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Finite Element Analysis of Functional Yarn with Thermal Management Characteristics

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Highlights

- Heat transfer analysis is performed for the multifilament yarn containing MPCM.
- Finite element model was successfully developed and validated using experimental results.
- The time dependant thermoregulating effect increases with the amount of phase change materials
- MPCM incorporated materials can protect wearer from extreme weather.

Abstract

Phase change materials (PCMs) provide thermal management solution to textiles for the protection of wearer from extreme weather conditions. PCMs are the substances which can store or release a large amount of energy in the form of latent heat at certain melting temperature. This research reports the heat transfer property of multifilament yarn incorporated with microencapsulated PCM (MPCM) using finite element method under ABAQUS environment. The results of simulation after post processing have been validated against experimental values which were tested through Differential Scanning Calorimetry. It shows a strong correlation between the predicted and experimental results. The time dependent thermoregulating effect of yarns containing different amount of PCMs has been predicted based on the validated finite element model.

Keywords

Heat transfer, finite element method, thermoregulating effect, MPCM, DSC, ABAQUS

1 Introduction

Smart materials are becoming more significant in different filed of science and technology. Phase change materials (PCM) are materials which are used in smart clothing for thermoregulating applications [1]. PCMs are the kind of smart materials which have been used in clothing by US National Aeronautics and Space Administration (NASA) in 1980 to make thermo-regulated garment for space and to protect apparatus in space with drastic temperature change [2-4]. This technology was then adopted by Outlast technologies based in Boulder, Colorado who used PCM in textile fibres and fabric coating [5].

PCMs are attractive due to the ability of storing energy in all the available heat energy storage techniques due to high density, compact storage system and high latent heat [6, 7]. The pioneer study of phase change material was applied for space crafts on small scale and then on large scale was applied in buildings and solar energy systems to build thermal energy storage system [8-10]. A large number of inorganic and organic PCMs are available in the temperature range of -5 °C to 190 °C [11-15]. The organic phase change materials are extensively used in textiles and buildings as thermal energy storage systems to store energy in the form of latent heat [16].

Heat transfer investigations on textiles have been performed by different researchers with or without PCM. Lamb et al [17] investigated heat loss by ventilation in the fabrics with and without PCM additives and claimed that incorporation of PCMs at the proper location of layered garment can significantly enhance the insulating properties of fabrics. Pause [18] studied the development of heat and cold insulating membrane structures containing PCMs and determined that thermal insulation of materials can be substantially enhanced using PCM but he did not use any numerical simulation for further theoretical study of thermal properties of PCM textiles. Nuckols [19] developed an analytical model for diver dry suit with comfortemp® foams containing MPCM and studied the thermal performance of fabric using different MPCMs. He concluded that octadecane microcapsules gave better thermal protection against hexadecane microcapsules due to higher melting temperature of octadecane. Shim et al [20] investigated quantitatively the effect of PCM in clothing for thermal performance of fabric and claimed that heating and cooling effect could last for 15 minutes depending on the number of PCM garment layers and combination of garments. Junghye et al [21] developed thermostatic fabrics treated with microencapsulated octadecane and compared the thermal storage/release properties with untreated fabric.

In 2004 Ghali et al [22] investigated the effect of PCM on clothing experimentally and numerically during periodic ventilation. They claimed that thermoregulating effect could last for approximately 12.5 minutes in fabric treated with MPCM depending on the amount of MPCM and outdoor temperature conditions. Li and Zhu [23] performed coupled analysis of heat and moisture transfer by developing a mathematical model with PCMs and simulated the thermal buffering effect of PCM in fabrics. They validated their model with experimental results by numerically computing the temperature distribution and moisture concentration in porous textiles with and without PCM. Fengzhi et al [24] developed a mathematical model of heat and moisture transfer in hygroscopic textiles containing MPCM and investigated the effect of fibre hygroscopicity on heat and moisture transfer properties of textile with MPCM. On the basis of proposed model they claimed that fibre hygroscopicity not only has influence on the distribution of water vapour concentration in the fabrics and water content in fibres but also on the effect of MPCM in delaying fabric temperature variation during environment transient periods.

In 2009, Fengzhi [25] investigated the effect of MPCM distribution on heat and moisture transfer in porous textile materials by numerical simulation and claimed that the total heat loss from body is the lowest when PCMs are located in the outer layer of fabrics. Ying et al [26] numerically simulated the heat and moisture transfer characteristics on multilayer PCM incorporated textile assemblies using finite difference volume method. Bendkowska et al [27] studied heat transfer in nonwoven with MPCM and determined the amount of latent heat per unit area of nonwoven fabrics. They reported that distribution of MPCM in fibrous substrate and position of PCMs layer in garments has significant effect on thermoregulating behaviour of the garments. Alay et al [28] studied the thermal conductivity and thermal resistance of fabrics containing MPCM under steady state conditions. Yoo et al [29] developed four layered garment treated with nanosilver nonadecane PCM and studied the thermoregulating properties with the effects of number and position of fabric layers. They found that outer layer containing PCM in garment assembly gives good thermoregulating properties by evaluating using Human Clothing Environment simulator.

Later on Hu et al [30] developed a one dimensional mathematical model based on finite difference technique to investigate the heat flow in protective clothing embedded with PCM for fire fighters. They simulated the temperature variation by comparing different thickness and position conditions of PCM in protective clothing as well as melting phase of the PCM and human irreversible burns. In 2014, Siddiqui and Sun [31] developed cotton, wool and Nomex woven models with MPCM in coating matrix using finite element (FE) method. They evaluated effective thermal conductivity of fabrics under ABAQUS environment in two steps by generating the two separate unit cell models for coating portion only and the coated composite fabrics. ABAQUS is useful tool which can provide an environment to solve many complex problems such as thermal and mechanical behaviour of textile structures.

The FE heat transfer analysis on PCM textiles has been reported in literature using PCM as a composite coated layer on fabric substrates by using binder. The binder itself affects the thermal properties of substrate depending on its chemical nature and different add which can affect the analysis [32, 33].

