Development of plug-ins to predict effective thermal conductivity of woven and microencapsulated phase change composite

Development of Plug-ins to Predict Effective Thermal Conductivity of Woven and Microencapsulated Phase Change Composite

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Abstract

The thermal property of textile structures plays an important role in the understanding of thermal behaviour of the clothing. In this work User friendly GUI plug-ins have been developed to generate both microscopic and mesoscopic scale models for finite element analysis. The plug-ins were developed by using Abaqus/CAE as a platform. The GUI Plug-ins enable automatic model generation and prediction of the effective thermal conductivity of woven composite and microencapsulated Phase Change Materials (MicroPCMs) composites via finite element analysis (FEA) by applying boundary conditions. The predicted effective thermal conductivities from plug-ins have been compared with the results obtained from published experimental research work based and an established mathematical model. They are correlated well. Moreover the influence of PCM on heat transfer behaviour of MicroPCMs composites was further analysed.

Keywords: MicroPCMs composites; woven composites; finite element analysis; plug-ins; Abaqus environment

1. Introduction

More recently, different commercial and open source software packages have been developed for modelling the geometry of textile structures at the mesoscopic scale such as TexGen [1], TexEng [2], WiseTex [3] etc. These software packages provide the user friendly environment by using many libraries such as: VTK, wxWidgets, OpenCascade, Python etc. and programs such as: Cmake, SWIG, Visual studio C++ etc. The geometrical models generated from these software packages can be imported into

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different finite element analysis (FEA) software in required formats. However when these geometrical models are imported into the FEA software there are difficulties in meshing due to of the sharp edges in the cross sectional geometry of yarns. If yarn or fabric geometrical models are exported in meshed form to FEA software, meshes are distorted because of too many faces in the geometry. In order to avoid this issue there is necessary to generate geometry of textile structures by inputting yarn and fabric parameters in Abaqus/CAE (Computer Aided Engineering) environment, therefore there is need to develop GUI plug-ins to incorporate into Abaqus/CAE.

In the meantime, the plug-ins are able to automatically predict the effective thermal conductivity of plain weave and MicroPCMs composites. The unique properties such as light weight, thermal and high strength of textile composites have been developed to replace many metallic parts in aeronautical, space and automobile industries.

Heat flow through the textile assembly mainly depends on the thermal conductivity of fibrous material, fibre volume content, construction of fabric, and orientation of fibre with respect to the heat flow direction [4, 5]. Effective thermal conductivity is one of the important thermal properties which describe the thermal behaviour of textile composites.

Heat flow mechanism of textile structures can be improved by special finishes [6]. Microencapsulated Phase Change Materials (MicroPCMs) have been widely used to develop thermo-regulating textiles; they can be applied on to fabric by various techniques including coating process [6]. Phase Change Material (PCM) has unique property of latent heat that can absorb and release energy over constant temperature range which enhances the thermal comfort of the clothing microenvironment [7-11].

PCMs have been widely used in thermo-regulating textiles by different application techniques [6]. Such textile structures can be used for making smart textiles and garments [12].

The microencapsulation of PCM involves enclosing PCM in thin and resilient polymer shell so that the PCMs can be changed from solid to liquid and back again within the shells [13]. Thermo-regulating textile was developed in the early 1980s under National Aeronautics and Space Administration (NASA) research programme by using PCM [14]. Microencapsulated PCM thermo-regulating textiles have been widely used in many application areas: protective clothing, sportswear, electronic textiles and many others.

Paula Sánchez reported that the use of microencapsulated PCM for fabric coating offers successful production of thermo-regulating textiles resulting in a substantial improvement of the thermal comfort [15].

The thermal conductivity and thermal resistance are the key parameters for heat flow in the textile structures for conduction and they can be evaluated by different ways: experimental method, analytical solution method and numerical method [16, 17].

There are numerous ways of obtaining the numerical formulation of a heat conduction problem, such as finite difference method, finite element method, boundary element method, and energy balance (or control volume) method [18]. In this research work finite element method (FEM) is used to evaluate the thermal property of plain weave composite fabric. It is a powerful computational process for imprecise solutions to a variety of applied engineering problems having complex domains subjected to general boundary conditions.

This research work also contains the methodology and validation of models and results obtained from the plug-ins.

2.   Design Methodology of Plug-ins in Abaqus/CAE

A plug-in is a customized software or program which can perform a single or multiple tasks and easily be installed and used as a part of already installed software. Research works have been carried out in different fields to develop the customized tools that used as plug-in in several commercial and open source software [19-25]. There appears no research work dedicated to plug-ins that can be used to generate textile-based structures in Abaqus/CAE environment; the present study is exploratory in nature.

One of the aims of this research is to develop user friendly GUI plug-ins. In this work the detailed information about how plug-ins were developed and worked in the Abaqus environment will be discussed.

Abaqus plug-ins execute Abaqus Scripting Interface and Abaqus Graphical User Interface (GUI) Toolkit commands. They provide ways to customize Abaqus/CAE for the specific needs or preferences. For example, a simple plug-in would automatically print the contents of the current viewport according to some predefined options. A more complex plug-in would provide a graphical user interface to a specialized post-processing routine that you have written [26].

In Abaqus two types of plug-in can be created: kernel and GUI [27, 28]. The kernel plug-in is composed of functions written by using the Abaqus scripting interface and requires no GUI infrastructure. In GUI plug-in it will allow the user to input all the necessary data in user interfaces within the Abaqus/CAE environment. In this research work a GUI plug-in was developed by using Abaqus GUI toolkit.

It is necessary to understand how the graphical interface of Abaqus works before going into the details of how GUI plug-in was developed and worked in Abaqus. When users start using the Abaqus graphical user interface Abaqus executes two processes, i.e. kernel and GUI process.

GUI process contains GUI command which displays the dialog box; for example, when users click a button a dialog box appears to allow entering the necessary information. When clicked 'ok' a kernel

command string passes to kernel process containing the data and method which Abaqus uses to perform different operations such as: create part, cut operation, merge operation, meshing and so on.

The process will be continued if there is no error in the input information otherwise a message will be displayed in the form of error dialog box. GUI plug-in works in the same way as Abaqus module works. GUI plug-in comprises of four sets of scripts.

The first script contains form modes that are of the type of AFXForm enabling to launch the dialog box of type AFXDATADIALOG (which is the second script). AFXDATADIALOG collects input data by user and then a command is sent to the Kernel script (third script) from the form mode (AFXForm). The third script performs the operation in Abaqus. The plug-in registration script (which is the fourth script) is to register the plug-in in the main plug-in menu as shown in **Error! Reference source not found.**. GUI plug-in execution process is shown in Figure 2.
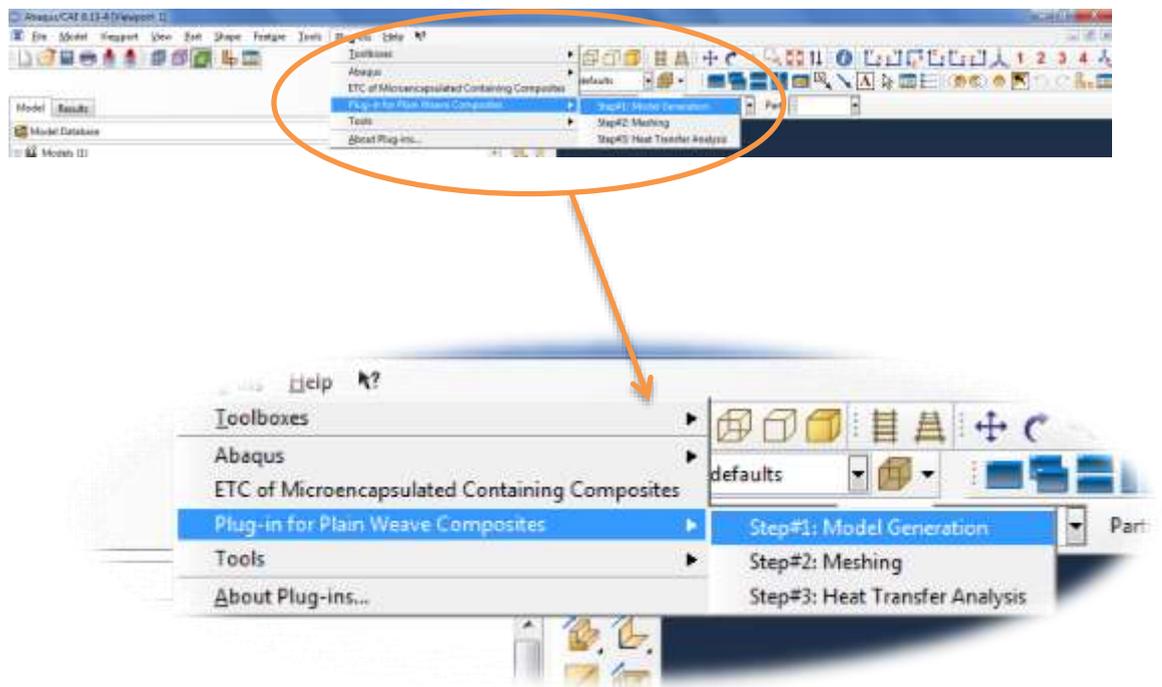

