Theoretical Calculation and Analysis Modelling for the Effective Thermal Conductivity of Lithium Metatitanate Pebble Bed

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Abstract: The effective thermal conductivity of lithium metatitanete (Li_2TiO_3) pebble bed is an important design parameter for the thermo-mechanical design of IN LLCB TBM (Indian Lead Lithium Ceramic Breeder Test blanket Module). In this paper, the 2D and 3D theoretical equations for the effective thermal conductivity of Li_2TiO_3 pebble bed are derived and compared with the modelling results obtained by using COMSOL as a numerical tool and also with available experimental results. The theoretical calculations and modelling analysis gives the preliminary result of the effective thermal conductivity of Li_2TiO_3 pebble bed.

Keywords: Effective thermal conductivity, Theoretical calculations, Modelling analysis, Li_2TiO_3 pebble bed, Fourier law.

1. Introduction

Lithium-based ceramics have been recognized as promising tritium-breeding materials for the fusion reactor blankets. India has proposed LLCB concept to be tested in ITER (International Thermonuclear Experimental Reactor). In this concept Li_2TiO_3 as lithium ceramic material will be adopted in the form of pebbles for tritium breeding and helium as coolant and purge gas [1]. The ceramic pebbles configuration has been the preferred option in most blanket designs due to its potential advantages like simpler assembly of breeder into complex geometry regions, uniform and stable pore network for purge gas transport, no thermal stress cracking because small thermal gradient across each pebbles, active control of bed thermal conductivity by varying the purge gas pressure [2]. The LLCB TBM consists of lithium metatitanate as ceramic breeder (CB) material in the form of packed pebble beds. The alloy lead–lithium eutectic (Pb–Li) flowing separately around the CB pebble bed to extract the generated nuclear heat from the CB zones, therefore heat is transferred from hot pebble beds to the coolant. The thermal properties of the lithium ceramic pebble beds have a significant impact on blanket's temperature profile and the heat extraction process. So, the effective thermal conductivity of pebble beds is an important design parameter for the temperature control in the pebble beds.

In this paper the theoretical calculation and modelling analysis for the effective thermal conductivity of Li_2TiO_3 pebble bed are performed. The 2D and 3D theoretical equations for the thermal conductivity of pebble bed are derived, and compared with the modelling results using COMSOL as a numerical tool [3]. The effective thermal conductivity of Li_2TiO_3 pebble bed can be preliminarily obtained by analysis modelling or theoretical calculation under the lack of experimental set-up at present. It might be a feasible choice to firstly calculate the effective thermal conductivity of pebble bed based on Fourier law of heat transfer [4] before going for experimental evaluation of pebble bed thermal conductivity. The mathematical model used in this paper for the calculation of effective thermal conductivity of Li_2TiO_3 pebble bed is based on a simple thermal conduction model, which only depends on the packing factor of pebble bed, thermal conductivity of purge gas helium and solid pebble material.

Nomenclatures

A	area
kg	thermal conductivity of helium gas
kp	thermal conductivity of Li_2TiO_3 pebbles
kx	theoretical thermal conductivity of 2D Li_2TiO_3 pebble bed in x (or y) direction
km	modelling thermal conductivity of Li_2TiO_3 pebble bed
ku	theoretical thermal conductivity of 3D Li_2TiO_3 mono-sized pebble bed
kb	theoretical thermal conductivity of 3D Li_2TiO_3 binary-sized pebble bed
ke	Experimental data for thermal conductivity of 3D Li_2TiO_3 pebble bed
ε	porosity of Li_2TiO_3 pebbles
r	radius of Li_2TiO_3 pebbles
R	thermal resistance
dRu	equivalent thermal resistance of upper Li_2TiO_3 pebble section
dRm	equivalent thermal resistance of middle helium gas section
dRb	equivalent thermal resistance of lower Li_2TiO_3 pebble section