More recently Iqbal et al [34] studied heat transfer of woven fabric incorporated with MPCM using finite element method and investigated the temperature delay of PCM fabric with respect to time. No theoretical research work has yet been reported in the effect of heat transfer behaviour of yarns incorporated with MPCM to predict the behaviour of PCM yarn. The aim of this research is to investigate the heat transfer properties of Multifilament polypropylene yarn incorporated with MPCM developed through an extrusion process. The heat transfer simulation is done using finite element method under Abaqus environment. Based on the validated model, the thermoregulating effect of yarn containing large amount of MPCM and bicomponent yarn (core/sheath) where PCM forms the core covered by polypropylene as sheath was predicted by exploiting the post processing in ABAQUS.

2 Materials and methodology

4% of MPCM was incorporated into the multifilament polypropylene yarn using melt spinning machine which is also called benchtop extrusion machine provided by Extrusion Systems Ltd. The development of MPCM multifilament yarn using benchtop extrusion machine has been provided elsewhere with parametric studies [35]. MPCM under the commercial name of MPCM 28-D was supplied by American company Microteklab Laboratories Inc. Capsules were composed of n-octadecane as phase change material in the core and melamine formaldehyde as shell material. Scanning electron microscopy (SEM) and USB microscope were used to capture the images of yarn for geometric model generation. The simulation was performed in computational software ABAQUS using the following finite element methodology as shown in Figure 1.

3 Finite element heat transfer of yarn

3.1 Geometric model generation

For theoretical heat transfer study of yarn, the geometric model was developed in ABAQUS and material properties were assigned to all the parts of MPCM yarn as shown in Table 1 and 2. All the steps mentioned in section 2 were followed to execute the simulation.

The thermo-physical properties of materials are shown in Table 2 which was used for transient phase change heat transfer analysis. Yarn was composed of three materials: polypropylene as fibre base material, melamine formaldehyde and n-octadecane as shell and core materials of MPCM capsules respectively.

The geometry of the yarn cross section and yarn part in the woven fabric was studied by using a USB microscope. The yarn is shown as a part of fabric and assumed to be taken from fabric to maintain its waviness. The yarn image is shown in Figure 2 which indicates the geometry of crimp path of yarn for the generation of geometric model.

The following assumptions were made for FE model generation:

- The yarn diameter was constant throughout the cross section;
- The MPCM were distributed evenly within the yarn; and
- The geometry of MPCM was created as assembly of many MPCM capsules to decrease the number of capsules for optimum mesh density and cost effective simulation.

Figure 3 shows the schematic diagram of unit cell that was created with the help of images taken by microscope. The cross section and path of the yarn were sketched in ABAQUS using spline with double length to show the repeat of yarn in a woven structure. The MPCM was created as separate part containing shell and core and were then merged together to develop complete MPCM yarn model by precise translation and rotation available in ABAQUS. The calculation of shell thickness and number of capsules can be found in the research published by Iqbal et al [34]. The material properties shown in Table 2 were assigned to each section of the parts in the PROPERTY module.

3.2 Meshing and boundary conditions

For discretization, DC3D4 tetrahedral element was selected and assigned to mesh the MPCM yarn model as shown in Figure 4. The minimum possible element size was assigned due to the small scales of capsules compared to the dimension of yarn. An optimal mesh density was obtained with 1854702 elements for the yarn containing 4% MPCM and 5.68 mmin length. The major and minor axis of yarn are stated in Table 3. Figure 4 shows the meshed images of yarn containing MPCM and the yarn discretized into tetrahedral elements for numerical evaluation.

4 Validation of simulated yarn model

Figure 5 shows heat flow results of yarn containing 4% MPCM which were obtained by DSC experimentally and ABAQUS theoretically. It clearly shows good agreement between the values obtained from experiment and from ABAQUS after post processing. The relative error of the maximum heat flow between the two methods is 9%. The phase change peak shown in Figure 5 is nearly 28 °C; it presents the same trend of maximum heat flow in the MPCM yarn between DSC tested and ABAQUS simulated results.

The ABAQUS curve shows higher peak value than DSC curve around the phase change melting temperature. The presence of static air among the filaments in actual MPCM yarn creates insulating effect resulting in the less heat flow in the MPCM yarn as shown in the DSC curve. On the other hand, the MPCM yarn model developed in ABAQUS was considered as solid which was described in the assumptions for model generation. Air among the filaments was not considered which causes more heat to flow through the yarn of the theoretical model. Later on the difference between the heat flow decreases for both of the two curves because air is not the dominant factor when the temperature goes higher.

5 Prediction of thermoregulating effect based on validated model

Based on the above validated model, the yarn containing 10% MPCM was simulated to predict the heat transfer properties based on the same assumptions stated in section 3. A bicomponent yarn consisting of core and sheath was also modelled using the same methodology to predict the thermal properties of the core/sheath yarn. The bicomponent (70/30 core/sheath) yarn model generated in ABAQUS is shown in Figure 6, where core is an organic PCM n-octadecane and sheath is composed of polypropylene.

In addition to the assumptions stated above, for the core/sheath yarn the PCM core was considered as fully filled within the sheath.

The MPCM in the yarn provides thermal protection through storing energy in the form of latent heat and does not allow the temperature to rise for certain period of time. This temperature delay with respect to time can be predicted using ABAQUS post processing which cannot be tested experimentally.

5.1 Thermoregulating zone of yarn containing phase change materials

The thermoregulating behaviour shown in Figure 7 was related to the following four yarns: control yarn without MPCM, yarn with 4% MPCM, yarn with 10% MPCM and a bicomponent yarn (70/30 core/sheath). The yarn without MPCM reaches the highest temperature very quickly while the yarn containing MPCM is delayed to reach the same level of temperature. As the percentage of MPCM increases, the time increases for yarn to reach the highest level of temperature. The increase in temperature with yarn containing 10% MPCM delays up to 8 minutes and yarn with core/sheath structure takes more than 17 minutes to reach the temperature of 28 °C due to the large amount of PCM contained. The three separate dashed boxes drawn in Figure 6 show the thermoregulating zone of each yarn containing different amount of MPCM, together with the core/sheath yarn.

