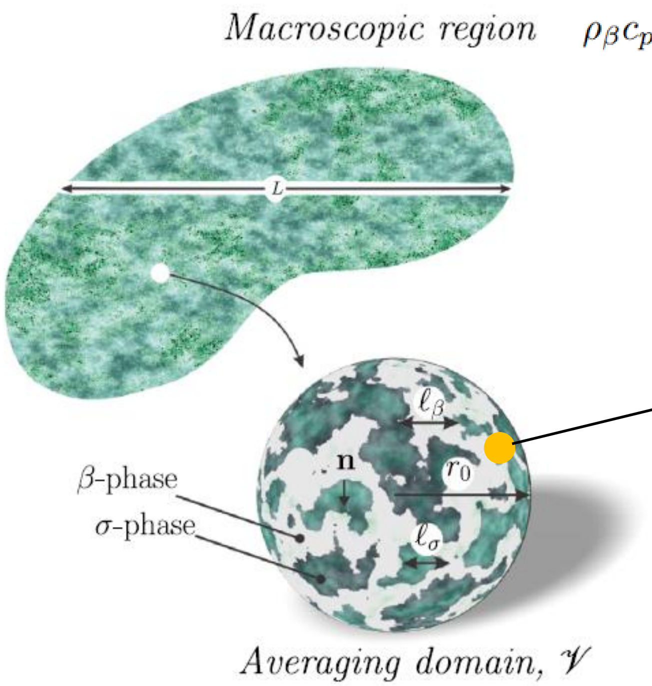
Figure 2: Snapshot of a shrinkage simulation with a THCM model on the imported mesh with CAST3M.



Video 2: Shrinkage simulation on the mesh exported from the real sample.

- Introduction
- **Mathematical Model**

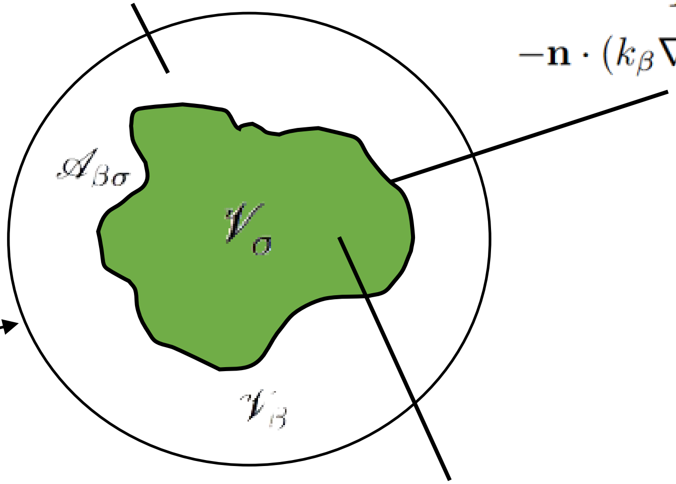
Mathematical Model: Meso-Scale Equations



$$\rho_\beta c_{p\beta} \frac{\partial T_\beta}{\partial t} = \nabla \cdot (k_\beta \nabla T_\beta)$$

$$T_\beta = T_\sigma$$

$$-\mathbf{n} \cdot (k_\beta \nabla T_\beta) = -\mathbf{n} \cdot (k_\sigma \nabla T_\sigma)$$



$$\rho_\sigma c_{p\sigma} \frac{\partial T_\sigma}{\partial t} = \nabla \cdot (k_\sigma \nabla T_\sigma)$$

1. Non Thermal Equilibrium;
2. Fourier's Law applicability;
3. Neglecting the interfacial resistance to heat transfer.

Figure 3: Sketch of a porous medium including a sample of the averaging volume and the characteristic length-scales. ***D. Lasseux and F.J.Valdés-Parada2025***. https://doi.org/10.1016/j.advwatres.2025.104899

Mathematical Model: Volume Averaging Method (*VAM*)

$$\begin{cases} \rho_\beta c_{p\beta} \dfrac{\partial T_\beta}{\partial t} = \nabla \cdot (k_\beta \nabla T_\beta), & \text{in } \mathscr{V}_\beta, \\ T_\beta = T_\sigma, & \text{at } \mathscr{A}_{\beta\sigma}, \\ -\mathbf{n} \cdot (k_\beta \nabla T_\beta) = -\mathbf{n} \cdot (k_\sigma \nabla T_\sigma), & \text{at } \mathscr{A}_{\beta\sigma}, \\ \rho_\sigma c_{p\sigma} \dfrac{\partial T_\sigma}{\partial t} = \nabla \cdot (k_\sigma \nabla T_\sigma), & \text{in } \mathscr{V}_\sigma \\ T_\alpha(\mathbf{r}, 0) = T_{\alpha 0}(\mathbf{r}) & \alpha = \beta, \sigma. \end{cases}$$

1. Applying the intrinsic average operator

$$\langle \cdot \rangle^\alpha = \frac{1}{V_\alpha} \int_{\mathscr{V}_\alpha} \cdot \, dV \quad \alpha = \beta, \sigma;$$

2. Separation of the length-scales: $max(\ell_\beta, \ell_\sigma) \ll r_0 \ll L$;
3. The media is statiscally homogeneous at r_0;
4. The media is pseudo-periodic;
5. Spatial averaging theorems (Whitaker 1999, 10.1007/978-94-017-3389-2);
6. Decomposition (Gray 1975, https://doi.org/10.1016/0009-2509(75)80010-8);

$$\psi_\alpha = \langle \psi_\alpha \rangle^\beta + \tilde{\psi}_\alpha \quad \alpha = \beta, \sigma.$$

7. $t_{\text{ref}} >> \max_{[t_0, t_{\text{fin}}]} \{\tau_\beta, \tau_\sigma\}, \quad \tau_\alpha = \dfrac{\rho_\alpha c_{p\alpha} l_a^2}{k_\alpha} \quad \alpha = \beta, \sigma.$

$$\rho_\beta c_{p\beta} \phi_\beta \frac{\partial \langle T_\beta \rangle^\beta}{\partial t} = \nabla \cdot \left(\mathbf{K}_{\beta\beta} \cdot \nabla \langle T_\beta \rangle^\beta + \mathbf{K}_{\beta\sigma} \cdot \nabla \langle T_\sigma \rangle^\sigma \right) + \mathbf{u}_{\beta\beta} \cdot \nabla \langle T_\beta \rangle^\beta + \mathbf{u}_{\beta\sigma} \cdot \nabla \langle T_\sigma \rangle^\sigma - \frac{a_v h}{\phi_\beta} \left(\langle T_\beta \rangle^\beta - \langle T_\sigma \rangle^\sigma \right)$$

$$\rho_\sigma c_{p\sigma} \phi_\sigma \frac{\partial \langle T_\sigma \rangle^\sigma}{\partial t} = \nabla \cdot \left(\mathbf{K}_{\sigma\sigma} \cdot \nabla \langle T_\sigma \rangle^\sigma + \mathbf{K}_{\sigma\beta} \cdot \nabla \langle T_\beta \rangle^\beta \right) + \mathbf{u}_{\sigma\sigma} \cdot \nabla \langle T_\sigma \rangle^\sigma + \mathbf{u}_{\sigma\beta} \cdot \nabla \langle T_\beta \rangle^\beta - \frac{a_v h}{\phi_\sigma} \left(\langle T_\sigma \rangle^\sigma - \langle T_\beta \rangle^\beta \right).$$