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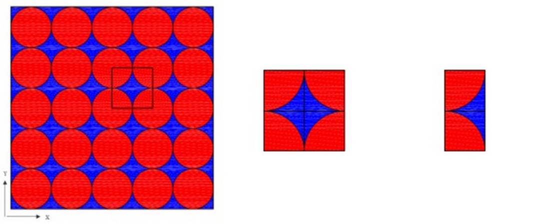
dRt	total thermal resistance of an infinitesimal layer in unit cell
Rt	total thermal resistance of a unit cell that used in the theoretical calculation
T	temperature
β	ratio (1−kg/kp)
δ	thickness
ϕ	packing factor

2. 2D Li_2TiO_3 pebble bed

Fig. 1(a) shows the 2D schematic array of Li_2TiO_3 pebbles with the theoretical packing factor of 78.5 %. The red colour is Li_2TiO_3 pebbles with the diameter of 1.0 mm and the blue colour is helium purge gas. Fig 1(b) and 1(c) shows the unit cell model and half unit cell model of 2D pebble bed array.



(a) 2D pebble bed (b) Unit cell (c) Half unit cell

Figure 1. 2D array of Li_2TiO_3 pebbles

In case of Fig. 1(a) with the infinite array of bed, it is could be approximately considered the thermal conduction is isotropy in xy plane, so the thermal–electrical analogy technique and the 1D heat conduction model [5] can be used to evaluate the effective thermal conductivity of Li_2TiO_3 pebble bed in x or y direction for two dimensional array.

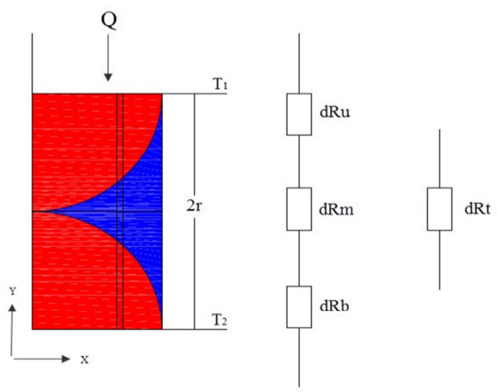


Figure 2. 2D heat transfer calculation model and thermal resistance network

As shown in Fig. 2, Q is the heat transfer rate along y direction, T_1 and T_2 are the temperatures on the top and bottom surfaces, respectively. The half unit cell model is divided into many infinitesimal layers with the thickness dx for each layer. The thermal resistance of different three sections inside an infinitesimal layer can be expressed using Fourier law of heat conduction for one dimension and steady state heat flow condition. The equivalent thermal resistance of upper pebble section (dRu) in fig.2 can be expressed,

$$dRu=\frac{\sqrt{r^2-x^2}}{kp*dx} \tag{1}$$

The equivalent thermal resistance of middle helium gas section (dRm),

$$dRm=\frac{2\left(r-\sqrt{r^2-x^2}\right)}{kg*dx} \tag{2}$$

Due to symmetry in fig.2 the thermal resistance for upper and lower pebble section will be same.

$$dRb=\frac{\sqrt{r^2-x^2}}{kp*dx} \tag{3}$$

The thermal resistance for different three sections inside all infinitesimal layers are in series combination. So, the total thermal resistance of an infinitesimal layer is,

$$dRt=dRu+dRm+dRb=\frac{2\left(r-\beta\sqrt{r^2-x^2}\right)}{kg*dx} \tag{4}$$

where, $\beta=1-\left(\frac{kg}{kp}\right)$.

All infinitesimal layers with definite value of thermal resistance dRt are in parallel combination. So the total thermal resistance, Rt of half of the unit cell is,

$$\frac{1}{Rt}=\int_0^r\frac{1}{dRt}=\left(-\frac{kg}{2*\beta}\right)*\left(\frac{\pi}{2}+\left(\frac{2}{-1+\beta}\right)\sqrt{\frac{-1+\beta}{-1-\beta}}\,\mathrm{arctg}\sqrt{\frac{-1-\beta}{-1+\beta}}\right) \tag{5}$$

