

Modelling method to evaluate the thermo-regulating behaviour of micro-encapsulated PCMs coated fabric

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SIDDIQUI MUHAMMAD OWAIS RAZA
BALOCH ZEHRA
NOORANI MUHAMMAD USAMA

IQBAL KASHIF
ZUBAIR MUHAMMAD
SUN DANMEI

ABSTRACT – REZUMAT

Modelling method to evaluate the thermo-regulating behaviour of micro-encapsulated PCMs coated fabric

Micro-encapsulated Phase Change Materials (MicroPCMs) have been widely used to enhance the thermal comfort of the clothing; they can be applied to fabric by various techniques including the coating process. Phase change material (PCM) has a unique property of latent heat that can absorb and release energy over a constant temperature range which enhances the thermal comfort of the clothing microenvironment. PCM textile structures are used in making smart textiles and thermo-regulated garments. An advanced modelling technique was successfully established to develop a finite element model of woven fabrics coated by MicroPCMs, the developed model was used to simulate and predict the effective thermal conductivity and thermal resistance.

Keywords: MicroPCMs, thermo-regulating, latent heat, FEM

Metodă de modelare pentru evaluarea comportamentului de termoreglare a țesăturii acoperite cu materialele cu schimbare de fază micro-încapsulate

Materialele cu schimbare de fază micro-încapsulate (MicroPCM) au fost utilizate pe scară largă pentru a spori confortul termic al îmbrăcăminteii; pot fi aplicate pe materialul textil prin diferite tehnici, inclusiv prin procesul de acoperire. Materialul cu schimbare de fază (PCM) are o proprietate unică de căldură latentă care poate absorbi și elibera energie într-un interval constant de temperatură, ceea ce sporește confortul termic al micromediului îmbrăcăminteii. Structurile textile PCM sunt folosite la realizarea de textile inteligente și articole de îmbrăcăminte cu termoreglare. O tehnică avansată de modelare a fost stabilită cu succes pentru a dezvolta un model cu elemente finite al țesăturilor acoperite cu MicroPCM, modelul dezvoltat a fost folosit pentru a simula și a preconiza conductivitatea termică efectivă și rezistența termică.

Cuvinte-cheie: MicroPCM, termoreglare, căldură latentă, FEM

INTRODUCTION

The demands for functional clothing increased with the growth of textile technology. The production of garments with comfort properties is worth considering [1]. One of the categories of clothing comfort is thermal comfort which mainly depends on the ability of the fabric to transmit heat and moisture from the body to the surroundings [2]. Phase change technology has been widely used to protect the thermal balance of the body and keep constant body temperature even if the physical activity or outer environmental condition changes. Textile products having thermal storage and regulation property can be manufactured by incorporation of phase change material to textiles [3].

In the early 1980s, thermo-regulating textile clothing was developed under the National Aeronautics and Space Administration (NASA) research program by using PCM. The effect of PCMs on the heat transfer behaviour of textiles has been investigated by many researchers [1–13]. Lamb and Duffy-Morris [4] studied the cooling rate, the permeability of fabrics and factors which influence the effectiveness of fabrics

containing phase change materials in improving insulation. They designed a rotating arm device through which heat loss through fabrics with and without PCM when a controlled amount of air is passed through it was monitored. It was concluded that a combination of PCM treated cotton fabric inside with polyester felts was used and the heat loss was nearly zero for some time.

Pause [5] studied the effect of the application of PCM for the development of heat and cold insulating membrane structures. The tests were carried out where basic thermal resistance and dynamic thermal resistance were measured separately, and the results were compared for the original membrane material, membrane material coated with foam and their different concentration. The test results showed that the dynamic thermal insulation is increased as the quantity of Microencapsulated Phase Change Materials (MicroPCMs) increased.

Kim and Cho [6] coated a fabric with MicroPCMs of octadecane, the effect of curing temperature and time on heat storage/release, durability and temperature sensing properties were studied and comparisons

were made between the treated and untreated fabrics. They concluded that as the concentration of MicroPCMs increased thermal storage or release also increased. Moreover, the treated fabric would be able to provide a better cooling effect than the untreated.

Ghali et al. [7] studied the effect of PCMs on body heat loss when environment condition changes from hot to cold in a numerical three-node ventilation model. When a PCM is incorporated in the fabric the sensible heat loss from the skin decreases. They concluded that the heating time depends on the amount of PCMs encapsulated in the fabric, the ventilation frequency, and the outdoor environmental temperature.