Macroscopic Thermal Non - Equilibrium Equations

Mathematical Model: Effective Coefficients

Problem **b**

$$\begin{cases} \nabla^2 \mathbf{b}_\beta = \frac{1}{V_\beta}\int_{\mathscr{A}_{\beta\sigma}} \mathbf{n}\cdot\nabla\mathbf{b}_\beta \, dA & \text{in } \mathscr{V}_\beta \\ \mathbf{b}_\beta = -\frac{k_\beta}{k_\sigma}\mathbf{b}_\sigma & \text{at } \mathscr{A}_{\beta\sigma} \\ -\mathbf{n}\cdot\nabla\mathbf{b}_\beta = -\mathbf{n}\cdot\nabla\mathbf{b}_\sigma + \mathbf{n} & \text{at } \mathscr{A}_{\beta\sigma} \\ \nabla^2 \mathbf{b}_\sigma = -\frac{1}{V_\sigma}\int_{\mathscr{A}_{\beta\sigma}} \mathbf{n}\cdot\nabla\mathbf{b}_\sigma \, dA & \text{in } \mathscr{V}_\sigma \\ \mathbf{b}_\alpha(\mathbf{r}) = \mathbf{b}_\alpha(\mathbf{r}+L_i\mathbf{e}_i), \quad i=1,2,3, \ \alpha=\beta,\sigma & \\ \langle \mathbf{b}_\alpha \rangle^\alpha = \mathbf{0} \quad \alpha = \beta,\sigma & \end{cases}$$

Problem s

$$\begin{cases} \nabla^2 s_\beta = \frac{1}{V_\beta}\int_{\mathscr{A}_{\beta\sigma}} \mathbf{n}\cdot\nabla s_\beta \, dA & \text{in } \mathscr{V}_\beta \\ s_\beta = 1 - s_\sigma & \text{at } \mathscr{A}_{\beta\sigma} \\ -\mathbf{n}\cdot k_\beta\nabla s_\beta = \mathbf{n}\cdot k_\sigma \nabla s_\sigma & \text{at } \mathscr{A}_{\beta\sigma} \\ \nabla^2 s_\sigma = -\frac{1}{V_\sigma}\int_{\mathscr{A}_{\beta\sigma}} \mathbf{n}\cdot\nabla s_\sigma \, dA & \text{in } \mathrm{A}_\sigma, \\ s_\alpha(\mathbf{r}) = s_\alpha(\mathbf{r}+L_i\mathbf{e}_i), \quad i=1,2,3, \ \alpha=\beta,\sigma & \\ \langle s_\alpha \rangle^\alpha = 0 \quad \alpha = \beta,\sigma & \end{cases}$$

$$\mathbf{K}_{\beta\beta} = k_\beta\left(\mathbf{I} + \frac{1}{V_\beta}\int_{\mathscr{A}_{\beta\sigma}} \mathbf{n}\otimes\mathbf{b}_\beta \, dA\right)$$

$$\mathbf{K}_{\beta\sigma} = -\frac{k_\beta}{V_\beta}\int_{\mathscr{A}_{\beta\sigma}} \mathbf{n}\otimes\mathbf{b}_\beta \, dA$$

$$\mathbf{K}_{\sigma\sigma} = k_\sigma\left(\mathbf{I} - \frac{1}{V_\sigma}\int_{\mathscr{A}_{\beta\sigma}} \mathbf{n}\otimes\mathbf{b}_\sigma \, dA\right)$$

$$\mathbf{K}_{\sigma\beta} = \frac{k_\sigma}{V_\sigma}\int_{\mathscr{A}_{\beta\sigma}} \mathbf{n}\otimes\mathbf{b}_\sigma \, dA$$

Dominant and Coupled heat conductivity tensors

$$\mathbf{u}_{\beta\beta} = \frac{k_\beta}{V_\beta}\int_{\mathscr{A}_{\beta\sigma}} \mathbf{n}\cdot(\nabla\mathbf{b}_\beta - s_\beta\mathbf{I}) \, dA$$

$$\mathbf{u}_{\beta\sigma} = \frac{k_\beta}{V_\beta}\int_{\mathscr{A}_{\beta\sigma}} \mathbf{n}\cdot\left(s_\beta\mathbf{I} - \frac{k_\sigma}{k_\beta}\nabla\mathbf{b}_\beta\right) dA$$

$$\mathbf{u}_{\sigma\sigma} = \frac{k_\sigma}{V_\sigma}\int_{\mathscr{A}_{\beta\sigma}} \mathbf{n}\cdot(s_\sigma\mathbf{I} - \nabla\mathbf{b}_\sigma) \, dA$$

$$\mathbf{u}_{\sigma\beta} = \frac{k_\sigma}{V_\sigma}\int_{\mathscr{A}_{\beta\sigma}} \mathbf{n}\cdot\left(\frac{k_\beta}{k_\sigma}\nabla\mathbf{b}_\sigma - s_\sigma\mathbf{I}\right) dA$$

Dominant Conduction and Co-Conduction heat corrective vectors

$$h = \frac{k_\beta}{A_{\beta\sigma}}\int_{\mathscr{A}_{\beta\sigma}} \mathbf{n}\cdot\nabla s_\beta \, dA = -\frac{k_\sigma}{A_{\beta\sigma}}\int_{\mathscr{A}_{\beta\sigma}} \mathbf{n}\cdot\nabla s_\sigma \, dA$$

Effective interfacial heat coefficient

Mathematical Model: Properties of Effective Coefficients

As showen in ***D. Lasseux and F.J. Valdés-Parada 2025*** (https://doi.org/10.1016/j.advwatres.2025.104899)

1) $\phi_\beta \mathbf{K}_{\beta\sigma} = \phi_\sigma \mathbf{K}_{\sigma\beta} := \mathbf{K}_c$

2) $\phi_\beta k_\sigma^2 \left(\mathbf{K}_{\beta\beta} - k_\beta \mathbf{I}\right) = \phi_\sigma k_\beta^2 \left(\mathbf{K}_{\sigma\sigma} - k_\sigma \mathbf{I}\right)$

3) $\phi_\beta \mathbf{u}_{\beta\sigma} = -\phi_\sigma \mathbf{u}_{\sigma\beta} := (k_\beta - k_\sigma)\mathbf{u}_c$

4) $\mathbf{u}_{\beta\beta} = \mathbf{u}_{\sigma\sigma} = \mathbf{0}$

5) $\mathbf{u}_c = \mathbf{0}$ if the unit cell is symmetric

6) $\mathbf{K}_{\alpha\kappa}$ $(\alpha, \kappa = \beta, \sigma)$ are positive definite and symmetric tensors.

Mathematical Model: Thermal Non - Equilibrium and Thermal Equilibrium

$$\rho_\beta c_{p\beta} \phi_\beta \frac{\partial \langle T_\beta \rangle^\beta}{\partial t} = \nabla \cdot (\phi_\beta \mathbf{K}_{\beta\beta} \cdot \nabla \langle T_\beta \rangle^\beta + \mathbf{K}_c \cdot \nabla \langle T_\sigma \rangle^\sigma) + (k_\beta - k_\sigma) \mathbf{u}_c \cdot \nabla \langle T_\sigma \rangle^\sigma - a_v h (\langle T_\beta \rangle^\beta - \langle T_\sigma \rangle^\sigma)$$

$$\rho_\sigma c_{p\sigma} \phi_\sigma \frac{\partial \langle T_\sigma \rangle^\sigma}{\partial t} = \nabla \cdot (\phi_\sigma \mathbf{K}_{\sigma\sigma} \cdot \nabla \langle T_\sigma \rangle^\sigma + \mathbf{K}_c \cdot \nabla \langle T_\beta \rangle^\beta) - (k_\beta - k_\sigma) \mathbf{u}_c \cdot \nabla \langle T_\beta \rangle^\beta + a_v h (\langle T_\beta \rangle^\beta - \langle T_\sigma \rangle^\sigma)$$

Macroscopic Thermal Non - Equilibrium Equations (2Eqs. Model)

$$\langle T_\beta \rangle^\beta = \langle T_\sigma \rangle^\sigma = \langle T \rangle$$

$$\langle \rho c_p \rangle \frac{\partial \langle T \rangle}{\partial t} = \nabla \cdot [(\phi_\beta \mathbf{K}_{\beta\beta} + 2\mathbf{K}_c + \phi_\sigma \mathbf{K}_{\sigma\sigma}) \cdot \nabla \langle T \rangle]$$