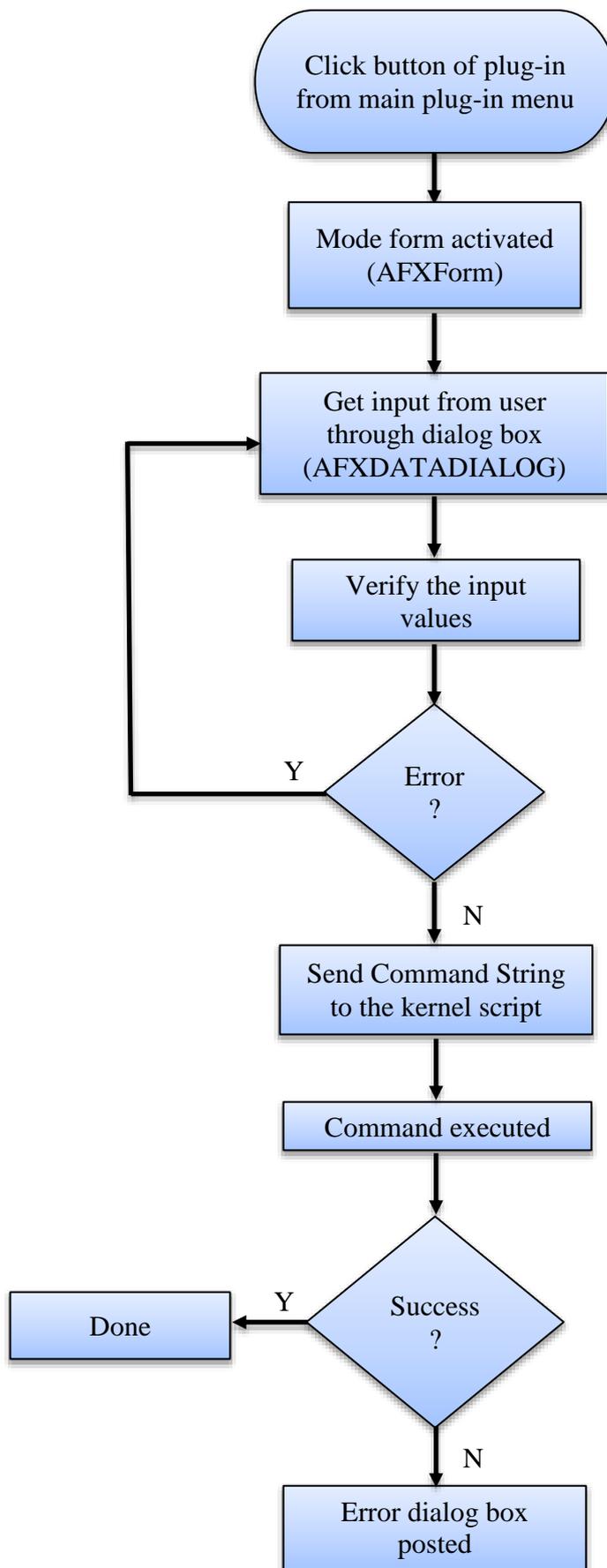**Figure 1:** Registered plug-in in plug-in menu

Figure 2: GUI plug-in processing sequence

2.1. Plug-in for Plain Woven Composite Fabric

The aim is to develop the plug-in to create a user friendly environment incorporated into Abaqus/CAE, enabling generation and accurate prediction of the effective thermal conductivity of plain woven fabric composite. The main advantages of the plug-in are: it generates a finite element model of single layer or multiple layer composite fabrics by only taking few necessary input parameters which is feasible in term of saving time and it automatically assigns the material orientation, and it is the critical task for woven fabric composite because material principal axis of yarn changes due to the waviness in warp and weft yarns. The Plug-in comprises the following three steps.

2.1.1. Step 1

In first step it generates the unit cell model of plain woven fabric composite by sweeping the lenticular cross-section of yarn along the yarn path which is defined by cubic spline curve as shown in Figure 3.
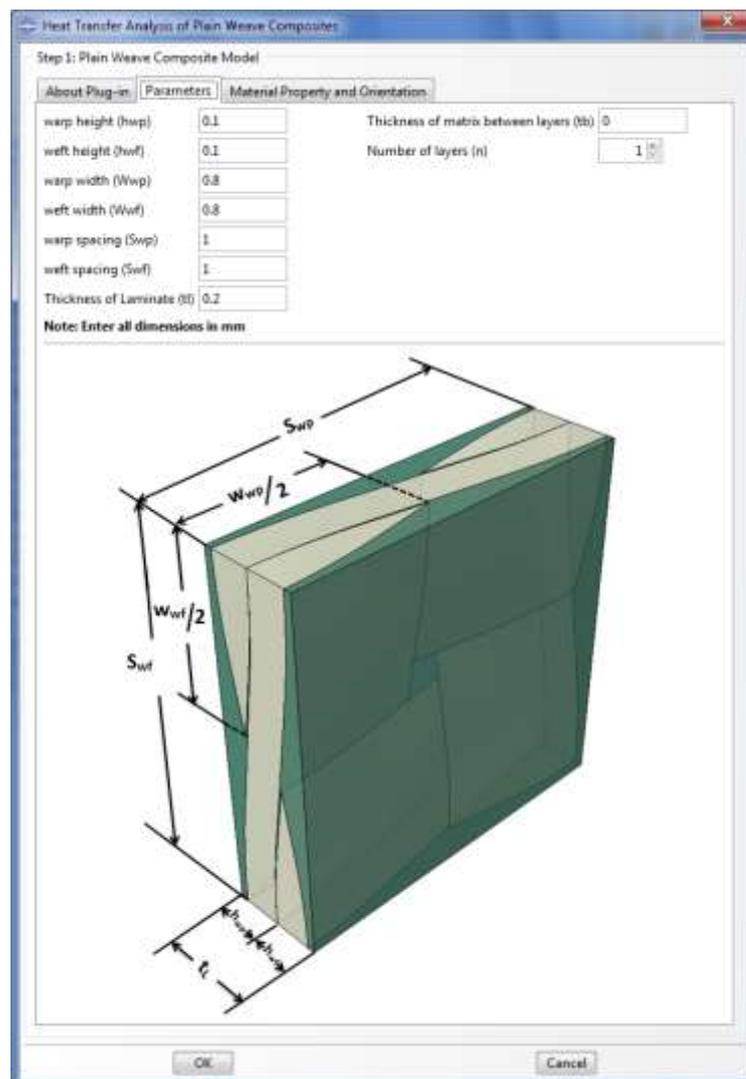

Figure 3: Plug-in main interface of plain woven composite fabric

Multilayer plain woven composites can be generated by using the idealized unit cell approach. In the same step material properties to the yarn and matrix can be assigned and material orientations can also be defined in this step.

Material orientation was defined by the discrete orientation technique in Abaqus/CAE as shown in Figure 5. Yarn is considered as solid orthotropic with the consideration of transversely isotropic. Transversely isotropic materials are those which have the equivalent physical properties at every point in the material about an axis that are normal to the plane of isotropy.