Li and Zhu [2] developed a mathematical model that takes account of the simultaneous heat and moisture transfer in porous textiles with PCM). The coupled heat and moisture transfer processes in porous textiles were simulated with different amounts of PCM using the finite volume method. For mathematical formulation, the mass balance of the vapour and liquid moisture, and the energy balance were considered. By specifying the initial and the boundary conditions, they calculated the distributions of temperature, moisture concentration, and water content in the fibres for different amounts of PCM in porous textiles. They computed temperature changes at the fabric surface during heat and moisture transfer into porous textiles based on theoretical predictions.

Ying et al. [8] conducted a series of experiments to establish a method to specify the effects of micro-PCM incorporated fabrics. The computed temperature changes at fabric surfaces were compared with experimental measurements and consistency between the experimental observations and the computational results were found. The analysis illustrates the complex multiple coupling effects among different moisture transport processes, as well as the heat transfer process, and there is reasonable agreement between the predictions and the measurements.

Li and Li [9] developed a mathematical model to predict the heat and moisture transfer behaviour of a permeable membrane incorporated with PCMs. The fibre hygroscopicity effect on heat and moisture transfer was investigated and the heat absorbing and releasing rate, distributions of temperature, moisture concentration and water content in the fibres with MicroPCMs were analysed. The ability of a PCMs fabric to react to the moisture content of the air by absorbing or releasing water vapour was investigated. It was found that the changes in environmental effects on fabric hygroscopicity due to the PCMs microcapsules took more time for temperature variation in the fabric.

Bendkowska and Wrzosek [10] studied the thermo-regulating properties of MicroPCMs coated nonwoven fabrics. Microcapsules of n-Octadecane and n-eicosane were applied using pad-mangle and screen-printing technique. Thermal properties such as thermal storage and thermal resistance were determined under steady-state condition whereas thermal performance was studied under transient

condition. Results showed that microcapsules presented in the interstitial spaces between the fibres whereas in the case of printed technique MicroPCMs formed a layer on one side of the nonwovens. All nonwovens with MicroPCMs exhibited a lower TRF value in the whole range of frequencies of heat flux changes compared to the reference nonwoven. This is due to the increase in nonwoven thermal capacitance resulting from the incorporation of MicroPCMs. There is a reduction in the thermal resistance of non-wovens resulting from the incorporation of MicroPCMs into the nonwoven structure. In the case of nonwoven without PCMs, there is a greater amount of trapped air, which has a very low thermal conductivity and is, therefore, a good insulator. Due to applying microcapsules to the nonwoven structure, the proportion of air is reduced, leading to the lowering of thermal resistance under steady-state conditions. The second important factor is the way of MicroPCMs distribution in the fibrous structure, the position of the MicroPCMs layer was proved to be of great importance for the thermoregulating properties of the printed nonwoven samples. In general, the heat control effect of a garment treated with MicroPCMs is determined by the quantity and the storage capacity of the MicroPCMs.

Yoo et al. [12] investigated the effect of the number and position of the PCMs treated fabric in the four-layer garments by using the Human Clothing-Environment (HCE) simulator. Garments consisted of different layer of fabrics. The temperature differences between garments with different layers of PCMs treated fabric were examined. It was found that with PCMs in the inner layer, which is in contact with skin, is more suitable for the thermal regulating effect. Alay et al. [1] investigated the thermal comfort properties of the fabrics treated with MicroPCMs under steady-state condition. MicroPCMs were applied to cotton and cotton/polyester blend fabrics. The thermal conductivity of treated fabrics decreases as compared to the untreated fabric.

In this work, a Novel Modelling technique is developed to evaluate the thermo-regulating behaviour of MicroPCMs coated fabrics via Finite Element Analysis (FEA) using commercial software Abaqus/CAE. Unit cell models of MicroPCMs coated woven fabric has been created, a novel modelling method has been established to simulate and predict the effective thermal conductivity and thermal resistance of MicroPCMs coated fabrics in a single unit cell model. The predicted effective thermal conductivity and thermal resistance of MicroPCMs coated fabrics have been compared with the previously developed method [13] to validate the model.

MATERIALS

A Nomex® III plain-woven fabric was coated at both sides with MicroPCMs, the coating mixture was applied through the screen coating technique, then dried and cured after the coating process. The fabric specifications are shown in table 1. The physical properties of Microcapsules are shown in table 2.

FABRIC SPECIFICATIONS	
Specifications	Nomex® III Fabric
Areal density (g/m ²)	170
Warp/Weft sett (per inch)	59/59
Warp/Weft yarn linear density (Tex)	33.3/33.3

The materials used for the core and shell of the Microcapsules are n-octadecane and melamine formaldehyde, respectively.

