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Comparison of methods for homogenizing the thermal properties of ultra-high performance fiber reinforced concrete

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Abstract. Ultra-high-performance fiber reinforced concrete (UHPFRC) stands out in the current context of civil construction as an alternative of great interest in the design of bold, slender and sophisticated structures. The performance under high thermal loads has been studied in order to understand the degradation of materials and a reduction in mechanical strength capacities, which indicates a loss of safety in structures. Computer simulations are a helpful tool for studying behavior patterns and identifying the mechanisms involved in the process of concrete damage when subjected to thermal stress. However, a challenge encountered in these models is the size difference between the fibers and the cementitious matrix in which they are embedded, which drives investment in homogenized models, as discrete modelling requires highly refined mesh generation and, consequently, high computational costs. In this context, this study aims to compare thermal models to represent the heating of synthetic UHPFRC specimens. Different models are discussed, including discrete fibers and homogenized systems, based on various methods in the literature. Analyses are carried out for concretes with fiber reinforcement rates ranging from 0 to 2% at temperatures of up to 600°C. The results show that the homogenized models have a good ability to approximate the thermal behavior observed in simulations with discrete fibers, with significant computational savings.

Keywords: Ultra-high-performance concrete, Steel Fibers, Homogenization, Heat Transfer, High-temperature behavior.

1 Introduction

The Construction Industry is situated in a context of seeking materials that are more economical from environmental, social, and financial perspectives, while still meeting the technical requirements for which they are used. In this regard, concrete, which stands out as the most widely used material in this sector, is the subject of various studies aiming to improve its limitations, among which are its low tensile strength, susceptibility to cracking, and limited deformability [1]. As a result of these efforts, ultra-high-performance concrete (UHPC) has been developed — a special type of concrete capable of withstanding high mechanical demands and meeting durability requirements, thus becoming an attractive alternative in the design of bold, slender, and sophisticated structures. It is worth highlighting that UHPC shows a significant increase in tensile strength, as well as improved tensile ductility and toughness due to the addition of fibers, as noted by Xue *et al*. [2].

The improvements presented by this material are due to a mix design with a high cement content, the use of admixtures (plasticizers and superplasticizers), and mineral additions such as silica fume, according to Bolina *et al*. [3]. The mix design for these concretes is based on the dense packing theory, with a low water-to-cement ratio, which results in low porosity and compressive strength exceeding 150 MPa and tensile strength above 7 MPa [1][4]. However, this increase in load-bearing capacity can make UHPC a brittle material. Therefore, it is very common, in order to enhance the ductile behavior of the material, to combine UHPC with steel, synthetic, mineral or organic fibers. When UHPC is combined with fibers, it is referred to as Ultra-High-Performance Fiber-Reinforced Concrete, identified as UHPFRC.

When analyzed under the issue of thermal loading, UHPC shows lower strength compared to conventional concrete. UHPC is more susceptible to spalling phenomena, as it consists of a less porous and less permeable matrix. As a result, the vapor generated from free water and the dehydration of paste components during heating causes a significant increase in pore pressure, as discussed by Kodur *et al*. [5]. This author further explains that the addition of fibers also helps to counteract the internal pressures generated by thermal loads. In general, fibers contribute to the mechanical strength of concrete; however, polypropylene fibers reduce pore pressure, as they melt at elevated temperatures and create pores that relieve vapor pressure [6].

The development of numerical models has supported the analysis of material behavior, as they allow for the simulation of various problems in a simplified manner and enable the study of processes experienced by bodies based on theoretical models. Accordingly, the literature contains numerous studies presenting a numerical approach to UHPC and UHPFRC. Xue *et al*. [7] investigated the influence of fiber orientation on the improvement of mechanical properties through experimental, microstructural, and numerical investigation. Saeed and Hejazi [8] analyzed the use of UHPFRC as reinforcement for conventional concrete structures, employing computational tools to carry out the proposed analysis. Reddy *et al*. [9] presented experimental and numerical results for flexural tests of steel fiber-reinforced UHPFRC, indicating that the simulated models provided a good representation of the observed phenomena.