Figure 4 shows the material orientation in yarn of woven fabric generated in Abaqus/CAE. Axis 11 refers to the axis which is parallel to yarn axis, axis 22 and 33 are transverse (perpendicular) to the fibre direction by using discrete orientation technique. Because of the waviness in warp and weft yarn the material principal may vary from point to point. A discrete orientation defines a spatially varying orientation at the centroid of each native or orphan mesh element. The orientations are based on the topology of the part, allowing defining a continually varying orientation. Once the normal axis and primary axis are defined, Abaqus/CAE uses these axes to construct a right-handed Cartesian coordinate system [26]. For that purpose the surface of the yarn is divided into small faces by partition and the edges and surfaces are selected for primary and normal axis.
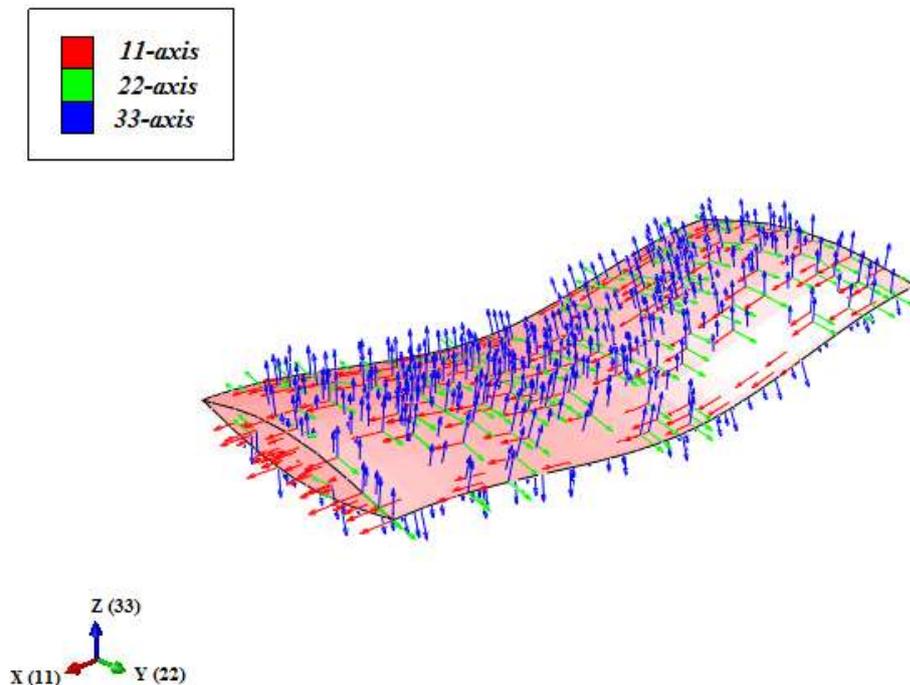
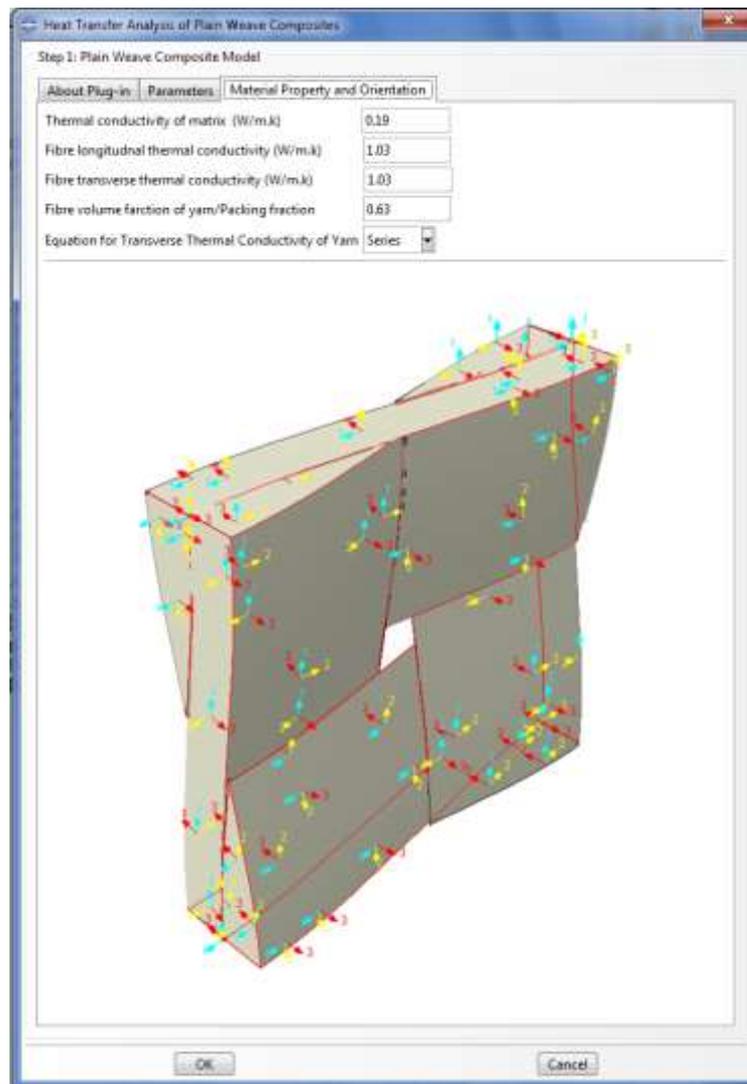**Figure 4:** Material orientation of yarn in woven fabric

Figure 5: Material orientation interface

2.1.2. Step 2

In second step it generates the mesh of unit cell by using 4-node linear tetrahedral elements (DC3D4) because this is the most suitable mesh element to completely mesh the complex geometrical shape [26] as shown in Figure 6 .

2.1.3. Step 3

In this step the temperature specified boundary conditions are applied and job is submitted for analysis. The steady state heat transfer of unit cell will be analysed.

Heat flux and surface area extracted can be obtained by using command within plug-in. The effective thermal conductivity across the thickness can be calculated by Fourier's law of conduction as shown in Equation (**1** and displayed in the message area of Abaqus/CAE.

$$K_{eff} = \frac{\text{Heat Flux across the thickness}}{\text{Surface Area} \times \Delta T} \times \text{thickness of composite} \qquad (1)$$
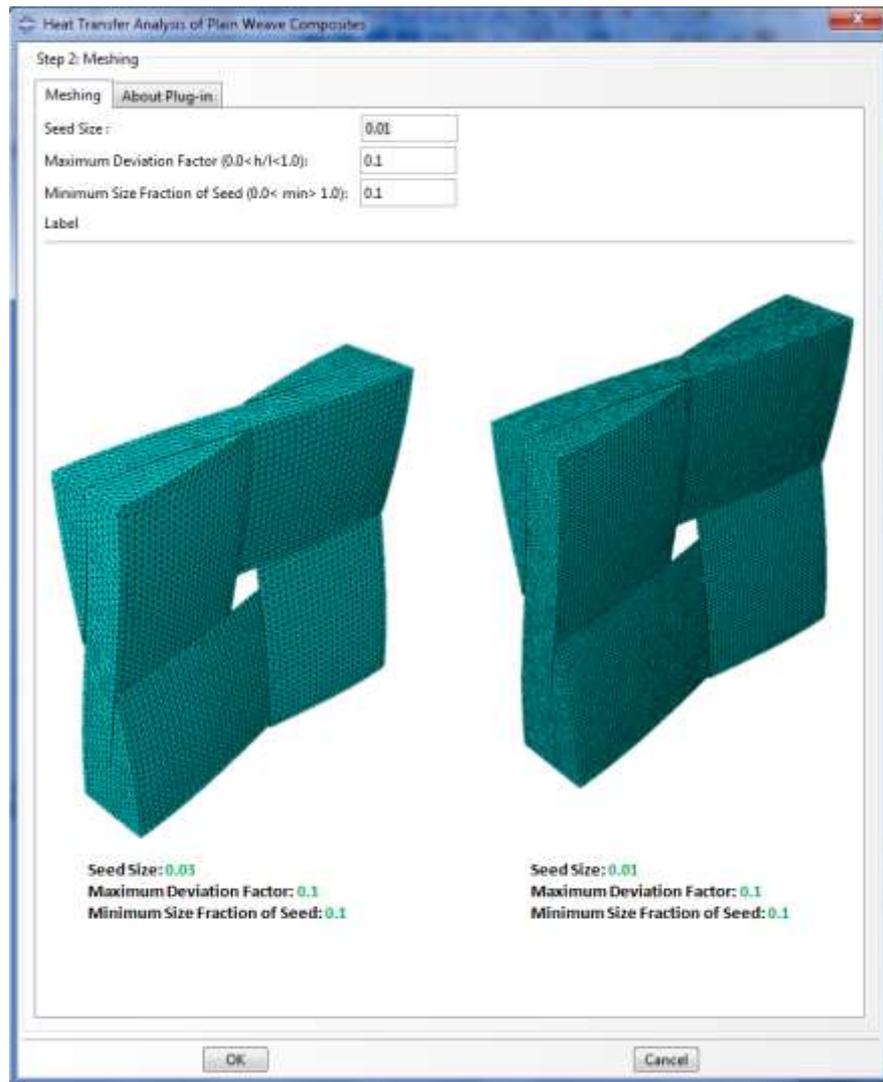

Figure 6: Mesh interface

2.1.4. Validation

In order to validate the predicted effective thermal conductivity of plain woven fabric composite obtained from the developed plug-in, results from FE models generated by the plug-in are compared with Dasgupta's results [29]. The homogenization scheme was developed in their researchto predict the effective thermal conductivity of woven composite fabric. Their method and analysis technique have been positively utilized by many authors in their research work which shows the accuracy of work. Figure 7 shows the comparison of the effective thermal conductivity between results obtained from plug-in and Dasgupta's work.   It was found that they are highly correlated. Figure 8 shows the plug-in environment of step 3.