METHODOLOGY

A unit cell model of MicroPCMs coated composite fabric has been developed to evaluate the effective thermal conductivity by finite element method. The developed unit cell model of coated composite fabric consists of four sections i.e., the woven fabric section, MicroPCMs section which is submerged inside the binder section and the air-fluid matrix section. Scanning Electron Microscope images were inspected, for the establishment of geometrical unit cell models of MicroPCMs coated composite fabrics. It was revealed that the capsules were only present at the surface of the fabric. The steps to develop a finite element model follow: (i) develop a model of MicroPCMs then analyse it; (ii) develop a unit cell model of uncoated fabric; (iii) develop a unit cell model of coated fabric; (iv) the above models were merged to form a final model which was then analysed to compute the effective thermal conductivity of the coated fabric. The technique used to develop a finite element unit cell model of coated composite fabric is shown in figure 1.

While analysis of model certain presumptions has been taken into consideration: (i) heat transfer through convection and radiation phenomena is neglected; (ii) no variation in the density of the PCM with temperature change; (iii) no internal heat generation in the model. For analysis, the parts were meshed using tetrahedral shaped four-node elements.

PHYSICAL PROPERTIES OF MICRO PCMS	
Capsule composition	85–90 wt.% PCM
Core material	n-octadecane
Shell material	Melamine formaldehyde
Particle size (µm)	17–20
Melting point (°C)	28.2
Heat of fusion (J/g)	180–195
Specific gravity	0.9

The seed size of the elements was optimized. The temperature specified boundary conditions were applied. The model was simulated under transient condition. It is visible from temperature contours that MicroPCMs act as conductive material and heat transfer takes place from shell to core as shown in figure 2. Latent heat of fusion was calculated using

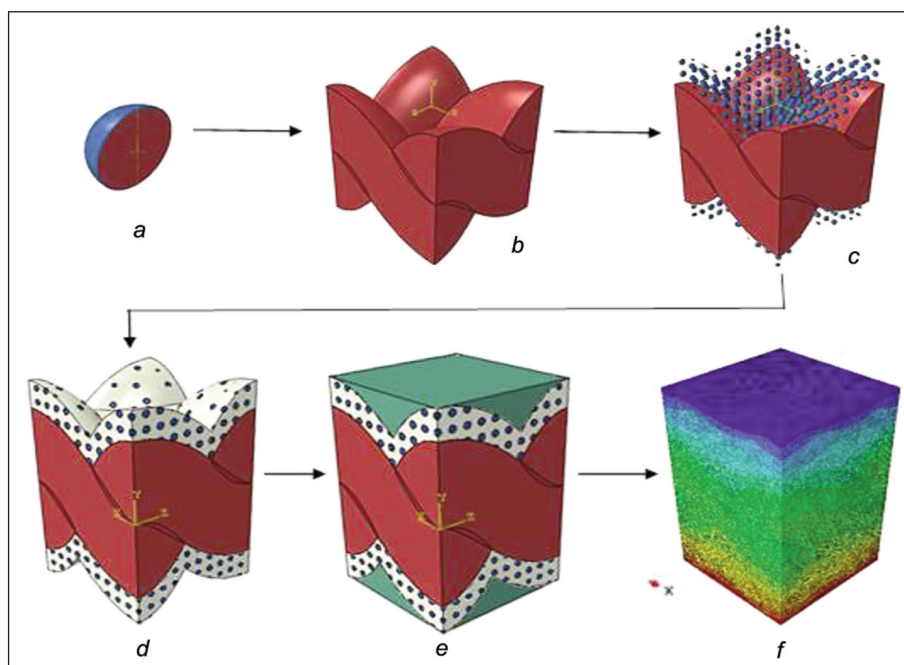


Fig. 1. Stages of modelling: *a* – model of Micro-PCMs; *b* – unit cell model of woven fabric only; *c* – unit cell model of woven fabric with Micro-PCMs; *d* – unit cell model of woven fabric with Micro-PCMs and binder; *e* – unit cell model of woven fabric with Micro-PCMs, binder and air; *f* – heat flow through the unit cell of MicroPCMs coated Nomex® III fabric