The thermoregulating zone is also called the thermal arrest zone which means that the temperature is arrested for some time because of the phase change effect. In Figure 7 the curve of yarn without MPCM proceeds linearly over time showing no temperature arrest whereas the yarn containing MPCM shows thermal arrest which lasts as long as the PCM changes its phase completely from solid to liquid. After the latent heat effect completes, the temperature again starts rising and leaves the thermoregulating zone.

5.2 Temperature delay in yarn due to phase change effect

Figure 8 shows the comparison of heat transfer in all types of yarns during the analysis with the heat applied at the back side of the yarn. The temperature contour for the yarn without MPCM shows the temperature of 33 °C transferred to the face of the yarn while the temperature transferred to the yarn containing 4% MPCM is 31.5 °C at the end of the analysis. This is because the transfer of heat within the yarn slows down because of phase change materials and this effect prolongs as the amount of phase change material contained in yarn increases. The yarn containing 10 % MPCM shows 26.5 °C temperature on the face of yarn and the surface area of blue regions showing least temperature is found where MPCMs are present as shown in Figure 9, ensuring the phase change characteristic. Hence as the amount of phase change material increases in the yarn, the increase in temperature or transfer of heat delays in the yarn.

Figure 10 shows the images of yarn without MPCM and bicomponent yarn with core sheath structure. The temperature found at the face of yarn is 33 °C in blue colour which is spread on the whole surface of the bicomponent yarn showing the least thermoregulating phenomenon. On the other hand the bicomponent yarn containing 70% of PCM in core with large amount of latent heat does not allow temperature to increase for certain period of time, hence significant thermoregulating effect can be achieved.

The heat transfer inside the cross section of simulated yarn with and without MPCM with respect to time is shown in Figure 11. The yarn without MPCM reaches the temperature of 31-32 °C after 2000 seconds, whereas the yarn with MPCM reaches the temperature of 27.4 °C in the same time. There is no big difference for the simulated MPCM containing yarns where capsules are not present compared to the yarn without MPCM. However the change in temperature slows down for the MPCM containing yarn where capsules are present compared to the yarn without MPCM, due to the phase change characteristic of MPCM. Similarly the bicomponent yarn containing PCM in core reaches to 26 °C after 2000 sec and the larger blue region indicates the better thermoregulating effect. Therefore the bicomponent simulated yarn provides the best thermoregulating effect as compared to other simulated yarns because of large amount of PCM in the core. Hence from the simulation results it is clear that as the amount of PCM increases in yarn, the thermoregulating effect also increases.

6 Conclusion

The heat transfer analysis of yarn incorporated with MPCM was carried out by finite element method using ABAQUS. The results of simulated models were compared with experimental results for model validation. The prediction of thermoregulating effect from ABAQUS can help in determining the amount of phase change materials to protect wearer against extreme weather.

The yarn model containing 4% MCPM was successfully developed and heat flow of the model was investigated through ABAQUS to compare with results of DSC heat flow. The relative error of 9% was found against phase change temperature between simulated and experimental results. Further models were developed containing 10% of MPCM and core/sheath yarn containing 70% of PCM to study the time dependent thermoregulating effect and this provides useful information in yarn design to meet the effective thermal regulation for required period of thermal regulating time. Thermoregulating effect was found approximately to be 2 min, 5 min and 17 minutes for the yarns containing 4% MPCM, 10% MPCM and 70% PCM in core respectively.

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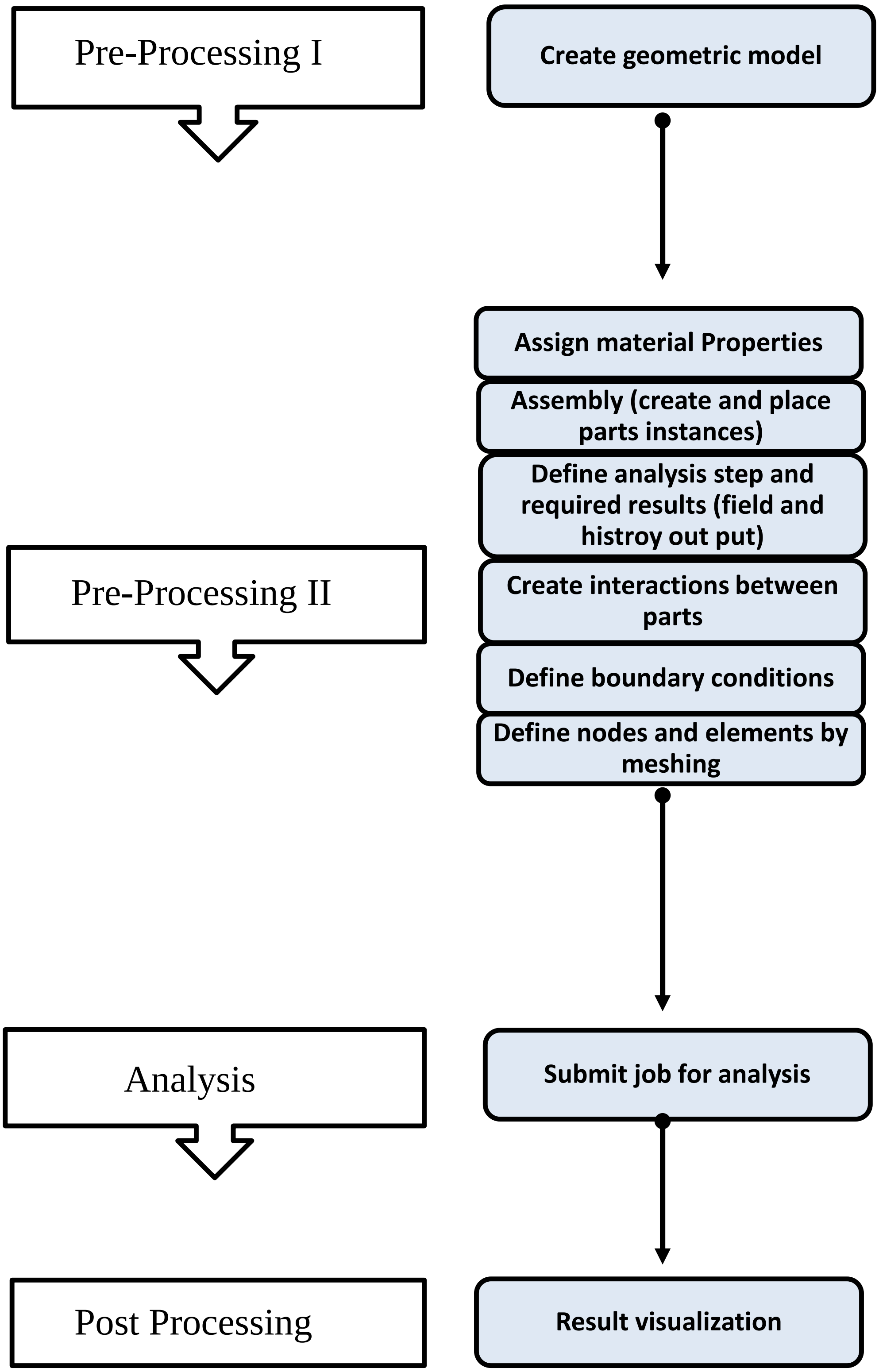