The effective thermal conductivity of two dimensional array for Li_2TiO_3 pebble bed in x or y direction is expressed as follows,

$$kx=\frac{2r}{r}*\frac{1}{Rt}=-\frac{kg}{\beta}*\left(\frac{\pi}{2}+\left(\frac{2}{-1+\beta}\right)\sqrt{\frac{-1+\beta}{-1-\beta}}\,\mathrm{arctg}\sqrt{\frac{-1-\beta}{-1+\beta}}\right) \tag{6}$$

According to Eq. (6) the effective thermal conductivity kx for 2D pebble bed depends on the thermal conductivity of pebble material and thermal conductivity of helium gas, and not

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depends on the diameter of pebbles. Where, kg is the thermal conductivity of Helium gas [6] as a function of temperature (K) is given as,

$$kg=0.0294900023+(5.07655059*10^{-4}*T) -(4.22501605*10^{-7}*T^2)+(2.1209438*10^{-10}*T^3) \quad (7)$$

and kp is thermal conductivity of Li_2TiO_3 pebble [7] is given as,

$$kp=\left(\left((1-\varepsilon)^{2.9}\right)*(5.35-\left(4.78*10^{-3}*T\right)+\left(2.87*10^{-6}*T^2\right)\right) \quad (8)$$

$0.14 \leq \varepsilon \leq 0.25$ and $400\ K \leq T \leq 1400\ K$.

Note that, above Eq. (6) is obtained based on the assumption that the array of 2D Li_2TiO_3 pebble is infinite; however the size of pebble bed is always finite in the real-life, so based on the theoretical calculation, it is necessary to choose a finite model and analyse the effective thermal conductivity. Here the FEA (Finite Element Analysis) code COMSOL is used as numerical tool in the following analysis.

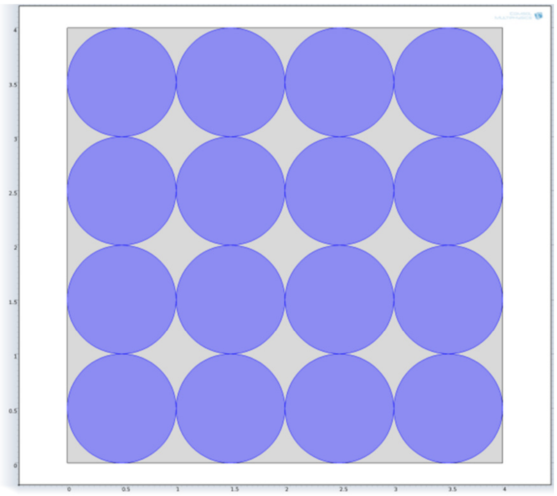


Figure 3. FEA model of 2D Li_2TiO_3 bed

Fig.3 is the 2D FEA model for the effective thermal conductivity of Li_2TiO_3 pebble bed. The model includes 16 pebbles with the same diameter of 1 mm. The heat transfer in the model is governed by the stationary heat transfer equations. The heat flux is applied on the top face, and both left and right side faces of model are thermally insulated (i.e. no heat will transfer across this boundary). The bottom side of model is convective cooled. Different values of convective heat transfer coefficient are used to obtain effective thermal conductivity at different mean temperature of pebble bed.

Fig. 4 shows the comparison of modelling km and theoretical kx results. Both km and kx increases with temperature increases. As temperature increases both modelling km and theoretical kx results come closer.

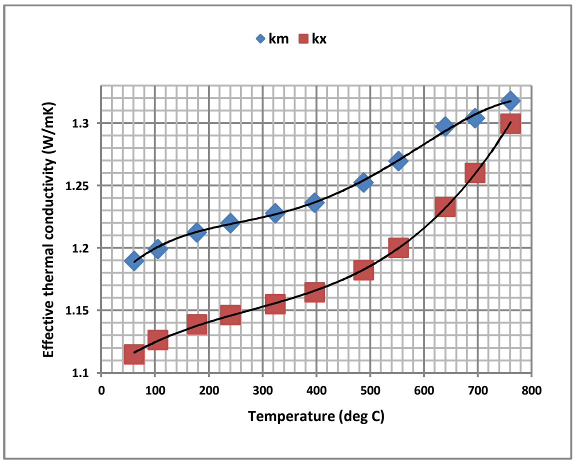
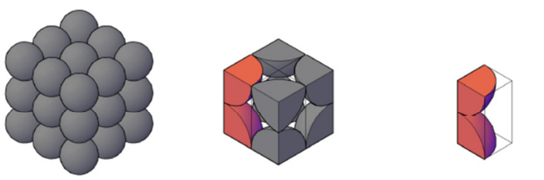