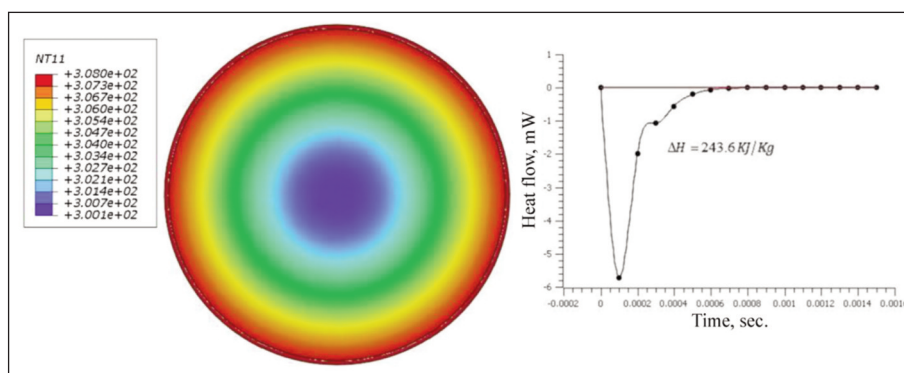


Fig. 2. Temperature contour of MicroPCMs

Table 3

THERMO-PHYSICAL PROPERTIES OF MICRO-PCMS			
Property	n-Octadecane [2]	Melamine formaldehyde [14]	Acrylic binder
Density (kg/m ³)	779	1500	1080
Specific heat (kJ/kg·K)	1.9 (solid) 2.2 (liquid)	1.2	2.4
Thermal conductivity (W/m·K)	0.4 (solid) 0.3 (liquid)	0.5	0.155 [15]
Latent heat of fusion (kJ/kg)	238.76	-	-
Melting point (°C)	28.2	-	-

post-processing data from the model and compared with the latent heat value of fusion provided by the manufacturer.

Model of MicroPCMs

In the FE model, the shell (formaldehyde) and core (octadecane) of MicroPCMs were considered as two separate parts. Both parts were assembled using surface to surface contact interaction property. Material properties were assigned to both parts separately. Thermo-physical properties of MicroPCMs shown in table 3, were used as material properties for finite element analysis.

Model of uncoated and coated fabric

The unit cell model of plain-woven fabrics was produced by taking the actual geometric parameters of fabric which are listed in table 4. The following parameters of the fabrics were needed for the geometric model of the fabric: warp/weft yarn spacing (W_{as}/W_{fs}), fabric thickness (t) and width of the warp/weft yarn (W_{ad}/W_{fd}), and yarn cross-sectional shape. Yarn spacing was determined using warp and weft set. The thickness of the fabric was determined through the FAST-1 compression meter. The appropriate force of 2 gf/cm² or 0.196 KPa was applied on the surface area of 10 cm². SEM was used to obtain the yarn cross-sectional shape.

Table 4

MEASURED GEOMETRIC DIMENSIONS OF UNIT CELL MODELS	
Dimensions	Nomex® III Fabric
(W_{as}/W_{fs}) (mm)	0.431/0.431
(W_{ad}/W_{fd}) (mm)	0.337/0.337
t (mm)	0.5
Total length of the unit cell (mm)	0.862
Total width of the unit cell (mm)	0.862
Unit cell volume (mm ³)	0.3715

After the generation of the uncoated fabric model being a base layer, a layer of MicroPCMs was created on top of the fabric which was submerged inside the layer of binder as a coating layer of the fabric. The coating layer contains 5% MicroPCMs which is

homogeneously distributed among the binder. A layer of air is also created above the layer of coating. All the layers were then merged together forming a unit cell model of MicroPCMs coated composite fabric. To mesh the unit cell model of MicroPCMs coated composite fabric 4-node linear tetrahedral element (DC3D4) has been used. It is the most suitable mesh element enabling completely mesh the unit cell model. It was examined that further refinement cannot change the results of mesh density.

Analysis of the model

It is important to consider the nature of the material for thermal analysis via FEA. Textile fibres are special orthotropic material. To find out the effective thermal conductivity of yarns thermal properties of fibres used are listed in table 5.

Table 5

FIBRE PROPERTIES	
Specifications	Nomex® III Fibre [16–20]
ρ_f (kg/m ³)	1380
K_{fa} (W/m·K)	1.3
K_{ft} (W/m·K)	0.13
C_{pf} (J/kg·K)	1200

The yarn is orthotropic in nature due to this reason of orthotropic nature of the yarn, the thermal conductivity of yarn in both axial (K_{ya}) and transverse direction (K_{yt}) are to be calculated. The thermal conductivity can be determined through equation 1 and equation 2 are listed in table 6.

$$K_{ya} = K_{fa}V_{fy} + K_{air}(1 - V_{fy}) \quad (1)$$

$$K_{yt} = \frac{K_{ft}K_{air}}{V_{fy}K_{air} + (1 - V_{fy})K_{ft}} \quad (2)$$

where K_{fa} is the thermal conductivity along the fibre axis, K_{ft} is the thermal conductivity perpendicular to the fibre's axis, K_{air} is the thermal conductivity of air and V_{fy} is the yarn fibre volume fraction.

To determine the effective thermal conductivity of the unit cell model of MicroPCMs coated composite fabric, two boundary conditions were specified: one was the temperature of the hot surface, and the other was

THERMAL CONDUCTIVITY OF YARN IN THE WOVEN FABRICS				
Yarn	Thermal conductivity in the axial direction, K_{ya} (W/m·K)		Yarn thermal conductivity in the transverse direction, K_{yt} (W/m·K)	
	Warp	Weft	Warp	Weft
Nomex® III Fibre				
	0.5356	0.5356	0.0382	0.0382

the temperature of cold surface assuming all other surfaces of the unit cell as insulated, shown in figure 3. This temperature difference causes heat flow through the unit cell as shown in figure 4.