Figure 1 Finite element analysis steps in ABAQUS

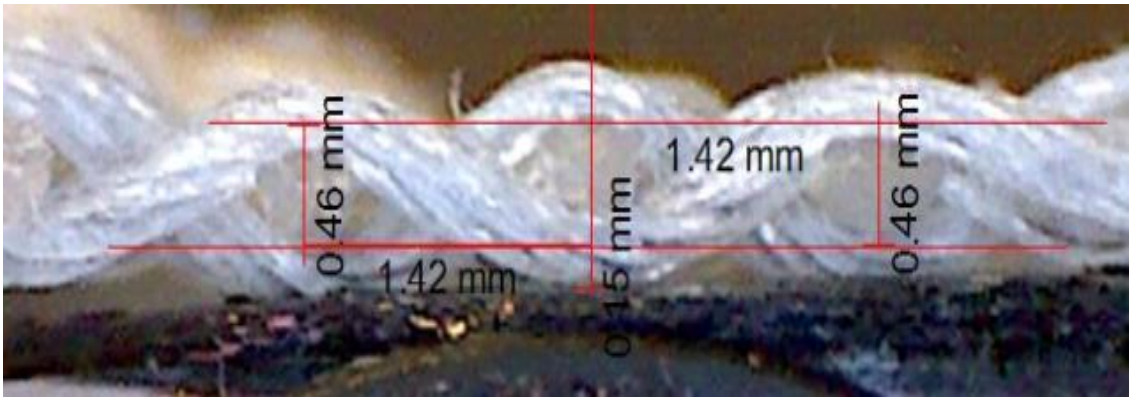

Figure 2 Yarn crimp path

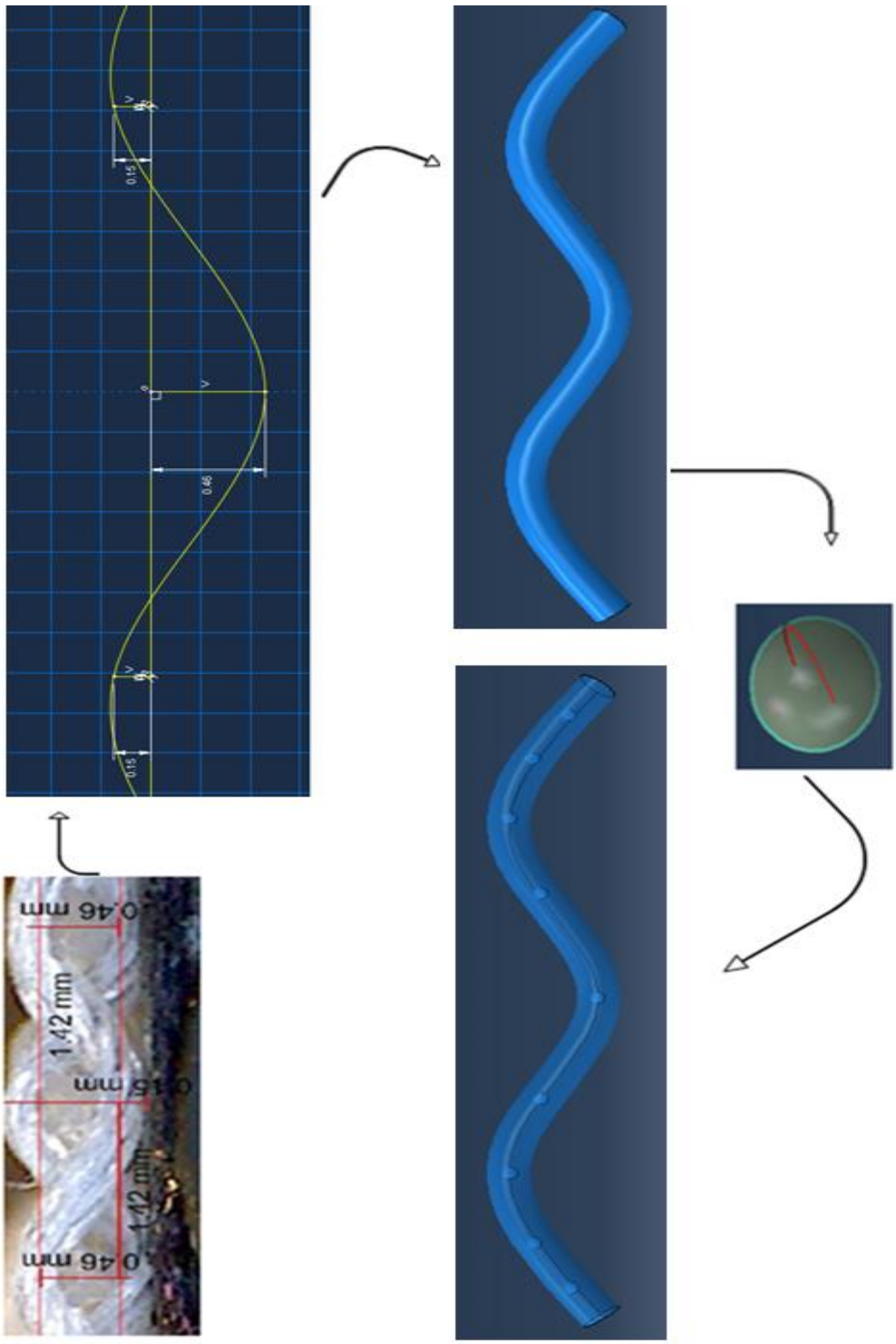

Figure 3 Schematic diagram of MPCM yarn geometric model

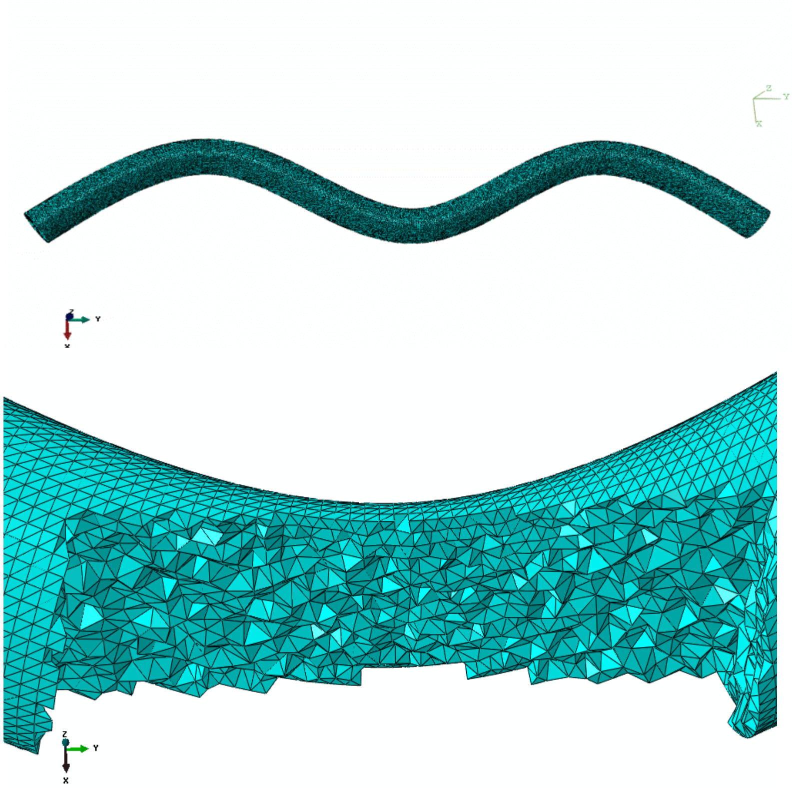

Figure 4 Meshed yarn model

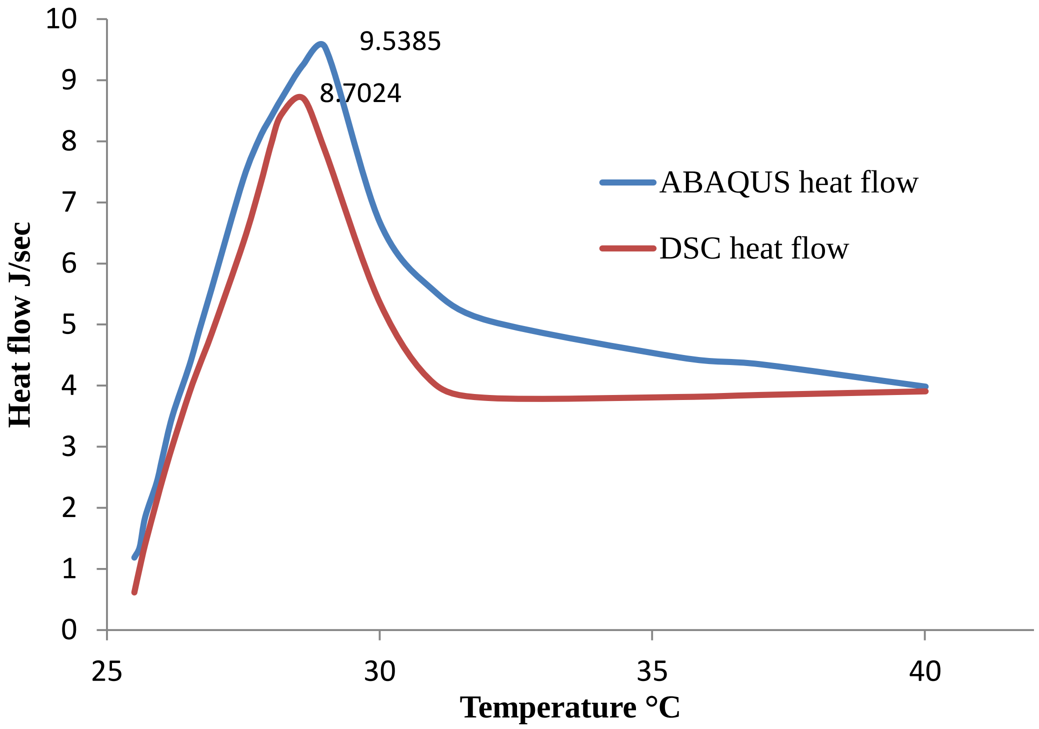