Figure 9 shows the process sequence of the developed plug-in. The limitation of the plug-in is that it can only generate yarns with lenticular cross-sectional shape and fabrics with low crimp.
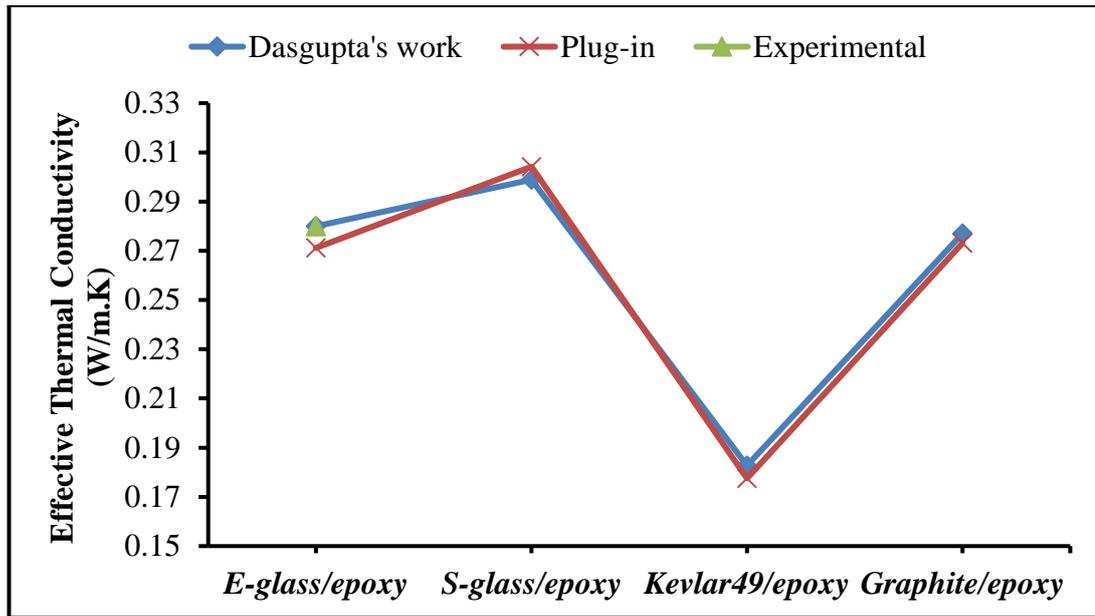

Figure 7: Comparison of effective thermal conductivity obtained from plug-in and Dasgupta's work
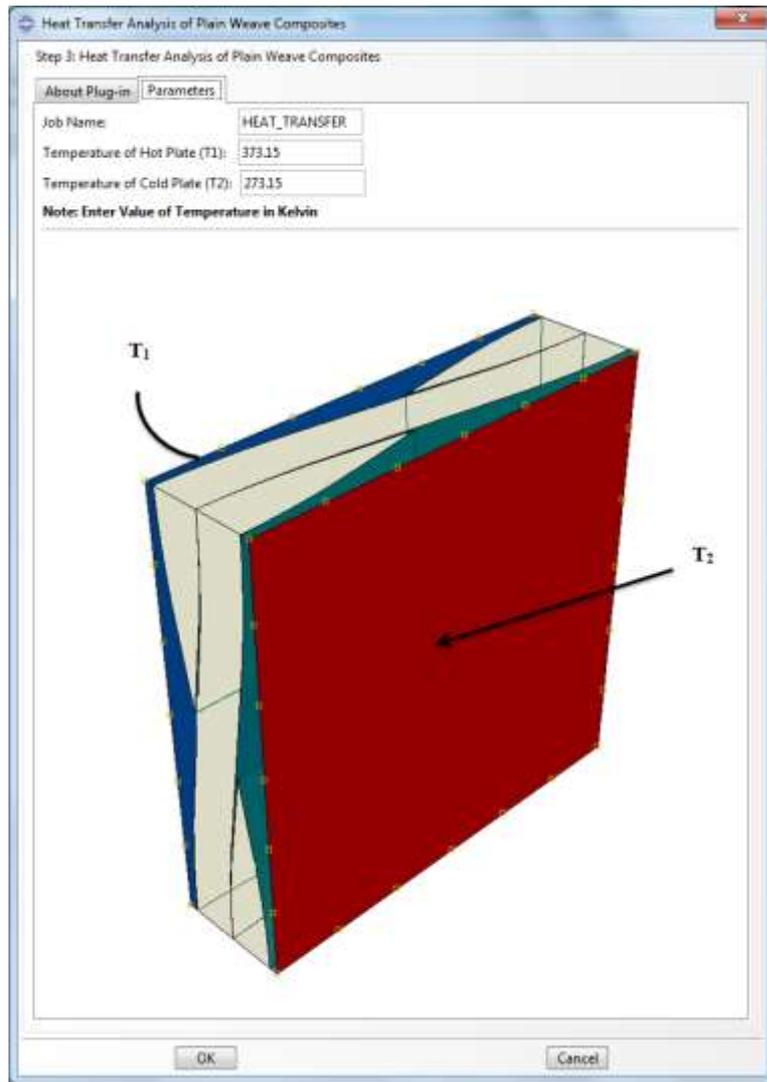
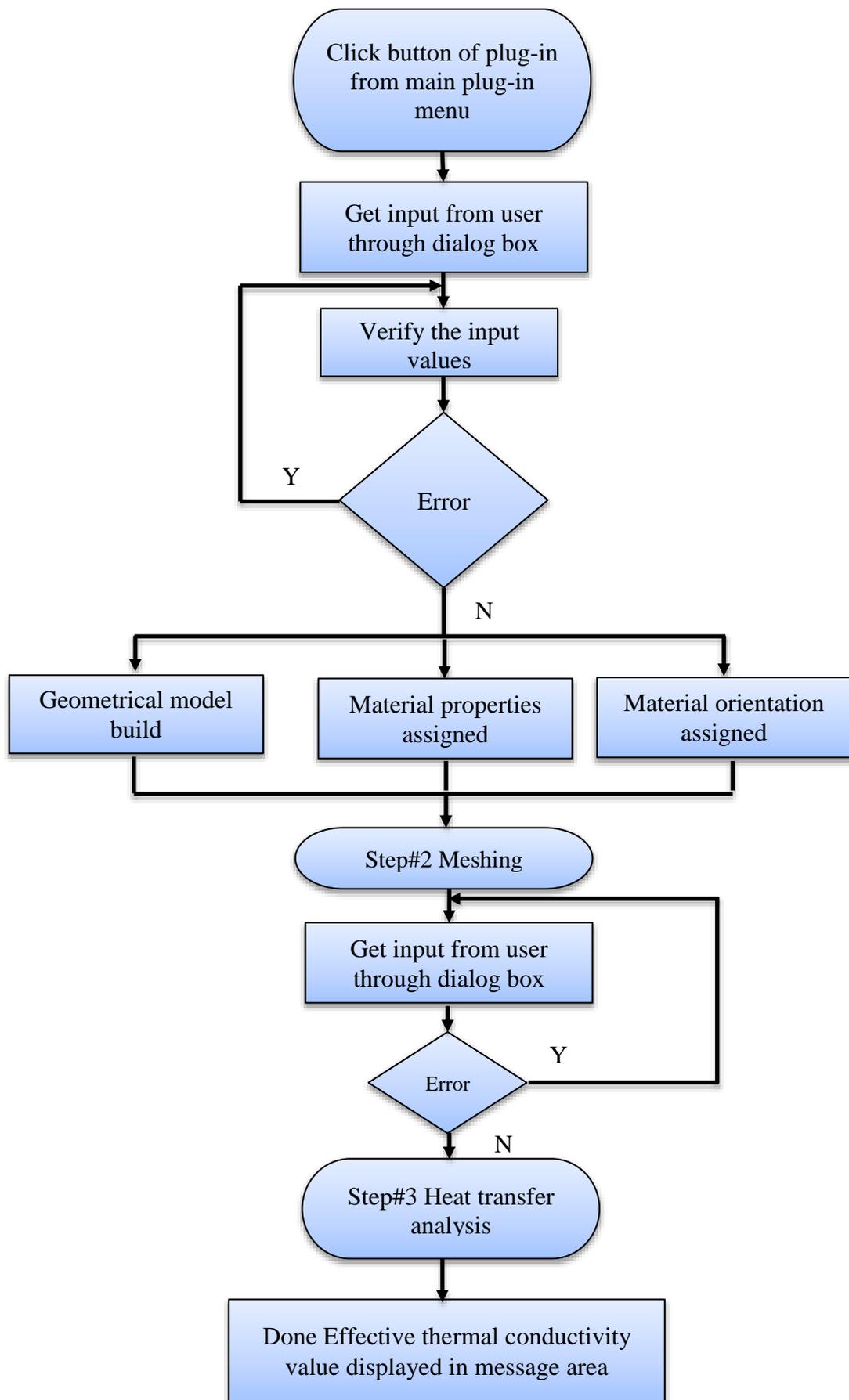**Figure 8:** Heat transfer analysis interface