There is a similarity among the most recent studies addressing the modeling of UHPFRC, namely the consideration of the material as a heterogeneous system, without discretizing the fibers embedded in the matrix. In this context, the present study aims to investigate the impact of the homogenization of UHPFRC for the simulation of thermal problems, by comparing different methods with the discrete model.

2 Methodology

This study presents a comparative analysis between computational models for the thermal simulation of UHPFRC specimens. Two types of approaches were implemented: a biphasic model, which explicitly represents the steel fibers embedded in the concrete, and homogeneous models obtained by homogenizing the thermal properties of the composite, considering two strategies: series averaging and parallel averaging. The objective is to evaluate the accuracy of the homogeneous models in comparison to the biphasic model for different fiber volume fractions.

The geometry adopted for the specimens consists of cylinders with 5 cm in diameter and 10 cm in height, fully represented within the computational domain. In the biphasic model, the fibers are represented as three-dimensional cylinders embedded within the concrete domain, with random orientations. Simulations were performed for the following fiber volume fractions: 0.25%, 0.50%, 0.75%, 1.00%, 1.23%, 1.50%, 1.75%, and 2.00%. The geometric generation of the fibers, as well as the calculation of the quantity corresponding to each volume fraction, was automated via a Python script.

The thermal properties of the concrete were obtained from Xue *et al*. [2], and those of the steel fibers from Li *et al*. [10], considering the following: thermal conductivity, specific heat, and density. These properties are presented in Table 1.

Table 1. Material properties

Properties	Concrete - Xue *et al*. [2]	Fibers - Li *et al*. [10]
Thermal Conductivity (W/mm°C)	$(2 \cdot 10^{-6} \cdot T^2 - 0.0035 \cdot T + 2.9631) \cdot 10^{-3}$	$(54 - 0.0333 \cdot T) \cdot 10^{-3}$
Specific Heat (J/kg°C)	$0.156 \cdot T + 1127.2, \quad 20 \leq T \leq 600$ $57.49 \cdot T - 33274, \quad 600 < T \leq 700$ $-35.49 \cdot T + 31812, \quad 700 < T \leq 800$	$425 + 0.773 \cdot T - 1.69 \cdot 10^{-3} \cdot T^2 + 2.22 \cdot 10^{-6} \cdot T^3$
Density (kg/mm³)	$(-0.00032 \cdot T + 1.023) \cdot 2400 \cdot 10^{-9}$	$7800 \cdot 10^{-9}$

The homogenization of thermal properties was carried out using two classical models: Series Homogenization (Equation 1) and Parallel Homogenization (Equation 1).

$$p = p_c \cdot v_c + p_f \cdot v_f \tag{1}$$

$$\frac{1}{p} = \frac{v_c}{p_c} + \frac{v_f}{p_f} \tag{2}$$

Where p represents the thermal property (conductivity or specific heat), v the volume fraction, and the subscripts c and f refer to concrete and fiber, respectively. The density was calculated using a simple weighted average in all cases.

The thermal analysis considers exclusively the heat conduction mechanism, disregarding internal heat generation. All external faces of the specimens were subjected to a prescribed temperature increase, with a linear variation from 20 °C to 600 °C over a period of 360 seconds. The governing equation is the transient heat conduction equation (Equation 3), implemented in the Abaqus software.

$$\kappa \nabla^2 T = \rho \, c_p \frac{\partial T}{\partial t} \tag{3}$$

Where κ is the thermal conductivity, ρ is the material's density, c_p is the specific heat, T is the temperature, and t is time.