Figure 5 Heat flow results obtained by ABAQUS vs DSC

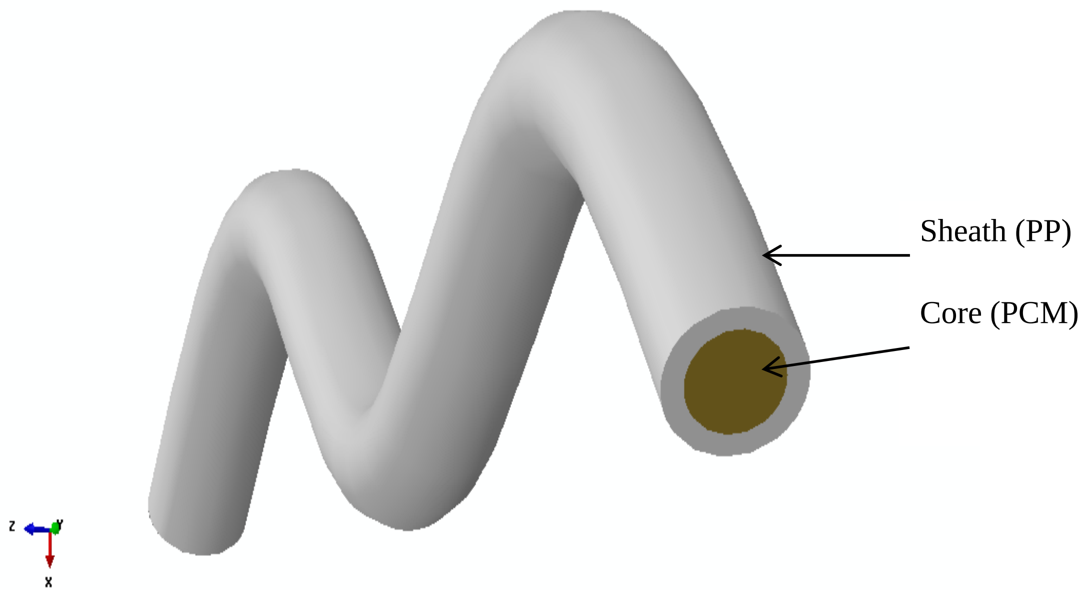

Figure 6 Geometry of Core/Sheath bicomponent yarn

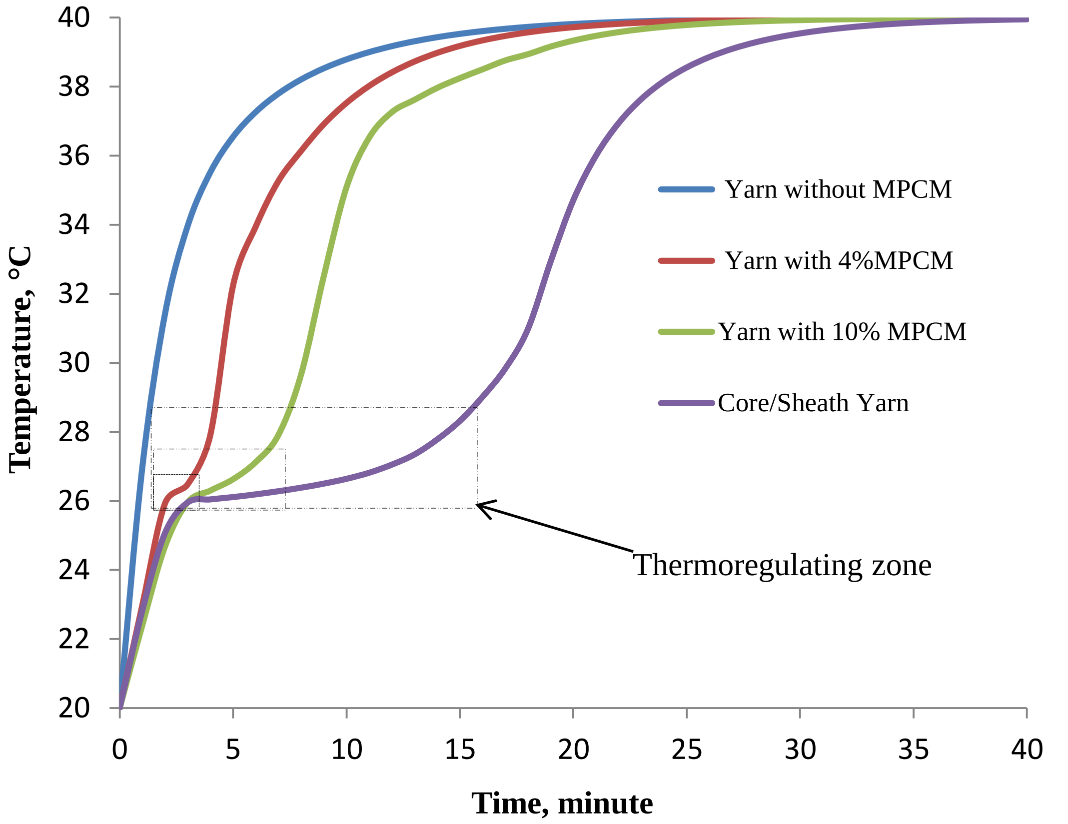

Figure 7 Delay in the rise of temperature over time

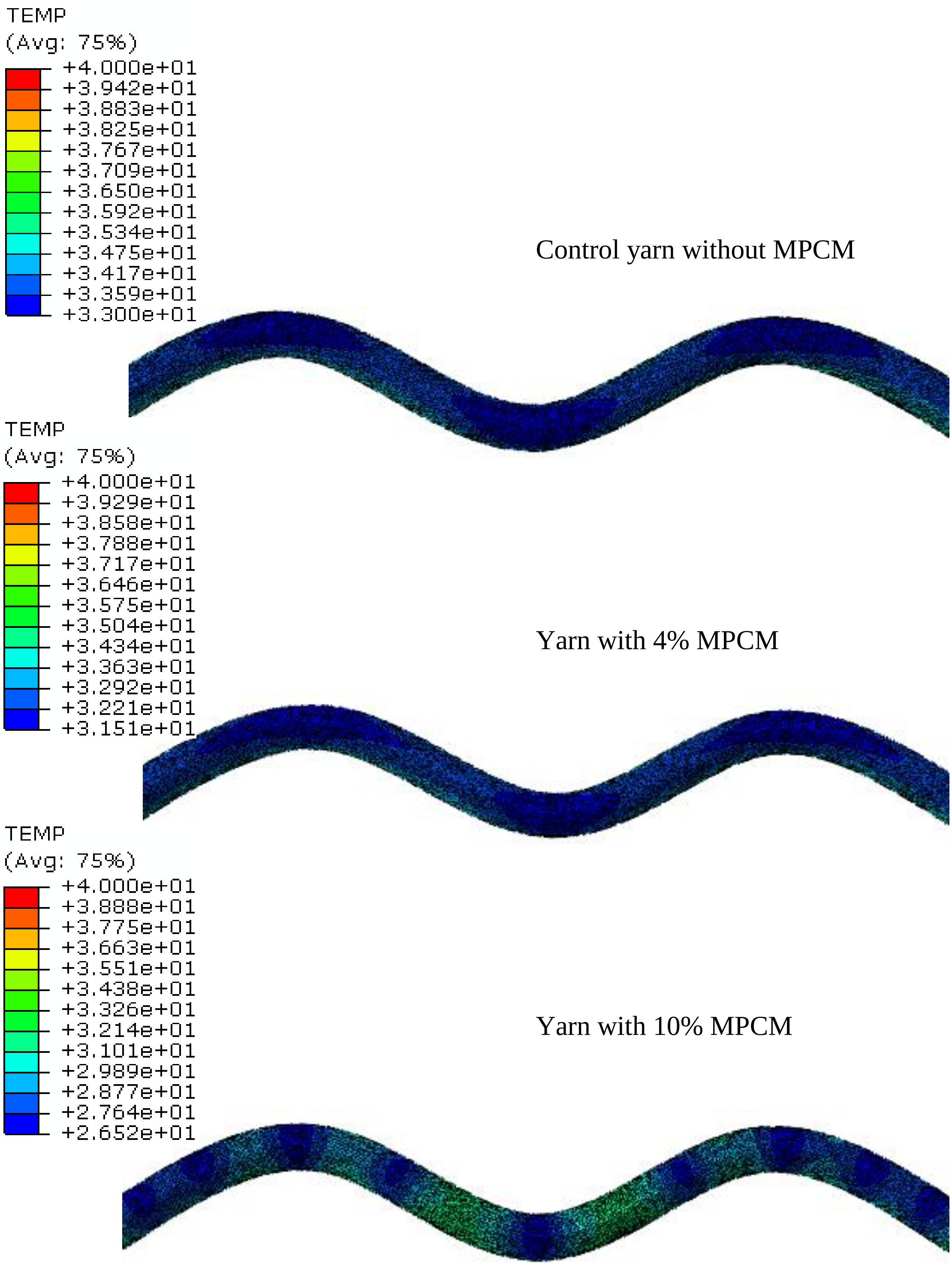

Figure 8 Temperature contour of yarn with and without MPCM at t= 2000 sec