Figure 9: Process sequence of the plug-in for plain woven composite fabric

2.2. Plug-in for MicroPCMs Composites

The unit cell model of MicroPCMs composite was created from GUI plug-in through micro-sphere filled composite material approach. Figure 10 shows the main interface of GUI plug-in which was created in Abaqus/CAE by python script. It can be used to automatically generate unit cell model of microencapsulated phase change material composites by simple cubic and body-centred cubic (BCC) structure as shown in Figure 11. The maximum volume fraction limit in simple cubic structure is 0.52 and in body-centred cubic structure is 0.68.
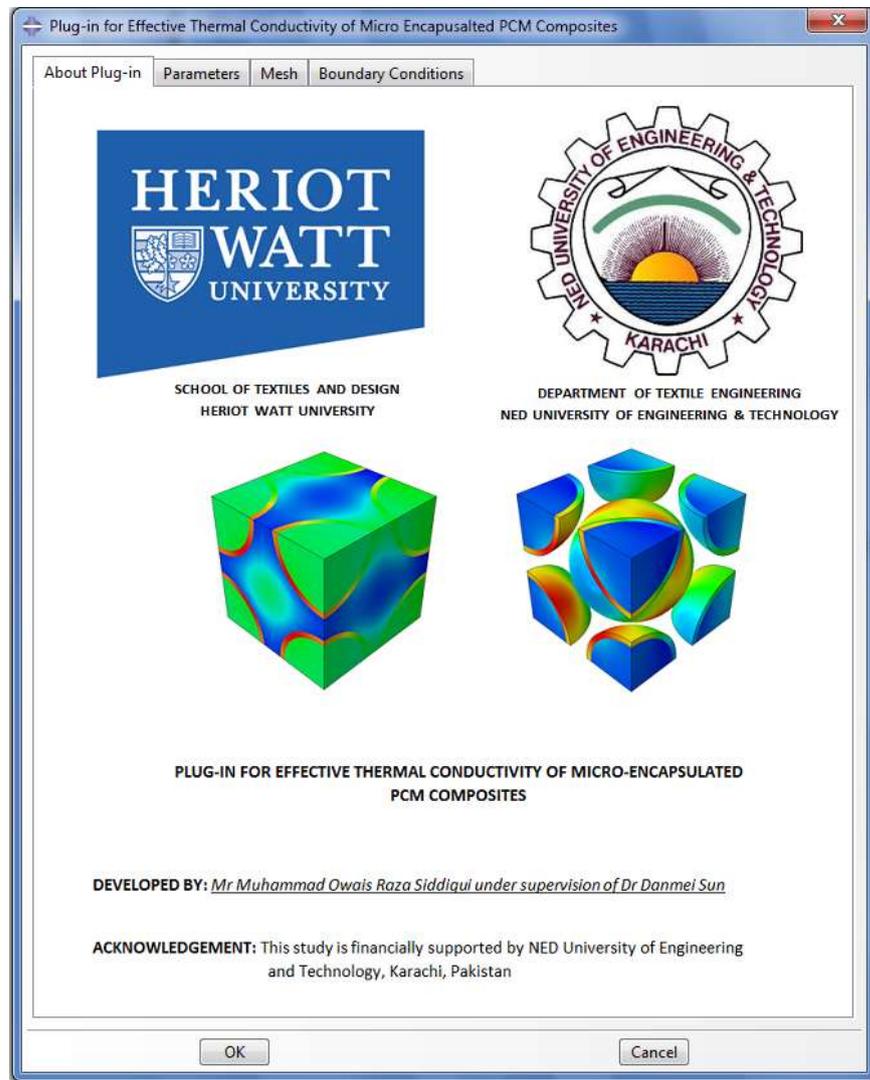

Figure 10: Main interface of GUI plug-in for microencapsulate PCM composites

Figure 12 shows the material interface of core, shell and matrix. The plug-in is capable to automatically predict the effective thermal conductivity of microencapsulated phase change composites.
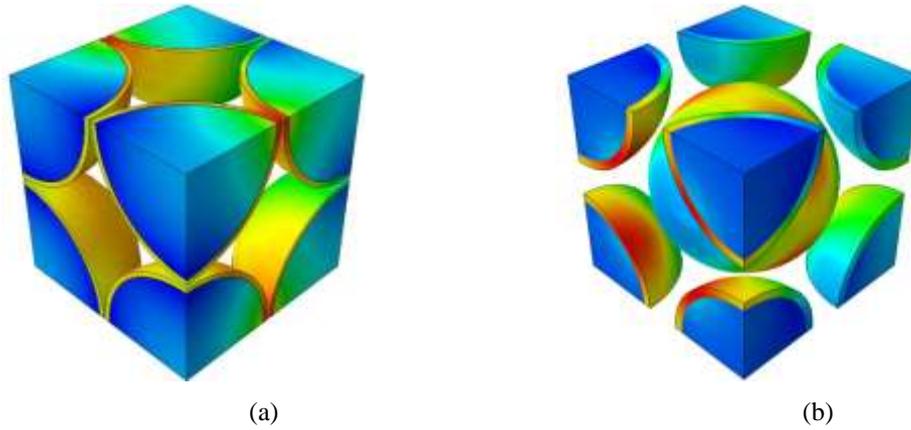
(a)   (b)

Figure 11: Packing arrangement: (a) Simple cubic and (b) Body-centred cubic (BCC)

2.2.1. Validation

In order to validate the finite element models of MicroPCMs generated from the plug-in, the effective thermal conductivity from plug-in are compared with well-established Maxwell's model. Different level of volume fractions of MicroPCMs (ϕ) were considered to evaluate the effectiveness of developed plug-in At higher volume fraction the values obtained from FEA were higher than the Maxwell's model due to the fact that Maxwell's equation was derived based on the assumption that the solid spheres apart from each other so there were no interaction and chain formation between them [7]. The results comparisons between the two methods are shown in Figure 13.

Table 1: Thermo-physical properties [7]

Property	n-Octadecane	Melamine Formaldehyde	Acrylic Binder (Matrix)
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
Latent Heat of Fusion (KJ/Kg)	238.76	-	-
Melting Point (˚C)	28.2	-	-
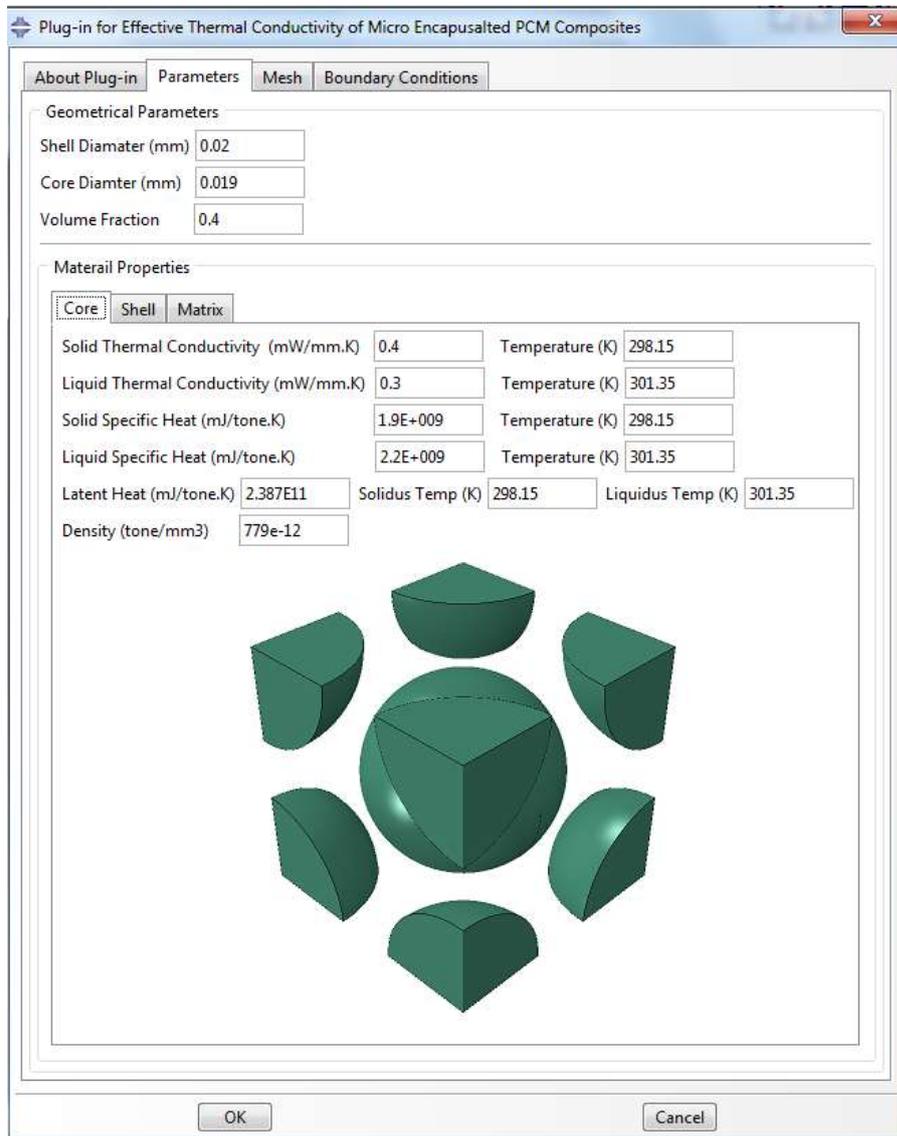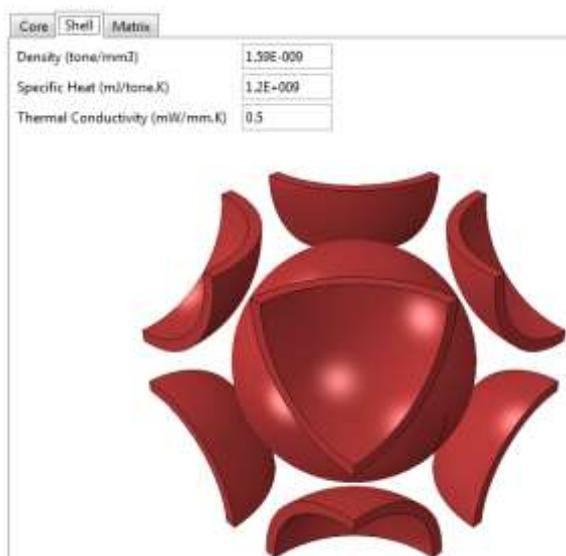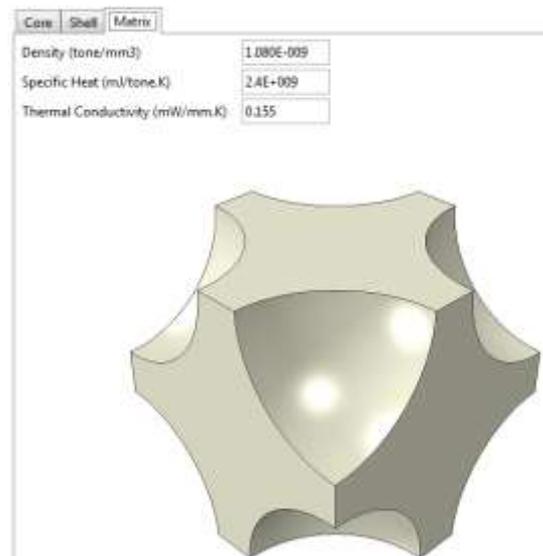
Figure 12: Material property interface: (a) Core; (b) Shell; and (c) Matrix