Macroscopic Thermal Equilibrium Equation (1Eq. Model)

- Introduction
- Mathematical Model
- **Numerical Simulations**

Numerical Simulations: Direct Numerical Simulation (DNS)

$$
\begin{cases}
\rho_\beta c_{p\beta}\dfrac{\partial T_\beta}{\partial t} = \nabla\cdot(k_\beta \nabla T_\beta), & \text{in } \mathscr{V}_\beta,\\
T_\beta = T_\sigma, & \text{at } \mathscr{A}_{\beta\sigma},\\
-\mathbf{n}\cdot(k_\beta\nabla T_\beta) = -\mathbf{n}\cdot(k_\sigma\nabla T_\sigma), & \text{at } \mathscr{A}_{\beta\sigma},\\
\rho_\sigma c_{p\sigma}\dfrac{\partial T_\sigma}{\partial t} = \nabla\cdot(k_\sigma \nabla T_\sigma), & \text{in } \mathscr{V}_\sigma\\
T_\alpha(\mathbf{r},0) = T_{\alpha 0}(\mathbf{r}) & \alpha=\beta,\sigma.
\end{cases}
$$

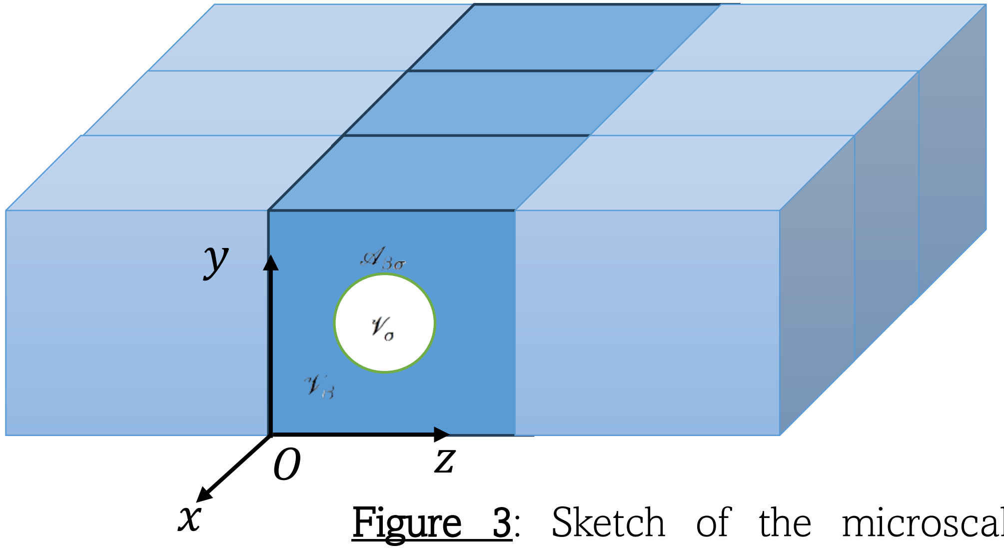


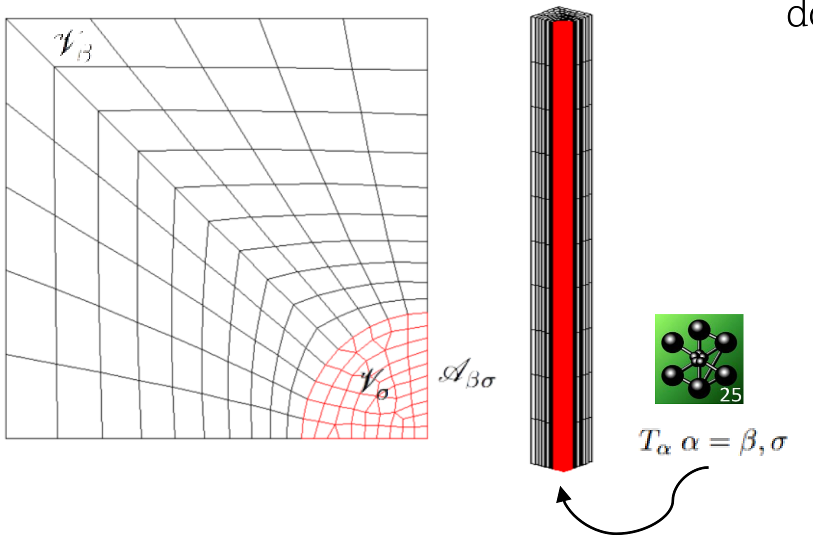
Figure 3: Sketch of the microscale domain considered for the DNS.

Table 1: Properties of micro-scopic domain (DNS).

Quantity	Symbol	Value	Unit of Measure
Volume fraction of phase β	ϕ_β	0.93	–
Volume fraction of phase σ	ϕ_σ	0.07	–
Characteristic length	L	0.1	m
Height	H	0.05	m
Radios of the inclusion	r	0.015	m

Table 2: Initial and boundary conditions (DNS).

Quantity	Symbol	Value	Unit of Measure
Imposed temperature	T_α $\alpha=\beta,\sigma$	200	C
Initial temperature	$T_{\alpha 0}$	20	C



Numerical Simulations: Direct Numerical Simulation (DNS)

```
PRO_ABSC = PROG;
PRO_ORDO = PROG;

N1 = 0;

REPETER BOU_TMOY (MESH_REF*24);
  DZ         = 1./(MESH_REF*24);
  SURF_MA1 = MAIL_IN PLUS (0. 0. (N1*DZ));
  TEMPE_T = CHAN CHAM TAB1.TEMPERATURES.time1 MOD_ACI;
  T_SURF_MA1 = PROI SURF_MA1 TEMPE_T;
  MOD_BID = MODE SURF_MA1 THERMIQUE;
  T_SURF_MA1 = EXCO 'T' (CHAN CHAM T_SURF_MA1 MOD_BID);
  INT_T_MA  = INTG  MOD_BID T_SURF_MA1;
  T_MOY_MA  = INT_T_MA / A_IN;
  LIST T_MOY_MA;
  PRO_ABSC = PRO_ABSC ET (PROG (N1*DZ));
  PRO_ORDO = PRO_ORDO ET (PROG T_MOY_MA);
  N1 = N1 + 1;
FIN BOU_TMOY;
EV_TIN1 = EVOL 'CYAN' MANU PRO_ABSC PRO_ORDO;
```

$$\langle T_\beta \rangle^\beta = \frac{1}{V_\beta} \int_{\mathcal{V}_\beta} T_\beta \, dV$$

```
PRO_ABSC = PROG;
PRO_ORDO = PROG;

N1 = 0;

REPETER BOU_TMOY (MESH_REF*24);
  DZ         = 1./(MESH_REF*24);
  SURF_MA1 = MAIL_MA PLUS (0. 0. (N1*DZ));
  TEMPE_T = CHAN CHAM TAB1.TEMPERATURES.time1 MOD_BET;
  T_SURF_MA1 = PROI SURF_MA1 TEMPE_T;
  MOD_BID = MODE SURF_MA1 THERMIQUE;
  T_SURF_MA1 = EXCO 'T' (CHAN CHAM T_SURF_MA1 MOD_BID);
  INT_T_MA  = INTG  MOD_BID T_SURF_MA1;
  T_MOY_MA  = INT_T_MA / A_MA;
  LIST T_MOY_MA;
  PRO_ABSC = PRO_ABSC ET (PROG (N1*DZ));
  PRO_ORDO = PRO_ORDO ET (PROG T_MOY_MA);
  N1 = N1 + 1;
FIN BOU_TMOY;
EV_TMA1 = EVOL 'CYAN' MANU PRO_ABSC PRO_ORDO;
```

$$\langle T_\sigma \rangle^\sigma = \frac{1}{V_\sigma} \int_{\mathcal{V}_\sigma} T_\sigma \, dV$$

Numerical Simulations: Closure Problems

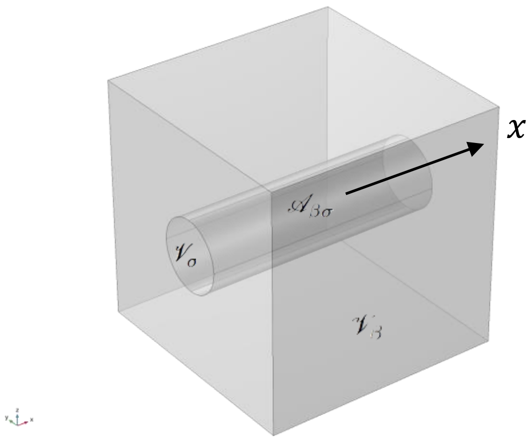


Figure 5: Periodic and symmetric unit cell for the closure problems solution.