Meshes were generated using hexahedral thermal conduction with reduced integration elements (DC3D8R), with a base size of 1.0 mm and a minimum refinement factor of 0.08. The mesh parameters were previously adjusted based on a convergence analysis, balancing computational cost, accuracy, and numerical stability. The analysis was conducted in the time domain with a transient solution.

A comparative evaluation was performed between the models for each fiber volume fraction, focusing on temperature and heat flux along the specimen's height at the end of heating, as well as at the central node over time. These data were used to identify the degree of agreement between the homogeneous models and the biphasic model, aiming to assess the fidelity of the adopted homogenization techniques.

3 Results

Based on the methodology discussed, the results obtained from the thermal simulations carried out with the three proposed numerical models are presented and analyzed: the biphasic model with discrete fibers, the homogeneous model with series homogenization, and the homogeneous model with parallel homogenization. The analysis was conducted for different steel fiber volume fractions, ranging from 0.25% to 2.00%, aiming to evaluate the accuracy of the homogeneous models against the biphasic reference model.

Figure 1 shows the heat flux profiles along the specimen height for all simulated fiber fractions. It can be observed that the homogeneous models yield results very close to each other, with smooth profiles and regular gradients. The biphasic model, although following the same general trend, exhibits significant oscillations along the analyzed direction.

These oscillations are attributed to the explicit presence of fibers, which create preferential heat conduction paths, locally increasing the heat flux in the regions where they are located. This effect becomes more evident as the fiber volume increases, intensifying the heat transfer peaks within the domain. It is also noted that the lowest heat flux values are recorded near the center of the specimens, which is expected since this point is the most internal and therefore the last to be reached by external heating.