Figure 4. Comparison of modelling km and theoretical kx results for 2D pebble bed

3. 3D Li_2TiO_3 pebble bed

3.1 Mono-sized pebble bed

Fig. 5(a) shows the 3D schematic array of Li_2TiO_3 pebbles with a uniform diameter of 1mm. It is only a simple cubic arrangement of pebble bed, having the theoretical packing factor is 52.33%. Fig. 5(b) and fig.5(c) shows the unit cell model and the quarter unit cell model respectively.



(a) 3D distribution (b) Unit cell (c) Quarter unit cell

Figure 5. Simple cubic arrangement of pebble bed

The unit cell which comprise eight number of 1/8 spheres with helium gas in the middle. Assumed that heat flows through the pebbles and the middle helium gas in parallel, so the effective thermal conductivity of the quarter of unit cell can be expressed as,

$$ku=\left(1-\frac{\pi}{4}\right)kg+\frac{\pi}{4}kc \quad (9)$$

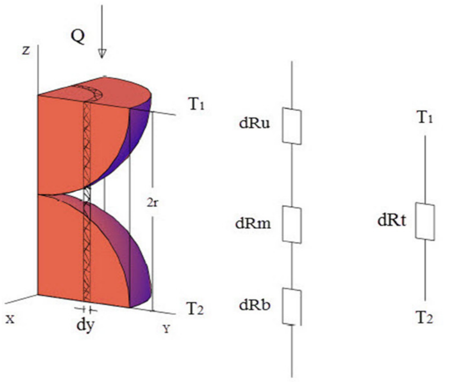


Figure 6. 3D heat transfer calculation model and the thermal resistance network

By using the thermal-electrical analogy and integral techniques kc can be obtained. The thermal–electrical analogy technique and the one-dimensional heat conduction model [8] used to evaluate effective thermal conductivity theoretically. As shown in fig.6, T_1 and T_2 are the temperatures on the top and bottom surfaces, respectively. The quarter of the unit cell column is divided into many infinitesimal layers with thickness of dy for each layer. Since, the thermal resistance of three different sections inside each infinitesimal layer are in series combination. The thermal resistance dRu, of the upper equivalent pebble section is,

$$dRu=\frac{2\left(\sqrt{r^2-y^2}\right)}{kp*\pi*y*dy} \tag{10}$$

Due to symmetry, the thermal resistance dRb of the bottom pebble section is equal to dRu. The resistance of the middle helium section dRm is,

$$dRm=\frac{4\left(r-\sqrt{r^2-y^2}\right)}{kg*\pi*y*dy} \tag{11}$$

Since, dRu, dRm and dRb are in series with each other, so the total thermal resistance of an infinitesimal layer is,

$$dRt=dRu+dRm+dRb=\frac{4\left(r-\beta\sqrt{r^2-y^2}\right)}{kg*\pi*y*dy} \tag{12}$$

However, since all infinitesimal layers with the resistance dRt of each layer are in parallel, the total thermal resistance of a quarter of the column can be obtained by

$$\frac{1}{Rt}=\int_0^r \frac{1}{dRt}$$

$$=\left(\frac{1}{4}\right)*\int_0^r \frac{kg*\pi*y*dy}{r-\beta\sqrt{r^2-y^2}}=\left(\frac{\pi*kg*r}{4*\beta}\right)*\left(\frac{1}{\beta}*\ln\left(\frac{1}{1-\beta}\right)-1\right) \tag{13}$$