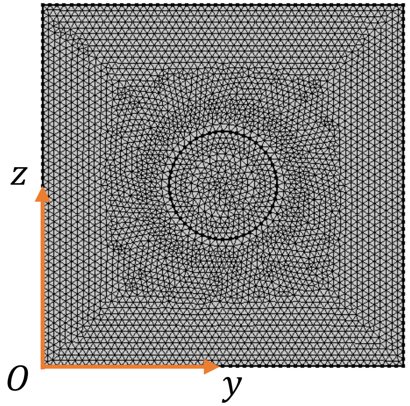


Figure 6: 2D - Periodic and symmetric unit cell for the closure problems.

Table 3: Properties of the unit cell.

Quantity	Symbol	Value	Unit of Measure
Volume fraction of phase β	ϕ_β	0.93	–
Volume fraction of phase σ	ϕ_σ	0.07	–
Characteristic length	l	0.01	m
Radios of the inclusion	r	0.015	m

Problem b

$$\begin{cases} \nabla^2 \mathbf{b}_\beta = \dfrac{1}{V_\beta} \displaystyle\int_{\mathscr{A}_{\beta\sigma}} \mathbf{n} \cdot \nabla \mathbf{b}_\beta \, dA & \text{in } \mathscr{V}_\beta \\ \mathbf{b}_\beta = -\dfrac{k_\beta}{k_\sigma} \mathbf{b}_\sigma & \text{at } \mathscr{A}_{\beta\sigma} \\ -\mathbf{n} \cdot \nabla \mathbf{b}_\beta = -\mathbf{n} \cdot \nabla \mathbf{b}_\sigma + \mathbf{n} & \text{at } \mathscr{A}_{\beta\sigma} \\ \nabla^2 \mathbf{b}_\sigma = -\dfrac{1}{V_\sigma} \displaystyle\int_{\mathscr{A}_{\beta\sigma}} \mathbf{n} \cdot \nabla \mathbf{b}_\sigma \, dA & \text{in } \mathscr{V}_\sigma \\ \mathbf{b}_\alpha(\mathbf{r}) = \mathbf{b}_\alpha(\mathbf{r} + L_i \mathbf{e}_i), \quad i = 1,2,3, \ \alpha = \beta, \sigma & \\ \langle \mathbf{b}_\alpha \rangle^\alpha = \mathbf{0} \quad \alpha = \beta, \sigma & \end{cases}$$

Problem s

$$\begin{cases} \nabla^2 s_\beta = \dfrac{1}{V_\beta} \displaystyle\int_{\mathscr{A}_{\beta\sigma}} \mathbf{n} \cdot \nabla s_\beta \, dA & \text{in } \mathscr{V}_\beta \\ s_\beta = 1 - s_\sigma & \text{at } \mathscr{A}_{\beta\sigma} \\ -\mathbf{n} \cdot k_\beta \nabla s_\beta = \mathbf{n} \cdot k_\sigma \nabla s_\sigma & \text{at } \mathscr{A}_{\beta\sigma} \\ \nabla^2 s_\sigma = -\dfrac{1}{V_\sigma} \displaystyle\int_{\mathscr{A}_{\beta\sigma}} \mathbf{n} \cdot \nabla s_\sigma \, dA & \text{in } \mathrm{A}_\sigma, \\ s_\alpha(\mathbf{r}) = s_\alpha(\mathbf{r} + L_i \mathbf{e}_i), \quad i = 1,2,3, \ \alpha = \beta, \sigma & \\ \langle s_\alpha \rangle^\alpha = 0 \quad \alpha = \beta, \sigma & \end{cases}$$

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Numerical Simulations: Macroscopic Model

CAST3M procedure:

- *CHARTHER* $a_v h(\langle T_\beta \rangle^\beta - \langle T_\sigma \rangle^\sigma)$

```
*****************************************************************
* CHARTHER
*****************************************************************
DEBP charther HTAB*'TABLE' tt*'FLOTTANT' ;
TAA=TABLE ;

* Altri parametri
AV   ;
HTRAN;

* Estrazione soluzione 1, w et 2 :
WORKTAB = PRECED   .'WTABLE';
THETA_W = WORKTAB . 'RELAXATION_THETA';
SOLU_1  = WORKTAB . 'CO1';
SOLU_2  = WORKTAB . 'CO2';
SOLU    = SOLU_1 + (THETA_W * (SOLU_2 - SOLU_1));

* Estrazione variabili primarie al passo w :
C1SC0 = ('EXCO' SOLU 'C1') 'NOMC' 'SCAL' ;
C2SC0 = ('EXCO' SOLU 'C2') 'NOMC' 'SCAL' ;

* Estrazione variabili primarie al passo n :
C1SC1 = ('EXCO' SOLU_1 'C1') 'NOMC' 'SCAL' ;
C2SC1 = ('EXCO' SOLU_1 'C2') 'NOMC' 'SCAL' ;

* Estrazione variabili primarie al passo (n+1) :
C1SC2 = ('EXCO' SOLU_2 'C1') 'NOMC' 'SCAL' ;
C2SC2 = ('EXCO' SOLU_2 'C2') 'NOMC' 'SCAL' ;

MO_THM   =  WORKTAB.'MOD_DIF';
ME_THM   = 'EXTR' MO_THM 'MAIL';

SOUR_C1     = ((C1SC0 - C2SC0) * AV * HTRAN) 'NOMC' 'SCAL';
FC0C1       = 'CHAN' 'CHAM' ((-1.) * SOUR_C1)  MO_THM;
SOURCE_C1   =  ('EXCO' 'QC1' ('SOUR' MO_THM FC0C1)) 'NOMC' 'QC1' ;

SOUR_C2 = -1 * SOUR_C1;
FC0C2       = 'CHAN' 'CHAM' ((-1.) * SOUR_C2)  MO_THM;
SOURCE_C2   =  ('EXCO' 'QC2' ('SOUR' MO_THM FC0C2)) 'NOMC' 'QC2' ;

* sortie du second membre
TAA . 'ADDI_SECOND' = SOURCE_C1 ET  SOURCE_C2;

FINP TAA;
*****************************************************************
```