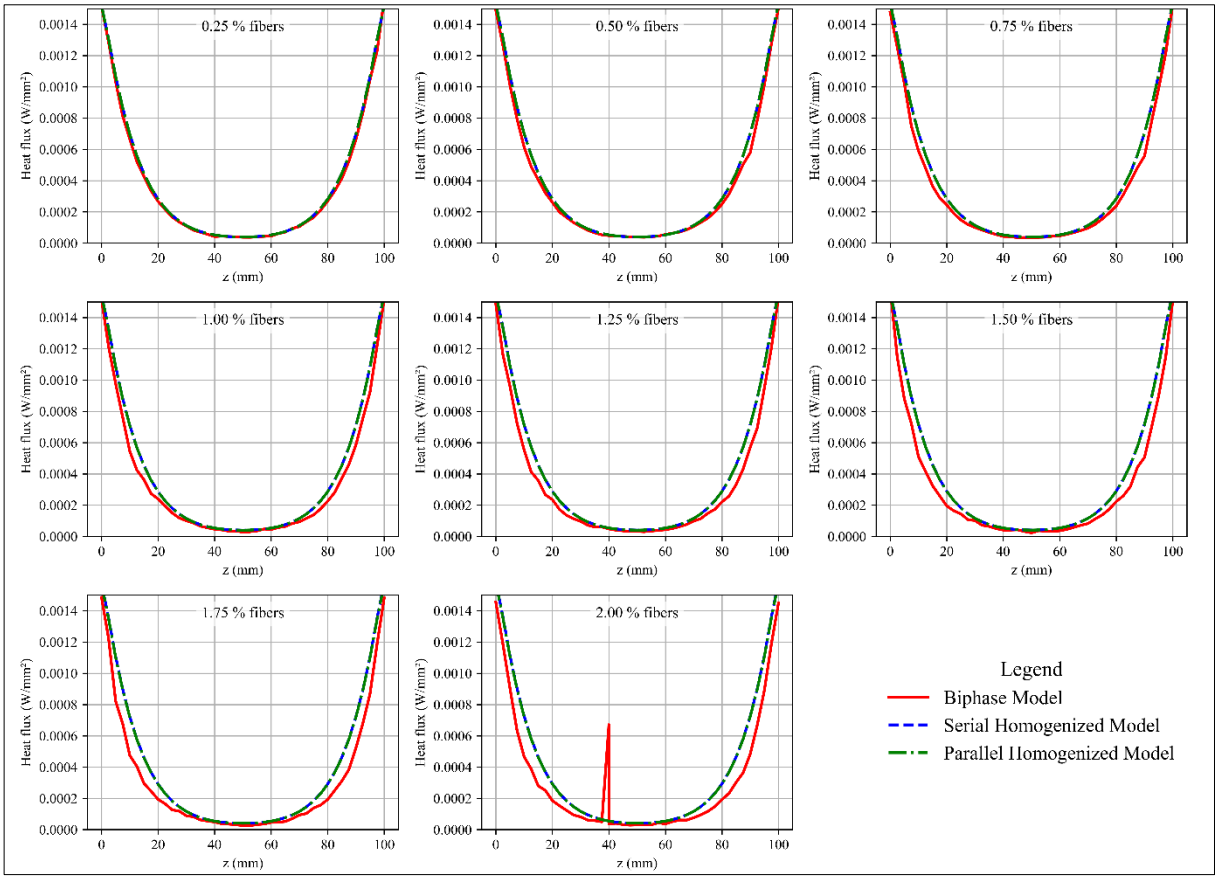


Figure 1. Heat flux distribution along the height

Figure 2 shows the temporal evolution of heat flux at the central node of the specimen. For the homogeneous models, the curves exhibit continuous and smooth behavior. However, for the biphasic model, significant oscillations over time are observed.

The fluctuating behavior of the biphasic model is a result of the local dynamics imposed by the steel fibers: at certain moments, the central node actively participates in heat conduction, while at others, heat is conducted through peripheral paths, depending on the spatial distribution of the fibers. Despite these local variations, the system tends towards a global thermal equilibrium as the thermal exposure time increases. This can be seen more acutely in the last excerpt, for a 2% volume of fibers, which shows a point intercepted by a fiber.

Figure 3 presents the temperature profiles along the height of the specimens at the end of the heating period. The three models agree reasonably well, but their behavior diverges as the fiber volume increases. The parallel model tends to deviate more noticeably from the biphasic model at higher fiber fractions, indicating an overestimation of the overall thermal conductivity. Conversely, the series model shows more consistent performance across the simulated cases, reproducing the temperature gradients obtained by the biphasic model with good fidelity.

Figure 4 depicts the final temperature recorded at the central node as a function of the fiber volume fraction for the three models. The results show that the series model closely follows the trend of the biphasic model, displaying a progressive increase in temperature with increasing fiber volume — a behavior consistent with the higher thermal conductivity of steel.

Despite the noted differences in values, the homogeneous models are able to reproduce the global thermal behavior of the biphasic model with good approximation. The simulated temperatures remain in the same order of magnitude and present small differences even at high fiber contents.

On the other hand, the parallel model exhibits non-physical behavior: as the fiber volume increases, the final temperature at the center decreases. This trend contradicts the physical expectation that the presence of metallic fibers — which are good conductors — would accelerate the heating of the specimen's interior. This indicates a significant limitation in the parallel homogenization formulation in this context, restricting its applicability in simulations of materials with strongly contrasting conductivities.