According to Fourier law of heat conduction, the effective thermal conductivity kc can be expressed as,

$$kc=\frac{2r}{\frac{\pi r^2}{4}}*\frac{1}{Rt}=\left(\frac{2*kg}{\beta}\right)*\left(\frac{1}{\beta}*\ln\left(\frac{1}{1-\beta}\right)-1\right) \tag{14}$$

Substituting Eq. (14) into Eq. (9), the effective thermal conductivity for mono sized pebble bed can be expressed as,

$$ku=\left(1-\frac{\pi}{4}\right)*kg+\left(\frac{\pi*kg}{2*\beta}\right)*\left(\frac{1}{\beta}*\ln\left(\frac{1}{1-\beta}\right)-1\right) \tag{15}$$

From eq. (15) it can say that the effective thermal conductivity of mono sized pebble bed only relates with thermal conductivity of pebble material and helium gas and arrangement of pebbles (packing fraction).

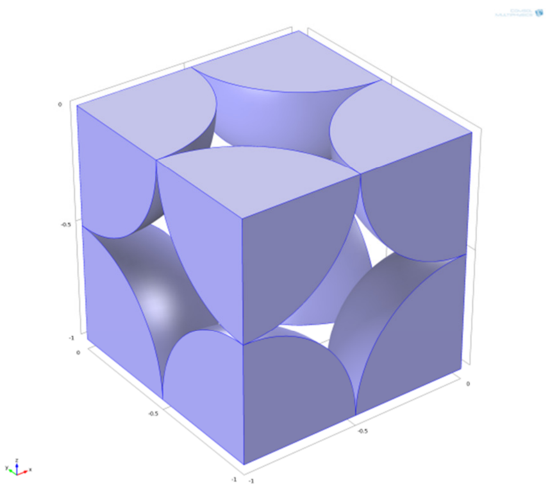


Figure 7. FEA model of mono-sized pebble bed

The theoretical effective thermal conductivity using above equation is compared with modelling results using COMSOL as a numerical tool. Fig.7 shows a 3D FEA model of mono sized pebble bed having simple cubic arrangement. The heat transfer in the unit cell model is governed by steady state heat transfer equations. Due to symmetries in 3D array of pebble bed shown in fig. 5(a) only the unit cell is taken for meshing. Heat flux is applied at the top side and bottom side is convective cooled. All four sides are thermally insulated.

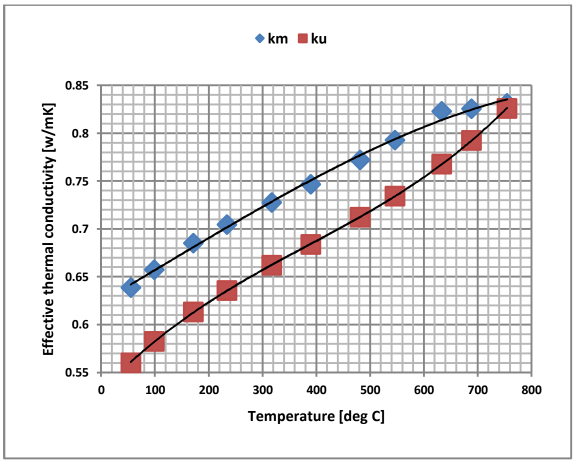
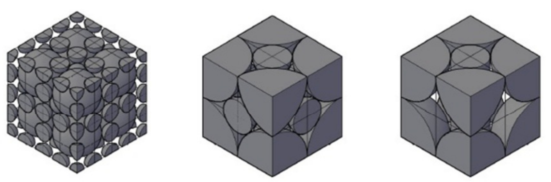


Figure 8. Comparison of theoretical ku and modelling km results for mono-sized bed

Fig. 8 shows the comparison of modelling estimated results km and theoretical estimated results ku for uniform diameter pebble bed. It can be seen that both km and ku are increasing functions depending on the temperature, and their results are gradually close to the same value as the temperature increases.

3.2 Binary sized pebble bed

In previous section, the theoretical calculation for uniform diameter pebbles or mono-sized pebble bed is performed. But it is not in the real condition, there are more or less differences in size of pebbles diameter.