- *diffu2.dgibi*

```
*--------------------- MODELE / CARACTERISTIQUES ----------------------*
*                                                                      *
* L'option 'INCO' de 'MODE' permet de definir le nom des inconnues     *
* primales et duales du modele (CO / QCO par defaut).                  *
* Attention ! limite a 2 caracteres pour le nom de l'inconnue primale  *
MOD1      = 'MODE' MESH1 'DIFFUSION' 'FICK' 'INCO' 'C1' 'QC1' ;
MOD2      = 'MODE' MESH1 'DIFFUSION' 'FICK' 'INCO' 'C2' 'QC2' ;

MAT1      = 'MATE' MOD1 'KD' (KD1 * (1. - V_FRACT)) 'CDIF' (RHO_BET*C_BET*(1. - V_FRACT));
MAT2      = 'MATE' MOD2 'KD' (KD2 * V_FRACT)        'CDIF' (RHO_ACI*C_ACI*V_FRACT) ;


************************************************************************
* Construction MATRICES de COUPLAGE :
* 1. on construit les matrices de diffusivite de chaque espece :       *
DC6QC6    = 'COND' MOD1 MAT1 ;
DC8QC8    = 'COND' MOD2 MAT2 ;
* 2. on renomme les noms d'inconnues sur lesquelles elles agissent :   *
* Pour DC6QC6, on a : C6 -> QC6, on veut : C8 -> QC6 :                 *
* Pour DC8QC8, on a : C8 -> QC8, on veut : C6 -> QC8 :                 *
* Attention ! il faut ajouter le mot-cle 'QUEL' pour indiquer a Cast3M *
*              que les matrices assemblees formeront un systeme qui ne *
*              sera pas symetrique (QUELconque).                       *
DC8QC6    = 'CHAN' 'INCO' DC6QC6 ('MOTS' 'C6')  ('MOTS' 'C8')
('MOTS' 'QC6') ('MOTS' 'QC6') 'QUEL' ;
DC6QC8    = 'CHAN' 'INCO' DC8QC8 ('MOTS' 'C8')  ('MOTS' 'C6')
('MOTS' 'QC8') ('MOTS' 'QC8') 'QUEL' ;
************************************************************************
```

$$\nabla \cdot (\phi_\beta \mathbf{K}_{\beta\beta} \cdot \nabla \langle T_\beta \rangle^\beta + \mathbf{K}_c \cdot \nabla \langle T_\sigma \rangle^\sigma)$$

$$\nabla \cdot (\phi_\sigma \mathbf{K}_{\sigma\sigma} \cdot \nabla \langle T_\sigma \rangle^\sigma + \mathbf{K}_c \cdot \nabla \langle T_\beta \rangle^\beta)$$

Numerical Simulations: Macroscopic Model

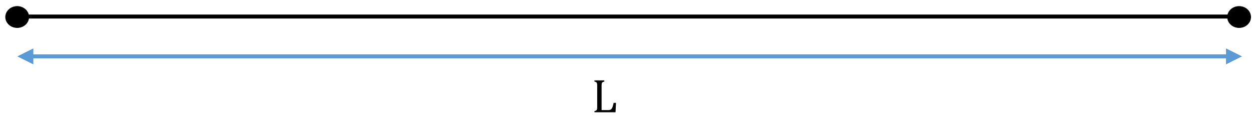


Figure 7: Macroscopic 1D representation of the considered geometry.

Table 4: Properties of macroscopic domain.

Quantity	Symbol	Value	Unit of Measure
Volume fraction of phase β	ϕ_β	0.93	–
Volume fraction of phase σ	ϕ_σ	0.07	–
Characteristic length	L	1	m

$$\rho_\beta c_{p\beta}\phi_\beta \frac{\partial \langle T_\beta\rangle^\beta}{\partial t} = \nabla \cdot \left(\phi_\beta \mathbf{K}_{\beta\beta} \cdot \nabla \langle T_\beta\rangle^\beta + \mathbf{K}_c \cdot \nabla \langle T_\sigma\rangle^\sigma\right) + (k_\beta - k_\sigma)\mathbf{u}_c \cdot \nabla \langle T_\sigma\rangle^\sigma - a_v h\left(\langle T_\beta\rangle^\beta - \langle T_\sigma\rangle^\sigma\right)$$

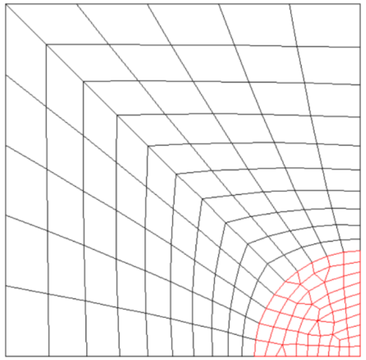
$$\rho_\sigma c_{p\sigma}\phi_\sigma \frac{\partial \langle T_\sigma\rangle^\sigma}{\partial t} = \nabla \cdot \left(\phi_\sigma \mathbf{K}_{\sigma\sigma} \cdot \nabla \langle T_\sigma\rangle^\sigma + \mathbf{K}_c \cdot \nabla \langle T_\beta\rangle^\beta\right) - (k_\beta - k_\sigma)\mathbf{u}_c \cdot \nabla \langle T_\beta\rangle^\beta + a_v h\left(\langle T_\beta\rangle^\beta - \langle T_\sigma\rangle^\sigma\right)$$

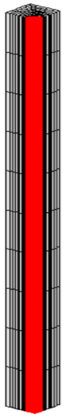
Macroscopic No-Thermal Equilibrium Equations (2Eqs. Model)

Numerical Simulations: Summery

Microscale Equations (DNS)

$$
\begin{cases}
\rho_\beta c_{p\beta} \dfrac{\partial T_\beta}{\partial t} = \nabla \cdot (k_\beta \nabla T_\beta), & \text{in } \mathscr{V}_\beta, \\
T_\beta = T_\sigma, & \text{at } \mathscr{A}_{\beta\sigma}, \\
-\mathbf{n} \cdot (k_\beta \nabla T_\beta) = -\mathbf{n} \cdot (k_\sigma \nabla T_\sigma), & \text{at } \mathscr{A}_{\beta\sigma}, \\
\rho_\sigma c_{p\sigma} \dfrac{\partial T_\sigma}{\partial t} = \nabla \cdot (k_\sigma \nabla T_\sigma), & \text{in } \mathscr{V}_\sigma \\
T_\alpha(\mathbf{r}, 0) = T_{\alpha 0}(\mathbf{r}) & \alpha = \beta, \sigma.
\end{cases}
$$



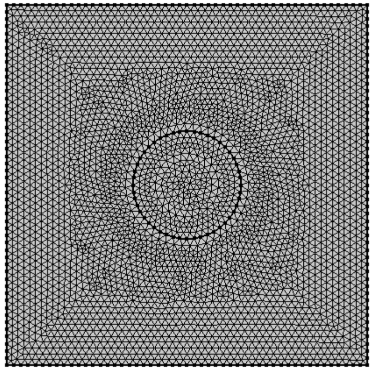


3D

Closure Problems

$$
\begin{cases}
\nabla^2 \mathbf{b}_\beta = \dfrac{1}{V_\beta} \displaystyle\int_{\mathscr{A}_{\beta\sigma}} \mathbf{n} \cdot \nabla \mathbf{b}_\beta \, dA \\
\mathbf{b}_\beta = -\dfrac{k_\beta}{k_\sigma} \mathbf{b}_\sigma \\
-\mathbf{n} \cdot \nabla \mathbf{b}_\beta = -\mathbf{n} \cdot \nabla \mathbf{b}_\sigma + \mathbf{n} \\
\nabla^2 \mathbf{b}_\sigma = -\dfrac{1}{V_\sigma} \displaystyle\int_{\mathscr{A}_{\beta\sigma}} \mathbf{n} \cdot \nabla \mathbf{b}_\sigma \, dA \\
\mathbf{b}_\alpha(\mathbf{r}) = \mathbf{b}_\alpha(\mathbf{r} + L_i \mathbf{e}_i), \quad i = 1, 2, 3, \ \alpha = \beta, \sigma \\
\langle \mathbf{b}_\alpha \rangle^\alpha = \mathbf{0} \quad \alpha = \beta, \sigma
\end{cases}
$$

$$
\begin{cases}
\nabla^2 s_\beta = \dfrac{1}{V_\beta} \displaystyle\int_{\mathscr{A}_{\beta\sigma}} \mathbf{n} \cdot \nabla s_\beta \, dA \\
s_\beta = 1 - s_\sigma \\
-\mathbf{n} \cdot k_\beta \nabla s_\beta = \mathbf{n} \cdot k_\sigma \nabla s_\sigma \\
\nabla^2 s_\sigma = -\dfrac{1}{V_\sigma} \displaystyle\int_{\mathscr{A}_{\beta\sigma}} \mathbf{n} \cdot \nabla s_\sigma \, dA \\
s_\alpha(\mathbf{r}) = s_\alpha(\mathbf{r} + L_i \mathbf{e}_i), \quad i = 1, 2, 3, \ \alpha = \beta, \sigma \\
\langle s_\alpha \rangle^\alpha = 0 \quad \alpha = \beta, \sigma
\end{cases}
$$