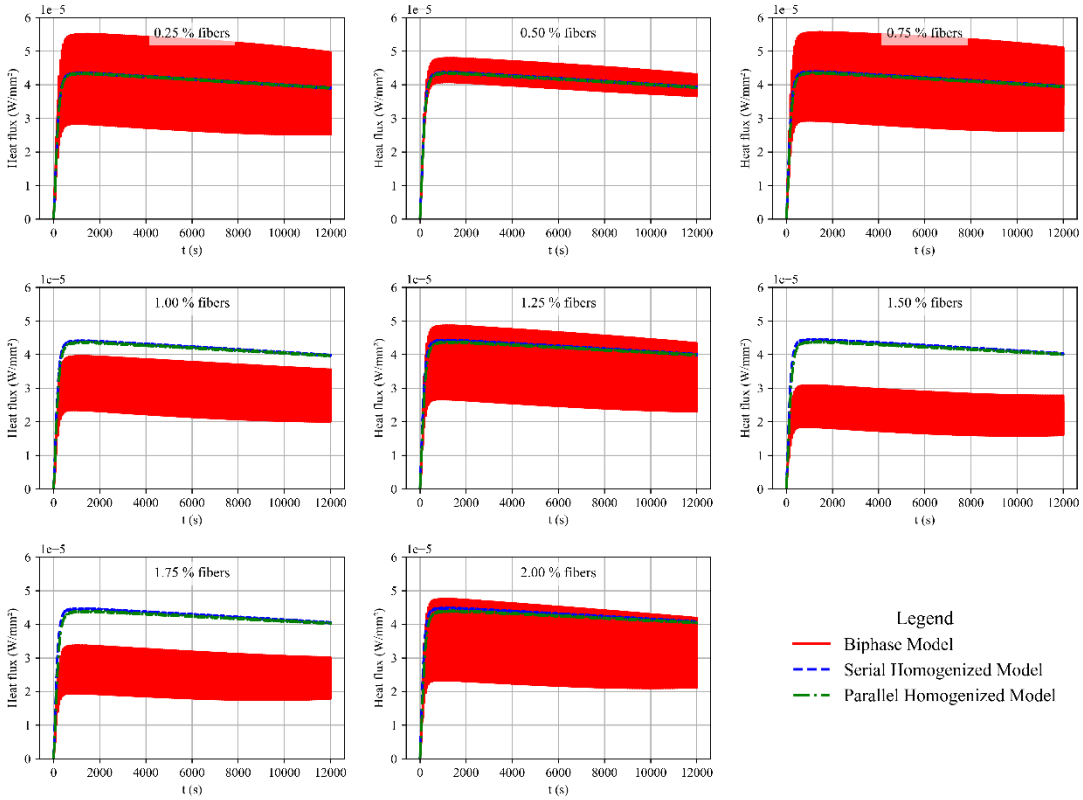


Figure 2. Time evolution of heat flux at the central node

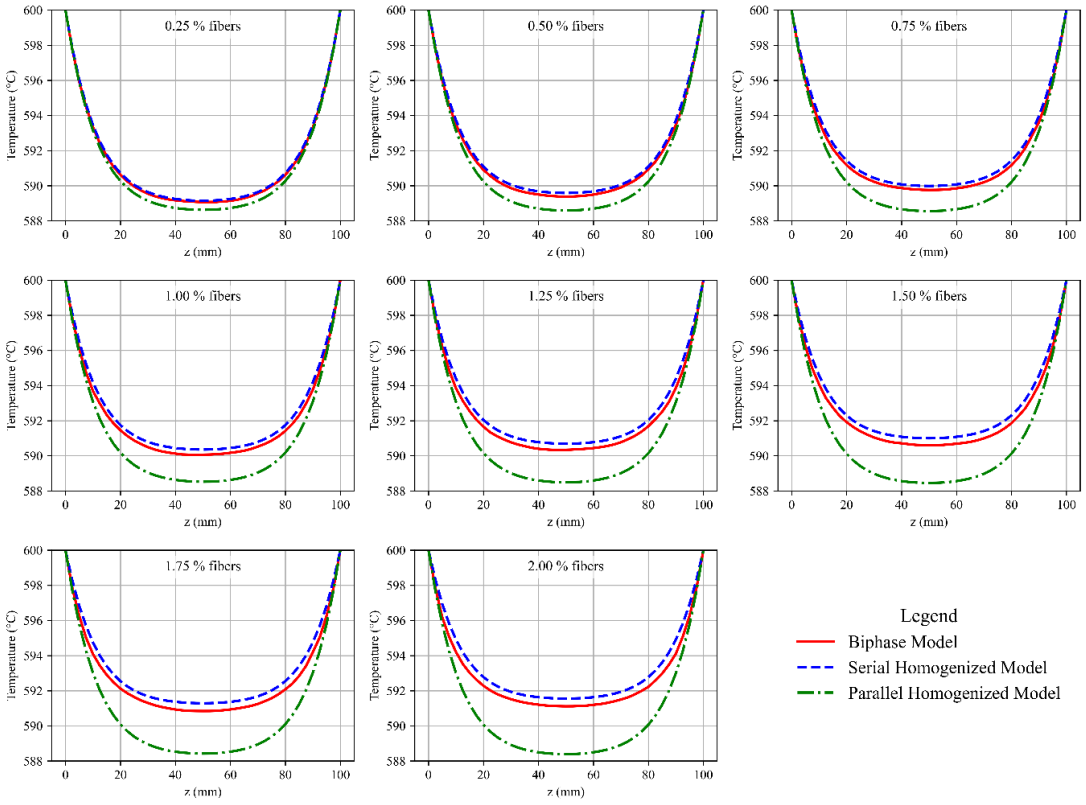


Figure 3. Temperature profiles along the height

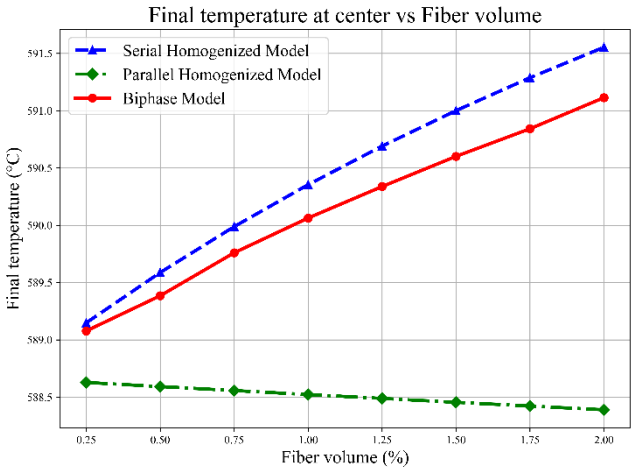


Figure 4. Final temperature at the central node as a function of fiber volume fraction

4 Conclusions

This study presented a comparative analysis of numerical models applied to the thermal simulation of UHPFRC specimens subjected to controlled heating from 20 °C to 600 °C. Three models were evaluated: the biphasic model, which explicitly represents of fibers, and two homogeneous models based on series and parallel homogenization of thermal properties.

The homogeneous models showed good approximation of the global thermal behavior of the biphasic model, particularly in the analysis of temperature at the center over time. The simulated curves were close and consistent even with increasing fiber volume fractions.

The biphasic modeling effectively captured relevant local effects, such as oscillations in heat flux along the specimen and at the central node, which are associated with the presence and random distribution of steel fibers. These phenomena are inherent to the heterogeneous nature of the material and are not captured by the homogeneous models.

The series homogenized model demonstrated greater compatibility with the biphasic model, both in terms of terms of temperature evolution and the trend of final temperature at the center as a function of fiber volume. Therefore, it represents a viable and more conservative alternative for thermal simulations of UHPFRC, especially in contexts where computational cost is a limiting factor.

The parallel homogenized model, on the other hand, presented physically inconsistent results at high fiber contents, such as a decrease in final central temperature with increasing overall thermal conductivity. This behavior compromises its applicability for representing materials with phases of widely differing conductivities.

In summary, the results confirm the feasibility of using homogeneous models as substitutes for the biphasic model in thermal simulations of UHPFRC, provided their limitations are respected. The choice of model should consider the required level of detail, the fiber volume fraction range, and the nature of the problem to be simulated. Future experimental investigations may complement and validate the findings of this numerical analysis.

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