The thermal conductivity of MicroPCMs was calculated by composite sphere approach [30] by using the properties given in Table 1.

$$K_p = \frac{2(1-\phi_c)K_s + (1+2\phi_c)K_c}{(2+\phi_c)K_s + (1-\phi_c)K_c} K_s \qquad (2)$$

where K_p, K_s and K_c are the thermal conductivity of MicroPCMs, shell and core of PCM microcapsule respectively and ϕ_c is the core volume fraction.

The effective thermal conductivity of acrylic binder (considered as matrix) and MicroPCMs can be calculated by Maxwell's model [31] using the thermal conductivity of MicroPCMs obtained from Equation (3).

$$K_{eff} = K_b \frac{2K_b + K_p + 2\phi(K_p - K_b)}{2K_b + K_p - \phi(K_p - K_b)} \qquad (3)$$

where K_{eff} is the effective thermal conductivity of binder and MicroPCMs, K_b and K_p are the thermal conductivity of binder (matrix) and MicroPCMs respectively and ϕ is the volume fraction of MicroPCMs.
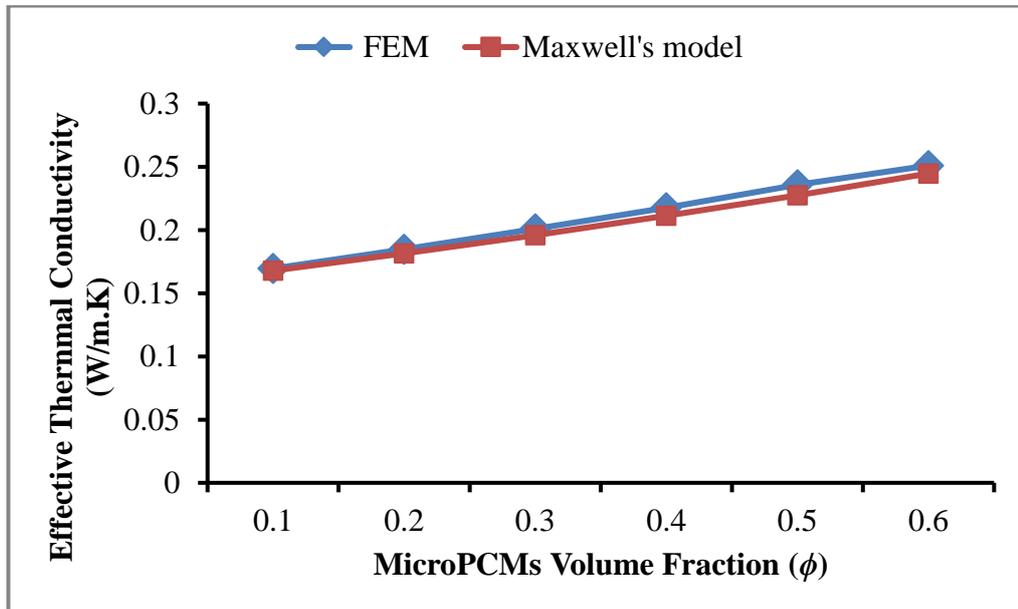

Figure 13: Results comparison between FEM and Maxwell's model

3. Parametric Analysis

3.1. Effect of Core Content of MicroPCMs on Effective Thermal Conductivity

The effect of core content on effective thermal conductivity of MicroPCMs composites has been investigated by keeping the volume fraction of MicroPCMs in matrix constant (10%). For that purpose the volume fraction of core within the microcapsules was decreased. It is found that the effective thermal conductivity increases with the decrease of core content. It is believed that this is caused by the higher thermal conductivity of shell material (melamine formaldehyde) compared to core material (n-octadecane) as shown in Figure 14. The results from FEA were agreed well with the results obtained from Maxwell's model as shown in Figure 14. The fact is that the shell thickness or core content has effect on effective thermal conductivity; it will increase or decrease depending on the thermal conductivity of both materials.
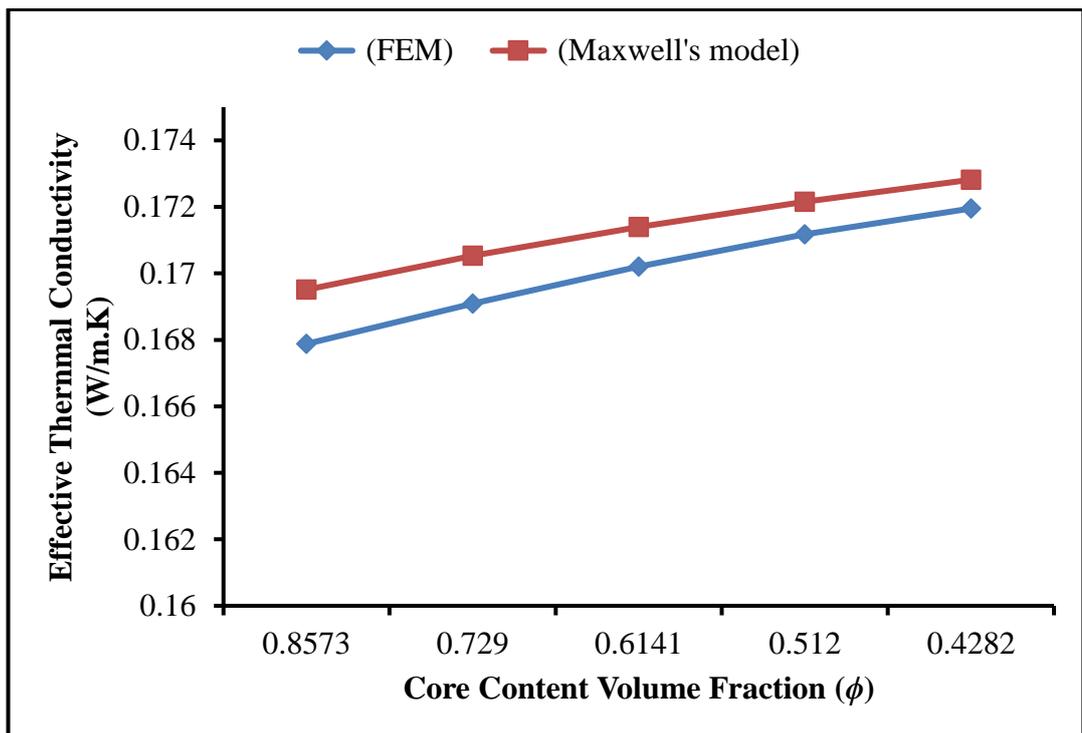

Figure 14: Effect of core content on effective thermal conductivity

3.2. Effect of PCM on Temperature Change vs Time

Figure 15 shows the unit cell model of MicroPCMs composite of acrylic binder as matrix and microcapsules which contain 20 percent volume fraction of Micro capsules. In order to evaluate the effect of PCM on temperature change with respect to time, a transient heat transfer analysis was carried on unit

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cell by applying temperature specified boundary conditions as shown in Figure 15. The initial temperature (273.15K) was applied on wall A, B, C, D and E at time zero second and a constant temperature (308.15K) was applied on wall E throughout the analysis.