2D

COMSOL MULTIPHYSICS®

Macroscale Equations

$$
\rho_\beta c_{p\beta} \phi_\beta \frac{\partial \langle T_\beta \rangle^\beta}{\partial t} = \nabla \cdot (\phi_\beta \mathbf{K}_{\beta\beta} \cdot \nabla \langle T_\beta \rangle^\beta + \mathbf{K}_c \cdot \nabla \langle T_\sigma \rangle^\sigma) + (k_\beta - k_\sigma) \mathbf{u}_c \cdot \nabla \langle T_\sigma \rangle^\sigma - a_v h (\langle T_\beta \rangle^\beta - \langle T_\sigma \rangle^\sigma)
$$

$$
\rho_\sigma c_{p\sigma} \phi_\sigma \frac{\partial \langle T_\sigma \rangle^\sigma}{\partial t} = \nabla \cdot (\phi_\sigma \mathbf{K}_{\sigma\sigma} \cdot \nabla \langle T_\sigma \rangle^\sigma + \mathbf{K}_c \cdot \nabla \langle T_\beta \rangle^\beta) - (k_\beta - k_\sigma) \mathbf{u}_c \cdot \nabla \langle T_\beta \rangle^\beta + a_v h (\langle T_\beta \rangle^\beta - \langle T_\sigma \rangle^\sigma)
$$

1D

Numerical Simulations: Test Cases $\frac{k_\sigma}{k_\beta} = 10, \phi_\beta = 0.93, \phi_\sigma = 0.07$

Table 5: Thermal properties Low Contrast (**LC**) case.

Quantity	Symbol	Value	Unit of Measure
Thermal conductivity of phase β	k_β	1.5	$\mathrm{W\,m^{-1}C^{-1}}$
Thermal conductivity of phase σ	k_σ	15	$\mathrm{W\,m^{-1}C^{-1}}$
Initial temperature	$T(0)$	20	C
Imposed temperature	T_0	200	C
Density of the phase β	ρ_β	2300	$\mathrm{Kg\,m^{-3}}$
Density of the phase σ	ρ_σ	1800	$\mathrm{Kg\,m^{-3}}$
Heat capacity of the phase β	$c_{p\beta}$	900	$\mathrm{J\,Kg^{-1}C^{-1}}$
Heat capacity of the phase σ	$c_{p\sigma}$	700	$\mathrm{J\,Kg^{-1}C^{-1}}$

Table 6: Effective parameters for (**LC**) case.

Quantity	Symbol	Value	Unit of Measure
Dominant conductive component of phase β	$K_{\beta\beta_{xx}}$	1.5	$\mathrm{W\,m^{-1}C^{-1}}$
Dominant conductive component of phase σ	$K_{\sigma\sigma_{xx}}$	15	$\mathrm{W\,m^{-1}C^{-1}}$
Co - Dominant conductive component of phase σ	$K_{c_{xx}}$	0	$\mathrm{W\,m^{-1}C^{-1}}$
Interfacial area per unit volume	a_v	9.379	$\mathrm{m^{-1}}$
Effective interfacial heat coefficient	h	127.45	$\mathrm{W\,m^{-2}C^{-1}}$

Numerical Simulations: DNS - Test Case LC -

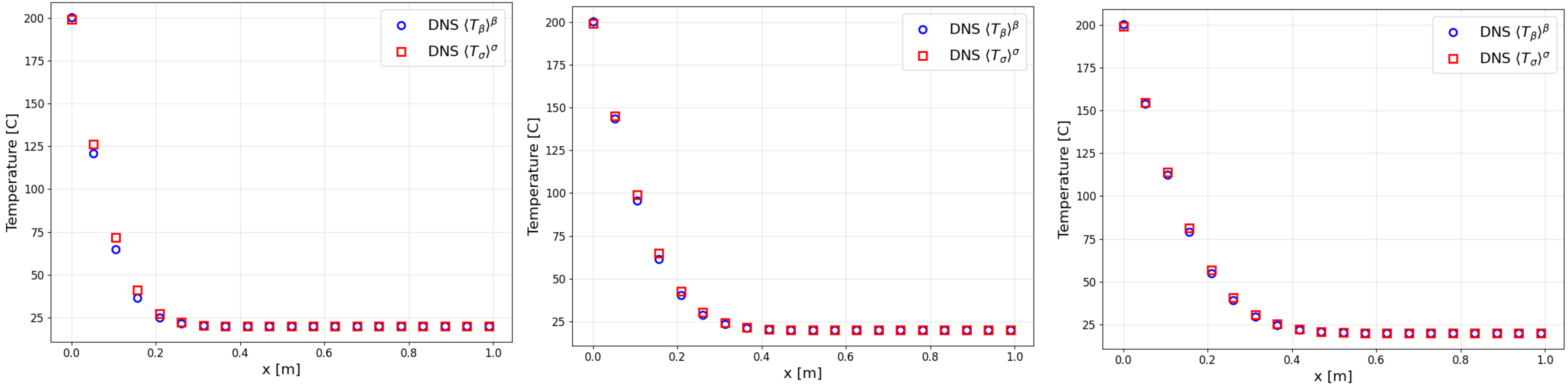


Figure 8: Direct Numerical Simulation (DNS) at different time of $\langle T_\alpha \rangle^\alpha$ for $\alpha = \beta, \sigma$ in LC-case.

Numerical Simulations: DNS vs 2 Eqs. vs 1 Eq. - Test Case LC -

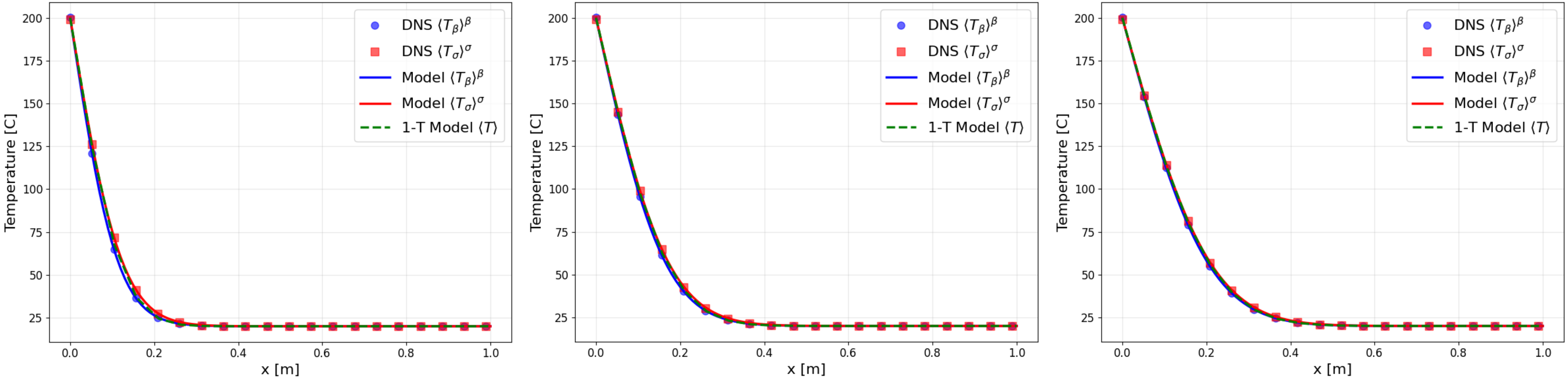


Figure 9: Comparison between Direct Numerical Simulation (DNS), 2Eqs. and 1 Eq. at different time of $\langle T_\alpha \rangle^\alpha$ for $\alpha = \beta, \sigma$ in LC-case.