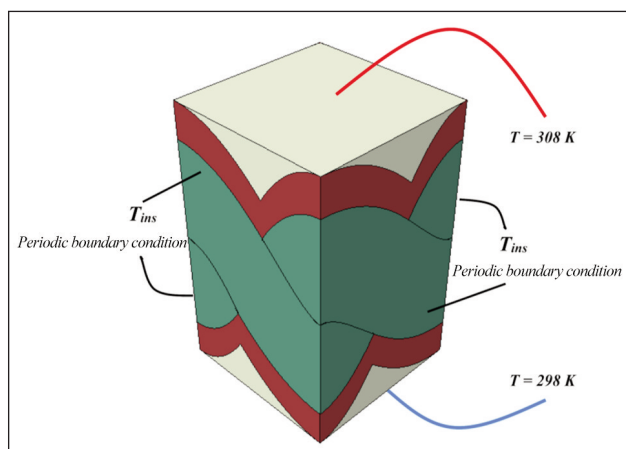


Fig. 3. Boundary conditions

Equations 3 and 4 are used to calculate the effective thermal conductivity (K_z) and thermal resistance (R_z) of the composite fabric model.

$$K_z = Q_z \frac{t}{\Delta T_z} \quad (3)$$

$$R_z = \frac{t}{K_z} \quad (4)$$

where Q_z is the overall heat flux, t is the thickness of the unit cell and ΔT_z is the temperature in the z-direction. To obtain K_z , Q_z needs to be calculated first by the following mean. Define the surface and then add the following lines:

*Section Print, Name = Section_name, Surface = Surface_name, freq = 1

SOH, SOAREA

$$Q_z = \frac{SOH}{SOAREA} \quad (5)$$

where *SOH* and *SOAREA* are built-in keywords in Abaqus/CAE that provide the value of the total section heat flux and the total surface area of the unit cell respectively. These values are then used in equation 5, equation 3 and equation 4 respectively.

After performing all the above calculations, the predicted effective thermal conductivity of the unit cell model of MicroPCMs coated composite fabric of Nomex® III is 0.08154 W/m·K.

Validation of model

The model was validated by using a two-step model which has already been validated by experimental results by Siddiqui and Sun [13]. Two finite element models were developed to determine the effective thermal conductivity MicroPCMs coated composite fabric. A unit cell model of coating that is MicroPCMs and binder was developed and analysed. The results from the coating model were used as input property for the second model which is a unit cell model of MicroPCMs coated composite fabric as shown in figure 5. The effective thermal conductivity of MicroPCMs coated Nomex® III fabric from the two-step and one-step model is found to be 0.08278 W/m·K. and 0.08154 W/m·K, respectively. The mean absolute error between the two models is 1.498%.

Furthermore, the thermo-regulating behaviour of PCMs coated composite fabric is analysed by comparing the heat flow through the thickness of the coated fabric as shown in figure 6, where transient analysis was used by applying temperature specified boundary conditions. Fabric without MicroPCMs reaches the highest heat flow Q_{max} very quickly, whilst the MicroPCMs coated composite fabric reaches the same level of heat flow but with much delayed time. With the increase of MicroPCMs applied, the time for the coated fabric to reach the highest level of heat flow increases. The increased PCMs in a fabric would improve the thermal comfortability of wear, but it would reduce flexibility. Therefore, a compromise between wear comfortability and flexibility needs to be considered, so as the amount of PCMs to be applied on fabric. This delay in heat flow is contributed by the phase change effect and latent heat contained in PCM, and the effect prolongs as the amount of MicroPCMs contained in the fabric increases. Such a thermal regulating zone created by MicroPCMs means that the temperature is arrested for some time because of the phase change effect. It is clearly evident from the enlarged view in figure 6 that the fabric containing 5% of MicroPCMs only reaches 60% of the maximum heat flow whilst the fabric without PCM reaches the maximum heat flow at the same time interval.