A node was selected shown in Figure 15 to analyse the effect of PCM (latent heat) on temperature. Figure 16 (a) shows the heating curve of the selected node of MicroPCMs composite with PCM and without latent heat (during the analysis latent heat property of core material was removed). It shows clearly that during the analysis temperature of the node with PCM is increased slowly as compared to that of without latent heat. The highlighted portion in the graph of Figure 16 (a) shows that the PCM absorbs energy and changes its phase from solid to liquid while in the case of without latent heat its temperature increment uniform. This phase change phenomena delayed the temperature change for the PCM composite.

Figure 16 (b) shows the cooling phenomena in which the initial temperature of 308.15K was used and 273.15K was applied on wall E. The effect is reverse to the heating phenomena. Without latent heat property of composite cooled and loses energy rapidly as compared to PCM composite.
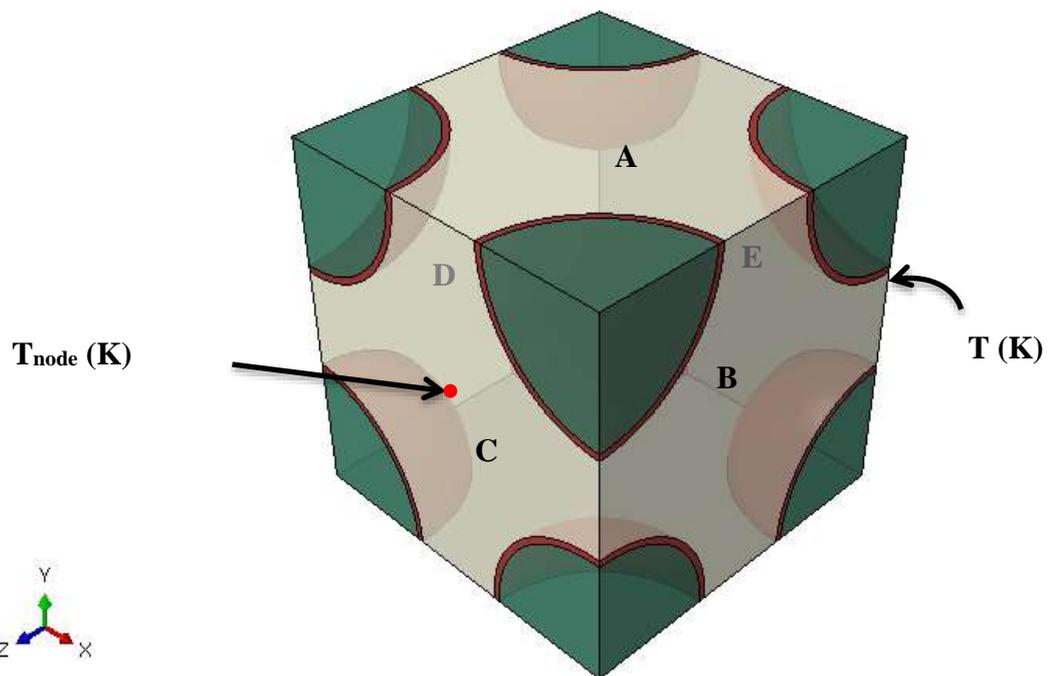

Figure 15: Unit cell model with boundary conditions

Figure 17 shows that heating and cooling curve of the node in composites with and without MicroPCMs. Figure 17 (a) shows the heating phenomena in which initial temperature of MicroPCMs composite rises more rapidly. Due to the fact that the thermal conductivity of microcapsules is high as compared to matrix material, when the simulation process reaches to the stage that phase change phenomena starts and the temperature of MicroPCMs composite drops down, or vice versa for the cooling case.
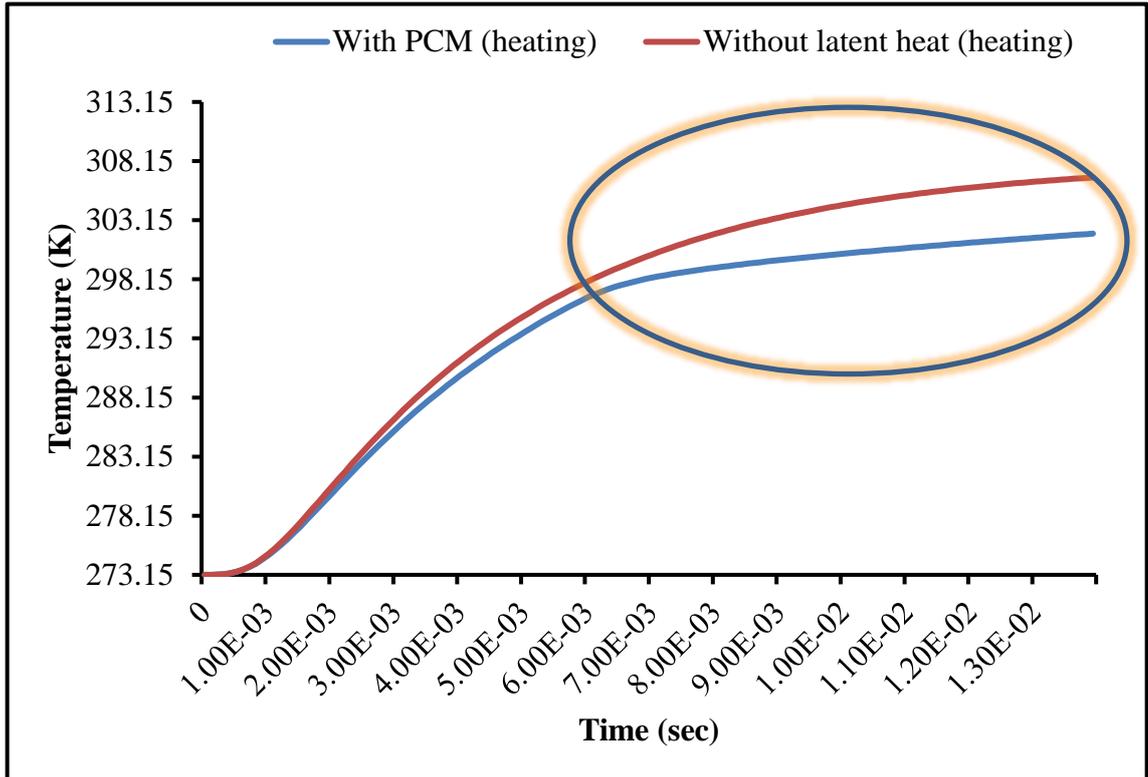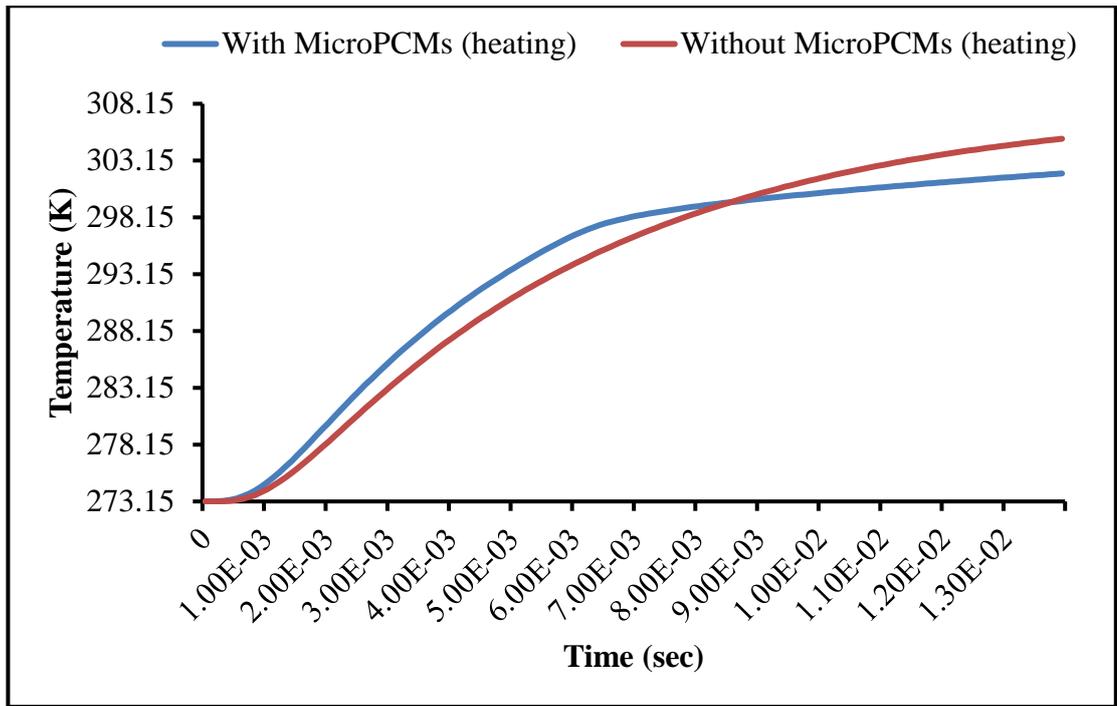
(a)
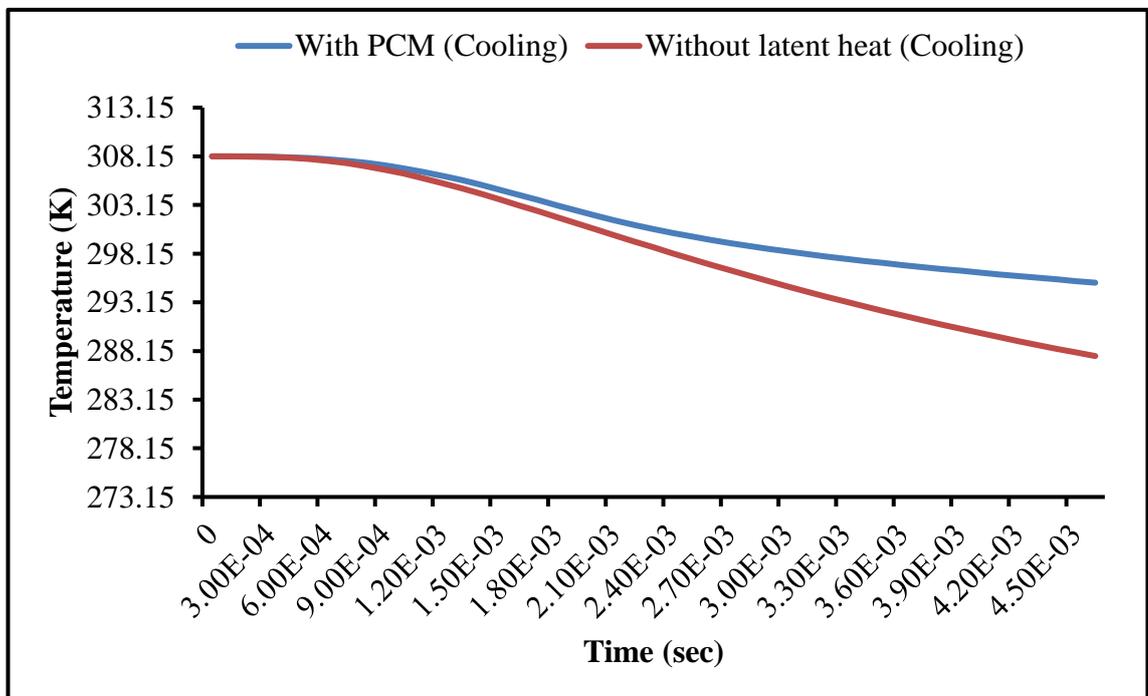
(b)