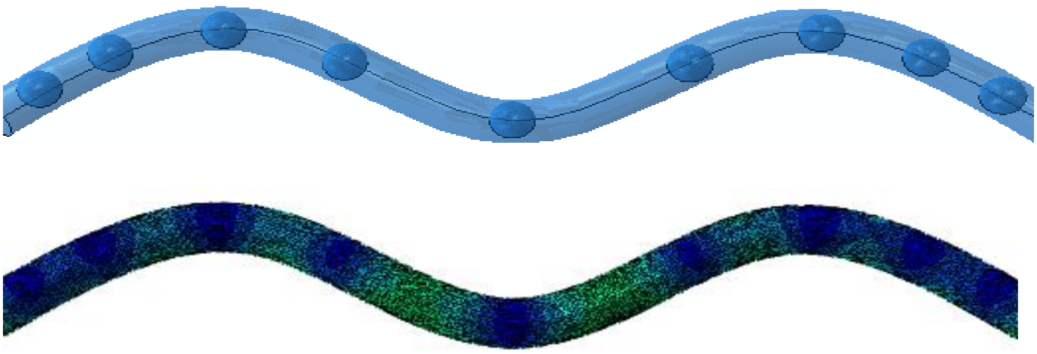

Figure 9 Yarn with 10% MPCM before and after post-processing analysis

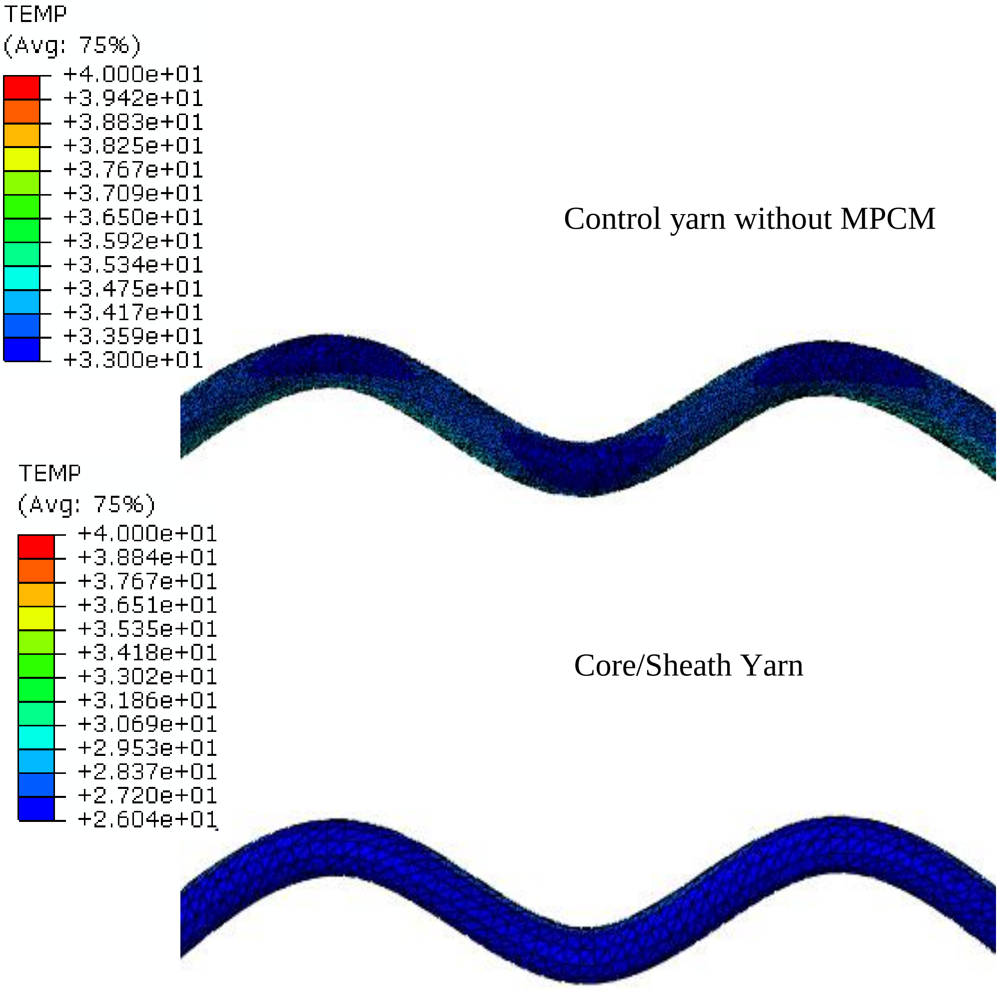

Figure 10 Temperature contour of bicomponent yarn

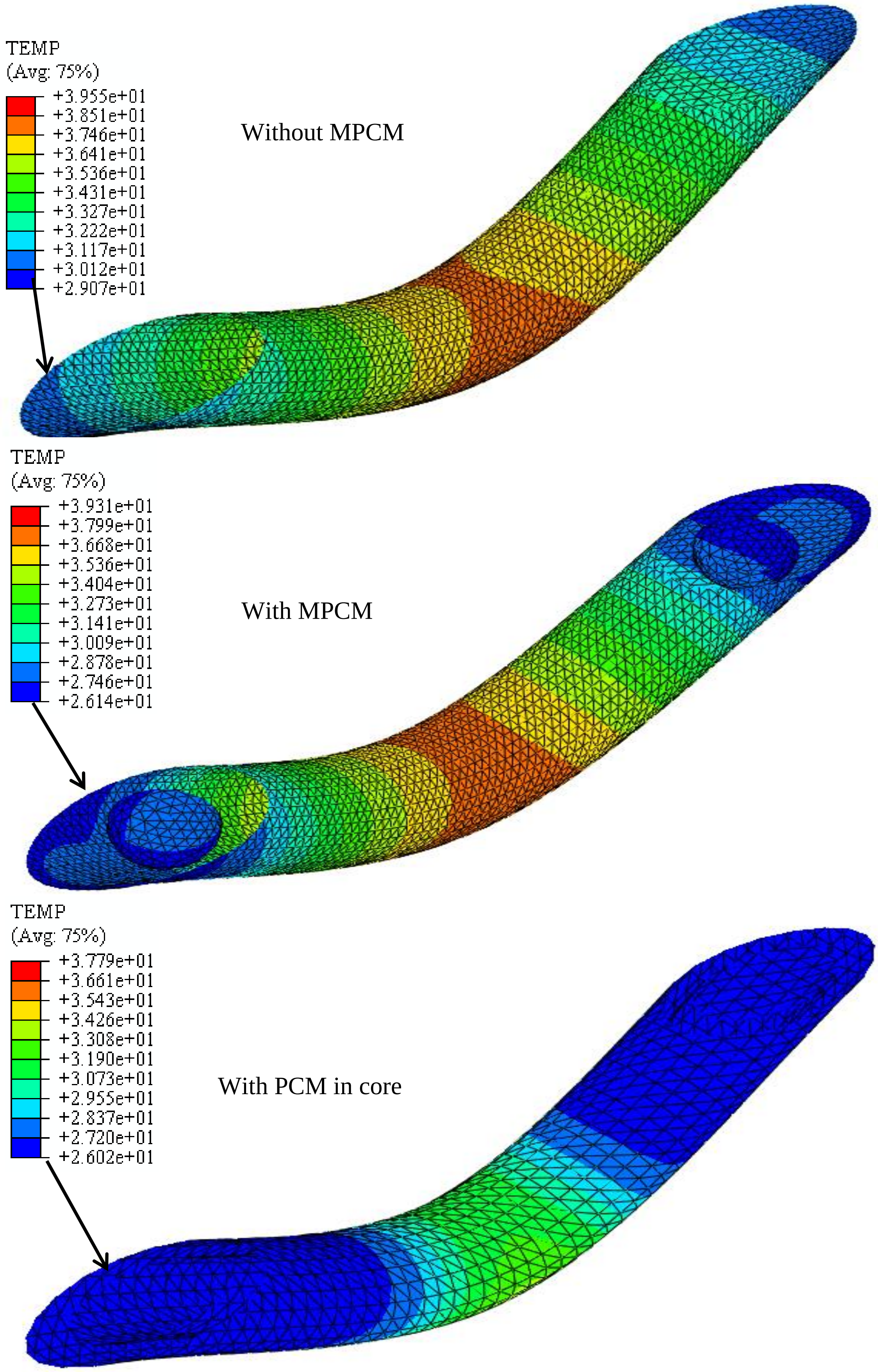

Figure 11 Thermoregulating effect in the yarns, an inside view

Table 1 Physical properties of MPCM

Properties of MPCM	
PCM	n-octadecane (C_{18})
Capsule Material	Melamine Formaldehyde
Particle size (µm)	17-20
Melting Point (°C)	28.2
Latent heat (KJ/Kg)	170-190

Table 2 Thermo-physical properties of materials in MPCM yarn

Property	n-octadecane	Melamine Formaldehyde	Polypropylene
Density (kg/m^3)	777	1500	910
Specific heat (KJ/Kg °K)	1.9	1.2	1.925
Thermal conductivity (W/m°K)	0.3	0.5	0.137
Latent heat of fusion (KJ/Kg)	238		

Table 3 Yarn parameters

Warp/Weft major axis (mm)	0.366
Warp/Weft minor axis (mm)	0.299

Boundary conditions were assigned as T_1 on one side of the yarn. The yarn was initially considered at room temperature which was assigned in predefined field.