These parameters were also reported useful to determine the thermal protective efficiency of fabrics containing PCM elements according to Hes and Lu [21]. They studied the effect of heat flow through fabric with and without PCM by using PC Tester, it was found that the heat flow through PCM containing fabric was much lower, only half of the maximum heat

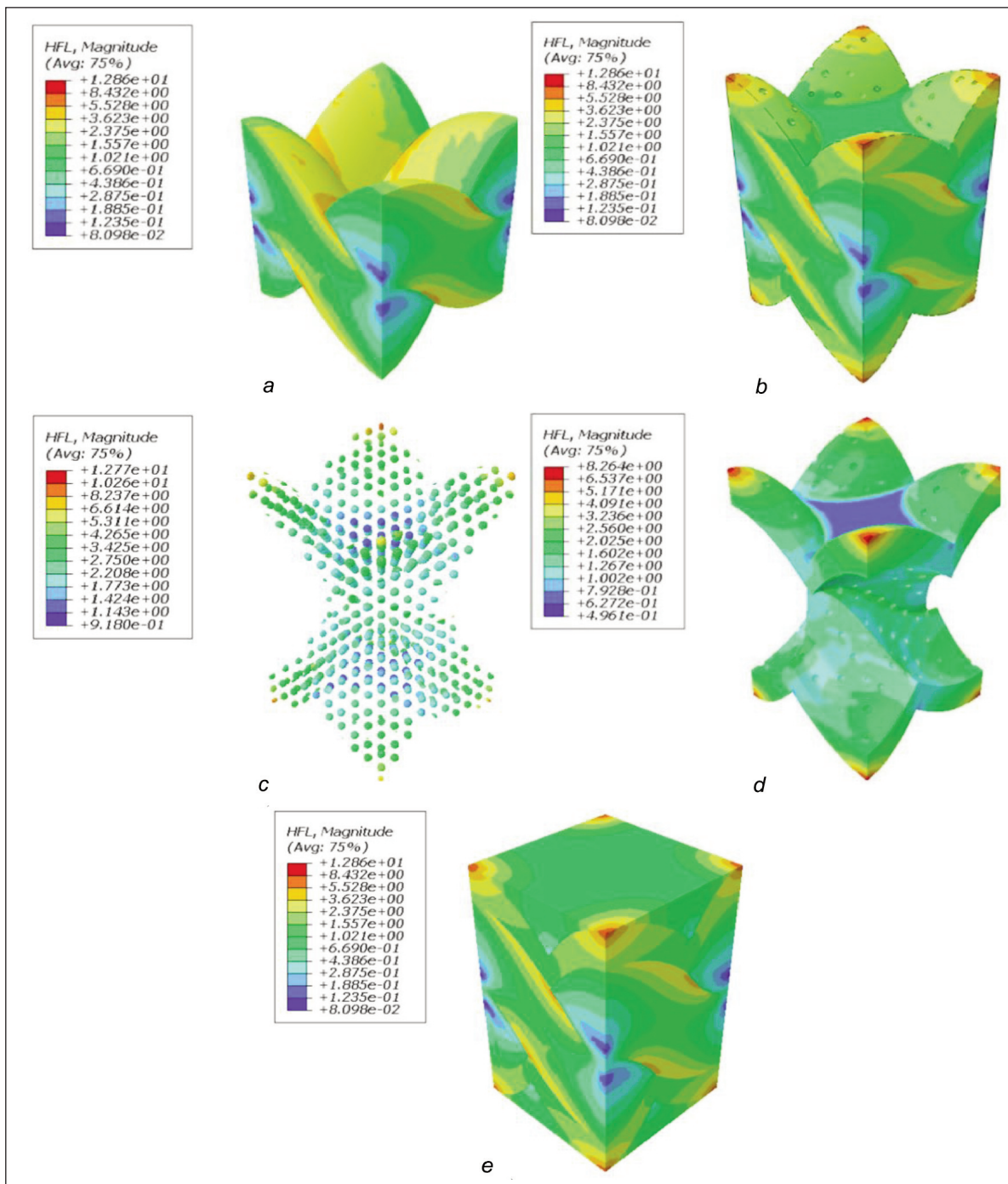


Fig. 4. Heat flux contours: *a* – unit cell model of woven fabric only; *b* – unit cell model of woven fabric with binder; *c* – unit cell model of Micro PCMs; *d* – unit cell model of binder only; *e* – heat flow through the unit cell of MicroPCMs coated Nomex® III fabric

flow rate through the fabric without PCM. In other words, PCM containing fabric had double thermal protection than the one without. As discussed above the highest thermal protection achieved is 1.67 times as shown in figure 6. This is caused by the much slower heat flow in the fabric containing PCM, attributed to the effect of heat accumulation needed for PCM to accomplish phase change. This thermal protection can be increased (even many times) depending on the amount of PCM to be applied onto fabric for a specified end-use application.