Numerical Simulations: Test Cases $\frac{k_\sigma}{k_\beta} = 38.6, \phi_\beta = 0.93, \phi_\sigma = 0.07$

Table 7: Thermal properties Medium Contrast (MC) case.

Quantity	Symbol	Value	Unit of Measure
Thermal conductivity of phase β	k_β	1.4	$\mathrm{W\,m^{-1}C^{-1}}$
Thermal conductivity of phase σ	k_σ	54	$\mathrm{W\,m^{-1}C^{-1}}$
Initial temperature	$T(0)$	20	C
Imposed temperature	T_0	200	C
Density of the phase β	ρ_β	2100	$\mathrm{Kg\,m^{-3}}$
Density of the phase σ	ρ_σ	7800	$\mathrm{Kg\,m^{-3}}$
Heat capacity of the phase β	$c_{p\beta}$	900	$\mathrm{J\,Kg^{-1}C^{-1}}$
Heat capacity of the phase σ	$c_{p\sigma}$	500	$\mathrm{J\,Kg^{-1}C^{-1}}$

Table 8: Effective parameters for (MC) case.

Quantity	Symbol	Value	Unit of Measure
Dominant conductive component of phase β	$K_{\beta\beta_{xx}}$	1.4	$\mathrm{W\,m^{-1}C^{-1}}$
Dominant conductive component of phase σ	$K_{\sigma\sigma_{xx}}$	54	$\mathrm{W\,m^{-1}C^{-1}}$
Co - Dominant conductive component of phase σ	$K_{c_{xx}}$	0	$\mathrm{W\,m^{-1}C^{-1}}$
Interfacial area per unit volume	a_v	9.379	$\mathrm{m^{-1}}$
Effective interfacial heat coefficient	h	121.814	$\mathrm{W\,m^{-2}C^{-1}}$

Numerical Simulations: DNS - Test Case MC -

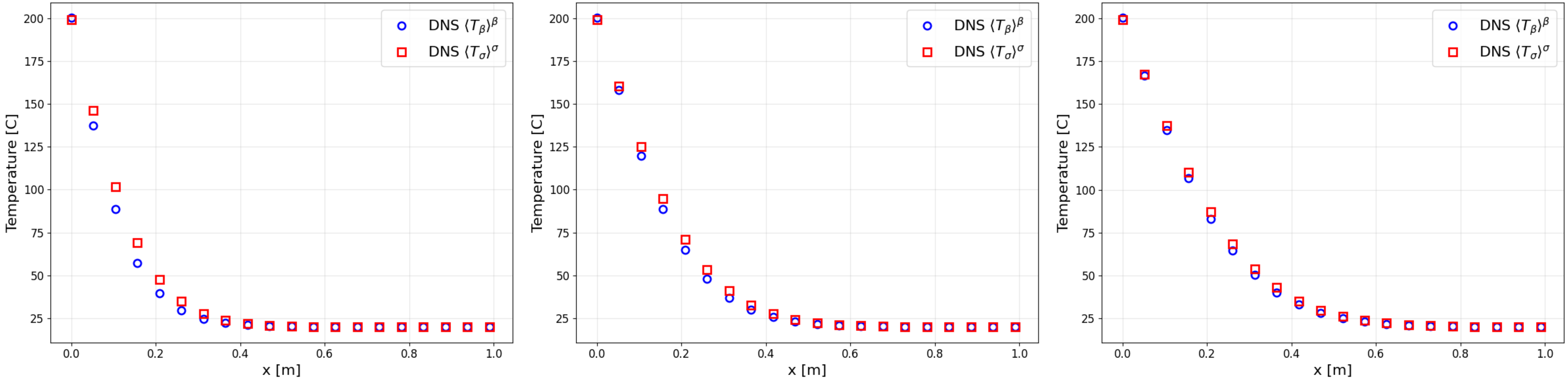


Figure 10: Direct Numerical Simulation (DNS) at different time of $\langle T_\alpha \rangle^\alpha$ for $\alpha = \beta, \sigma$ in MC-case.

Numerical Simulations: DNS vs 2 Eqs. vs 1 Eq. - Test Case MC -

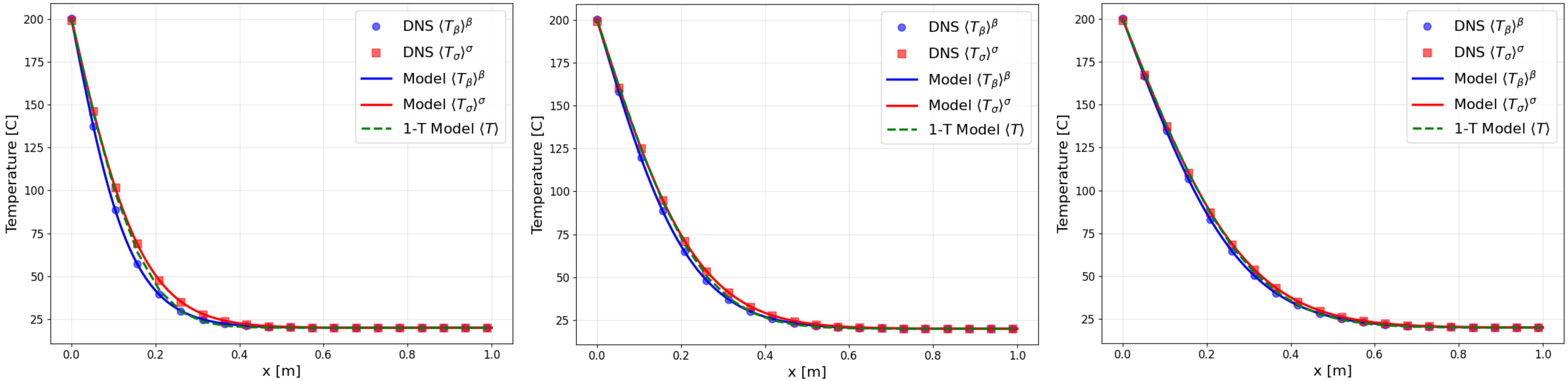


Figure 11: Comparison between Direct Numerical Simulation (DNS), 2Eqs. and 1 Eq. at different time of $\langle T_\alpha \rangle^\alpha$ for $\alpha = \beta, \sigma$ in MC-case.

Numerical Simulations: Test Cases $\frac{k_\sigma}{k_\beta} = 176.5, \phi_\beta = 0.93, \phi_\sigma = 0.07$

Table 9: Thermal properties High Contrast (**HC**) case.

Quantity	Symbol	Value	Unit of Measure
Thermal conductivity of phase β	k_β	0.17	$\mathrm{W\,m^{-1}C^{-1}}$
Thermal conductivity of phase σ	k_σ	30	$\mathrm{W\,m^{-1}C^{-1}}$
Initial temperature	$T(0)$	20	C
Imposed temperature	T_0	200	C
Density of the phase β	ρ_β	1150	$\mathrm{Kg\,m^{-3}}$
Density of the phase σ	ρ_σ	3900	$\mathrm{Kg\,m^{-3}}$
Heat capacity of the phase β	$c_{p\beta}$	1100	$\mathrm{J\,Kg^{-1}C^{-1}}$
Heat capacity of the phase σ	$c_{p\sigma}$	880	$\mathrm{J\,Kg^{-1}C^{-1}}$

Table 10: Effective parameters for (**HC**) case.