Figure 16: Heat and cooling curve at node of composites: (a) With PCM and (b) Without latent heat

(a)
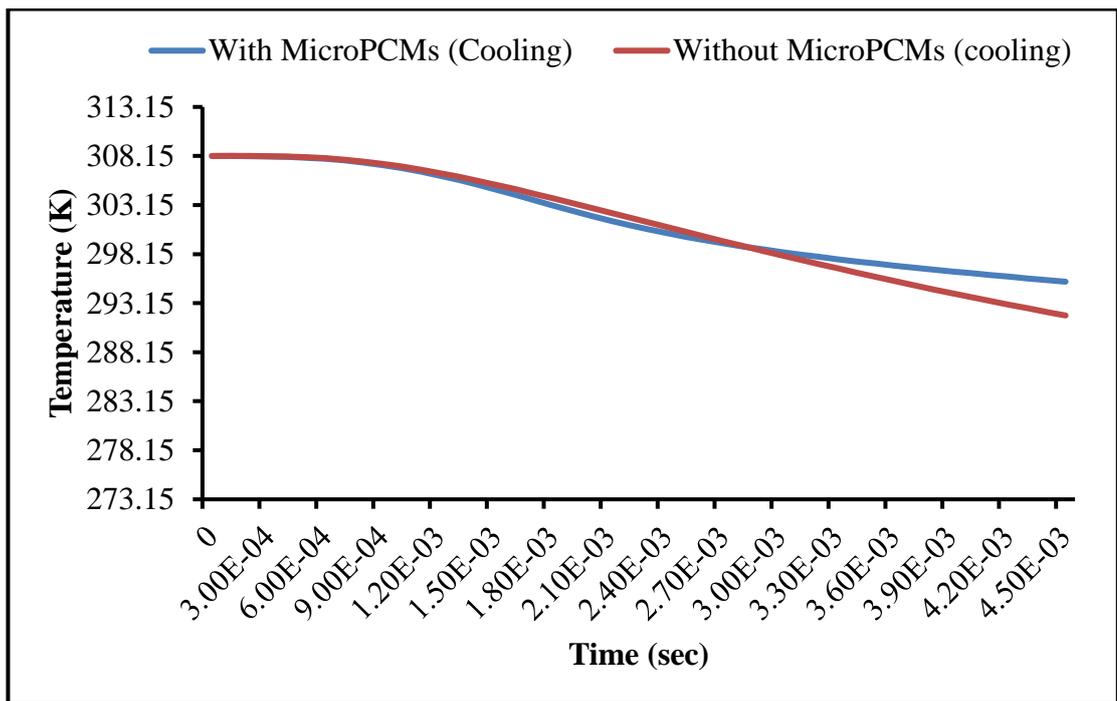
(b)

Figure 17: Heat and cooling curve at node of composites (a) With PCM and (b) Without PCM

Figure 18 shows the heating and cooling curves of the node of composites with different configurations within the solidus and liquidus temperature range of the core content (phase change material). The method described above is to predict the effective thermal conductivity of MicroPCMs composite and can be used for any kind of polymeric materials which contain microencapsulated phase change materials.

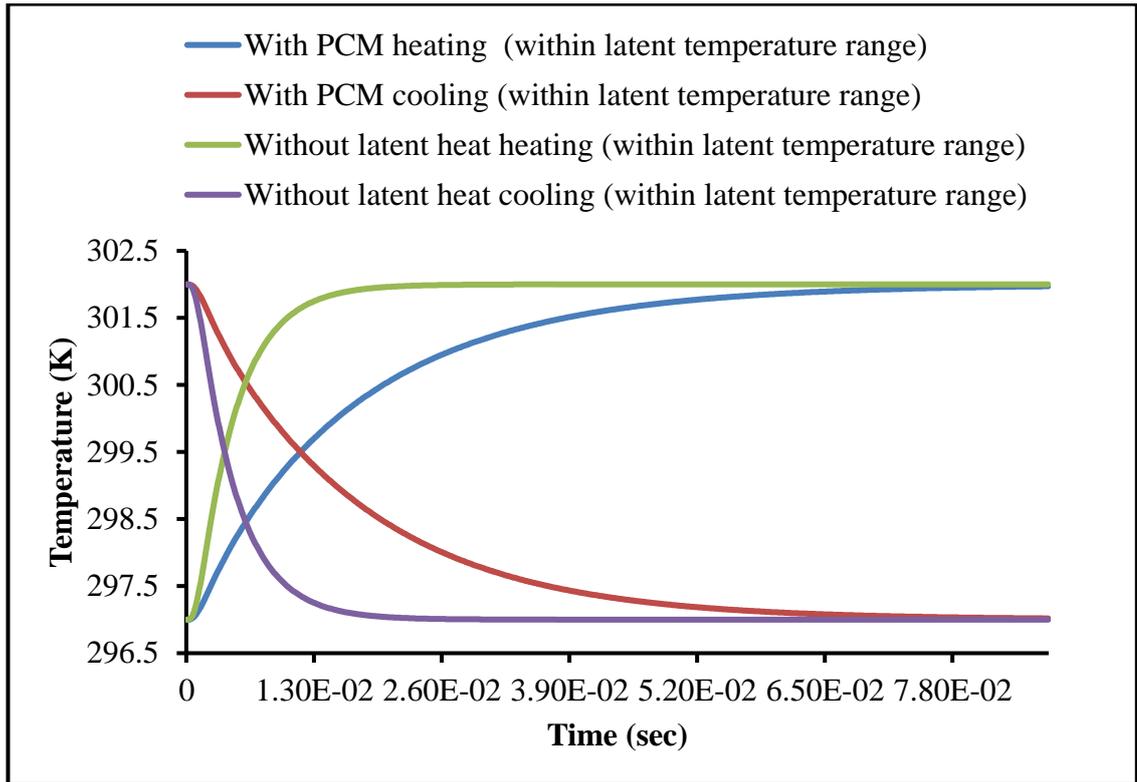**Figure 18:** Heating and cooling curves of Composite with different configuration

4. Conclusion

This research paper describes the development of the Plug-ins which can be used to generate the 3D solid model of MicroPCMs and plain woven composites. The plug-ins have been created to provide an instinctive and simple way for users to create models and predict fabric properties. They are validated by comparing post-processing results of finite element models in Abaqus environment to the results from previous published research work.

Based on the generated finite element models using the successfully developed Plug-ins, parametric studies were carried out to find out the effect of core content of MicroPCMs on effective thermal conductivity and heating and cooling effect of PCM.

Acknowledgement

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