CONCLUSIONS

In this research, a modelling technique has been established to evaluate the thermo-regulating behaviour of MicroPCMs coated Nomex® III woven fabric via finite element analysis. The orthotropic nature of the fibre, fibre orientation, accurate yarn cross-sectional shape, and fibre volume fraction of the fabric was considered for thermal analysis in order for the developed models to provide more realistic thermal properties of the MicroPCMs coated fabrics. The small mean absolute error (1.498%) shows the applicability of the developed technique for the

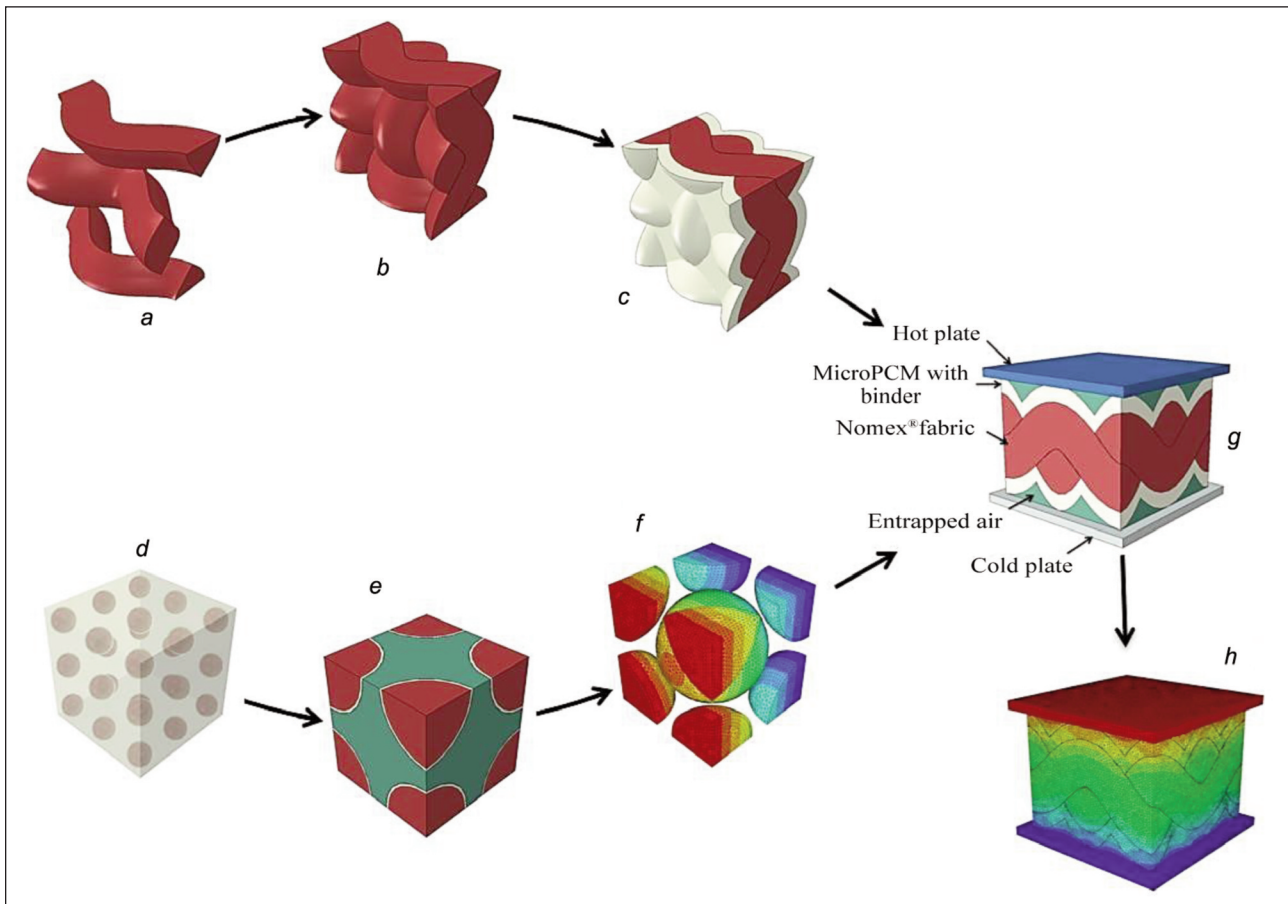


Fig. 5. Stages of modelling: *a* – model of yarn; *b* – unit cell model of woven fabric only; *c* – unit cell model of woven fabric with coated material; *d* – binder and MicroPCMs composite; *e* – unit cell model of binder and Micro-PCMs composite; *f* – simulated temperature profile of fabric composite [13]