Quantity	Symbol	Value	Unit of Measure
Dominant conductive component of phase β	$K_{\beta\beta_{xx}}$	0.07	$\mathrm{W\,m^{-1}C^{-1}}$
Dominant conductive component of phase σ	$K_{\sigma\sigma_{xx}}$	30	$\mathrm{W\,m^{-1}C^{-1}}$
Co - Dominant conductive component of phase σ	$K_{c_{xx}}$	0	$\mathrm{W\,m^{-1}C^{-1}}$
Interfacial area per unit volume	a_v	9.379	$\mathrm{m^{-1}}$
Effective interfacial heat coefficient	h	14.89	$\mathrm{W\,m^{-2}C^{-1}}$

Numerical Simulations: DNS - Test Case HC -

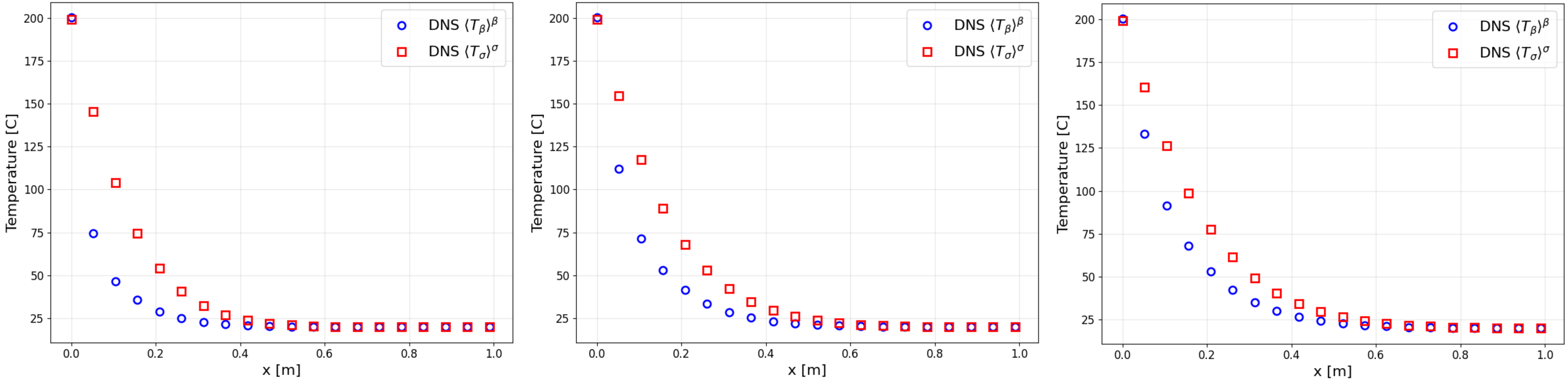


Figure 12: Direct Numerical Simulation (DNS) at different time of $\langle T_\alpha \rangle^\alpha$ for $\alpha = \beta, \sigma$ in HC-case.

Numerical Simulations: DNS vs 2 Eqs. vs 1 Eq. - Test Case HC -

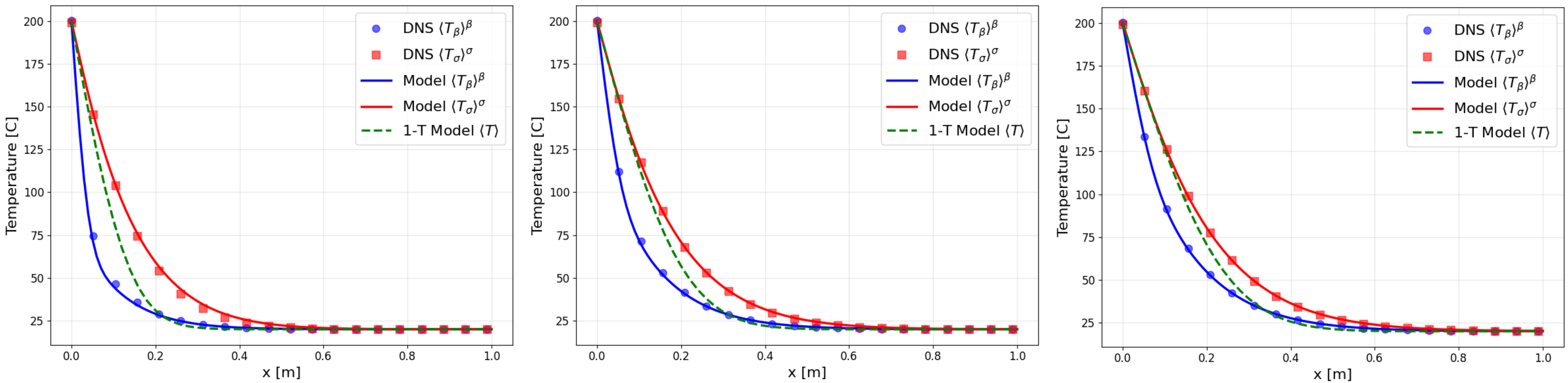


Figure 13: Comparison between Direct Numerical Simulation (DNS), 2Eqs. and 1 Eq. at different time of $\langle T_\alpha \rangle^\alpha$ for $\alpha = \beta, \sigma$ in HC-case.

Numerical Simulations: DNS vs 2 Eqs. vs 1 Eq. - Test Case HC -

$$\langle T \rangle = \langle T_\beta \rangle^\beta = \langle T_\sigma \rangle^\sigma$$

$$\langle \theta \rangle = \phi_\beta \langle T_\beta \rangle^\beta + \phi_\sigma \langle T_\sigma \rangle^\sigma$$

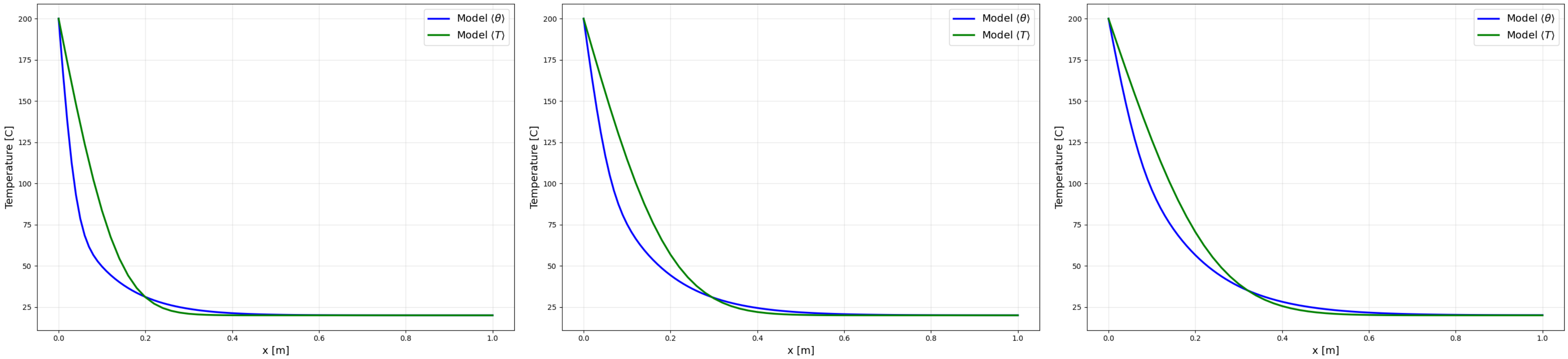


Figure 14: Comparison between 1 Eq. model and ⟨θ⟩ at different time in HC-case.

- Introduction
- Mathematical Model
- Numerical Simulations
- **<u>Conclusion</u>**

Conclusion: Objectives Achieved and Future Perspectives

I. Estimation of the effective parameters;
II. Good agreement between DNS and homogenized model;
III. Assessment of the applicability of the two-equation vs one-equation model.

I. Relax the time constraint hypothesis → (*Unsteady macroscopic one and two-equation models for equilibrium and non-equilibrium diffusive process in heterogeneous media*, **IN PREPARATION**) .

Promote the implementation of periodic boundary conditions in CAST3M to solve closure problems.

THANKS FOR YOUR ATTENTION

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