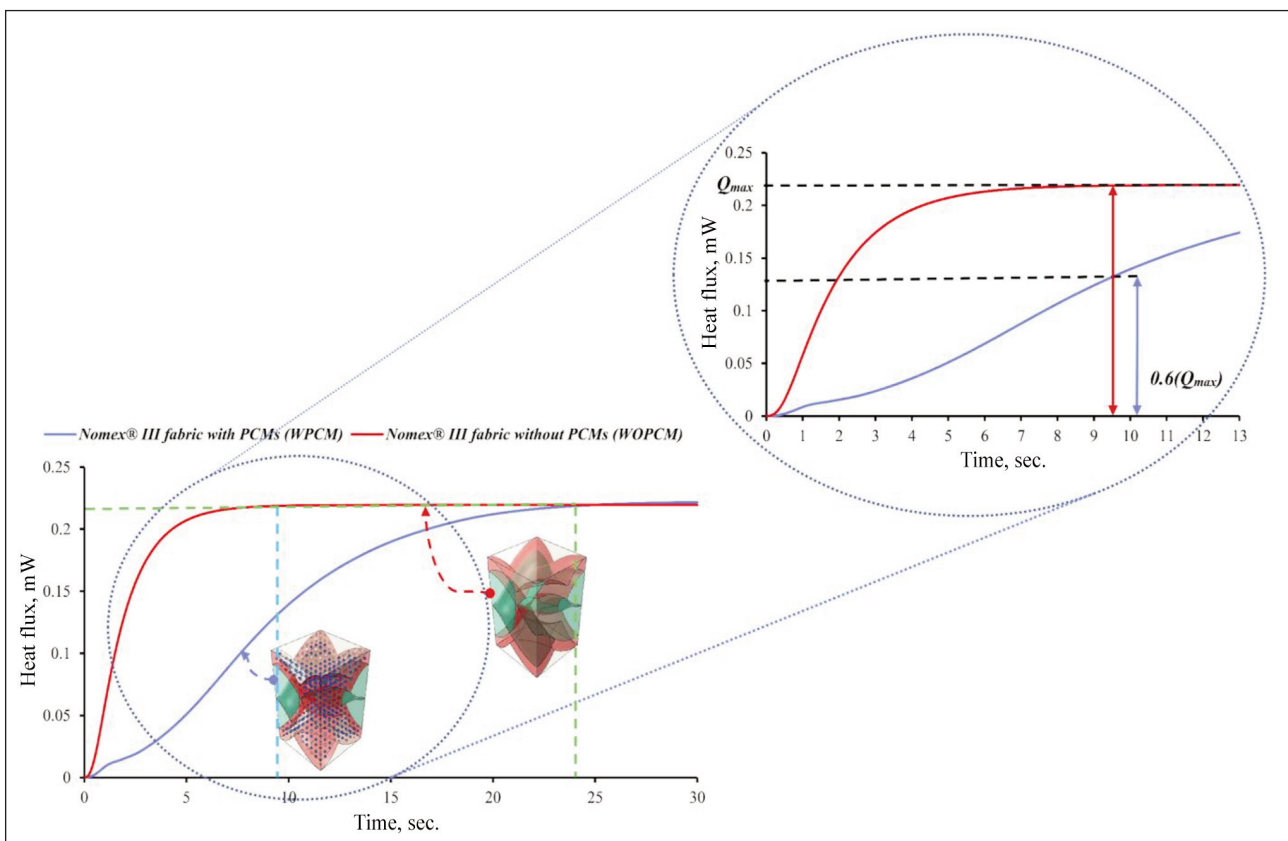


Fig. 6. Evaluation of PCM efficiency by comparing the heat flow behaviour through coated with and without MicroPCMs

prediction of thermal conductivity of MicroPCMs coated composite fabric. The model is capable of predicting the effect of thermo-regulating behaviour at various levels of MicroPCMs coating. The validated model is used to evaluate the thermo-regulating behaviour of coated with and without MicroPCMs which is useful in determining the amount of phase change materials to protect the wearer against extreme weather conditions. Furthermore, the estab-

lished novel simulation method from this research can be used to determine the thermo-regulating behaviour of fabrics treated using different PCM in the core of Microcapsules by applying various temperature boundary conditions according to the applications and specific temperature environment.

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Authors:

SIDDIQUI MUHAMMAD OWAIS RAZA¹, BALOCH ZEHRA¹, NOORANI MUHAMMAD USAMA¹, IQBAL KASHIF²,
ZUBAIR MUHAMMAD³, SUN DANMEI⁴

¹NED University of Engineering & Technology, Department of Textile Engineering,
University Road, 75270, Karachi, Pakistan

²National Textile University, Department of Textile Engineering,
Sheikhupura Road, 37610, Faisalabad, Pakistan

³North Carolina State University, Wilson College of Textiles,
1020 Main Campus Drive, Raleigh, 27606, NC, USA

⁴Heriot-Watt University, School of Textiles & Design, TD1 3HF, Galashiels, UK

Corresponding author:

SIDDIQUI MUHAMMAD OWAIS RAZA
e-mail: orazas@neduet.edu.pk