(a) 3D distribution (b) Unit cell (c) Simplified model

Figure 9. Binary sized pebble bed

Fig. 9(a) is a 2×2×2 simple cubic pile of Li_2TiO_3 pebbles, but the size of pebble diameter is binary, there are 32 little pebbles in the clearance among the 8 large pebbles, and the array formed by the large and little pebbles is symmetrical. For this array of Fig. 9(a), the diameter ratio of the little pebble to the large pebble is 0.4. The packing factor is about 65.76%.

The integral model for Fig. 9(b) is very complicated; therefore a simplified model used for the heat transfer calculation. The effective thermal conductivity for simplified model shown in fig. 9(c) is obtained by using the thermal-electrical analogy and integral techniques [5]. In simplified model a cylinder along z direction is used instead of four small size pebbles, where the diameter ratio of the cylinder to the large pebble is 0.4, the maximum value is (√2-1); thus its packing factor for this simplified model is equals 64.93%, which is almost as same as that of Fig. 9(b). According to the model of Fig. 9(c), assuming that the heat flows along z direction, an approximate result can be obtained and expressed in the following equation, which is a rough evaluation for the theoretical thermal conductivity of Li_2TiO_3 pebble bed under the distribution of Fig. 9(c). An approximate effective thermal conductivity kb can expressed for simplified model,

$$kb=\left(\frac{\pi}{4}*kc\right)+\left(\frac{\pi}{4}*\left(\sqrt{2}-1\right)^2*kp\right)$$
$$+\left(\left(1-\left(\frac{\pi}{4}+\left(\frac{\pi}{4}*\left(\sqrt{2}-1\right)^2\right)\right)\right)*kg\right) \quad (16)$$

Where, kc can be used from Eq. (14)

It can be seen from Eq. (16) because of the small pebbles are replaced by the cylinder, among the clearance of large pebbles, the effective thermal conductivity kb relates with the thermal conductivity of helium and Li_2TiO_3 material, and also with the diameter ratio of the small pebbles (cylinder) to the large pebbles, that relates with the packing factor of Li_2TiO_3 pebble bed.

Fig.10 is a FEA model for binary sized pebble bed. Model consisting one large size pebble and four small size pebbles and helium gas inside voids created by large and small size pebbles based on the array of figure 9(a). The diameter ratio for small diameter spheres to large diameter sphere is 0.4. The same thermal boundary conditions are used that was used in the case of uniform diameter pebble bed. The heat transfer in the unit cell model is governed by steady state heat transfer equations. The experimental data of the effective thermal conductivity for 1.91 mm diameter pebble bed with 60 % of packing fraction [9] is used for comparison with modelling and theoretical results. Fig. 10 shows the comparisons of theoretical kb, modelling km and experimental ke.

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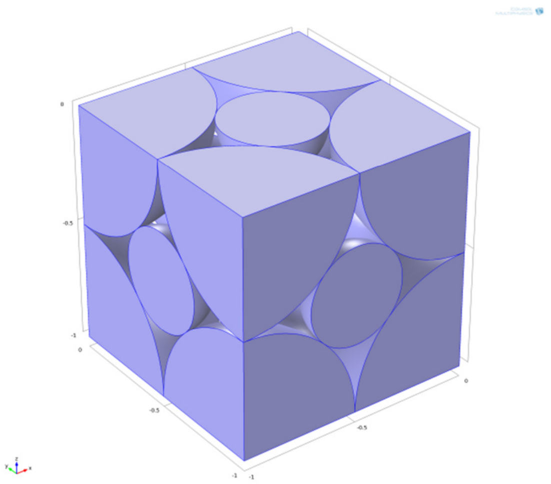

Figure 10. FEA model of binary-sized pebble bed.

Fig.11 shows the comparisons of theoretical, modelling and experimental results. It can be seen from comparisons that both experimental ke and modelling km increases with temperature. The approximate results of theoretical kb are also increasing function of temperature but the effective thermal conductivity value is lower than both ke and km. The reason may be come from the assumption taken in the simplified model of theoretical calculations.

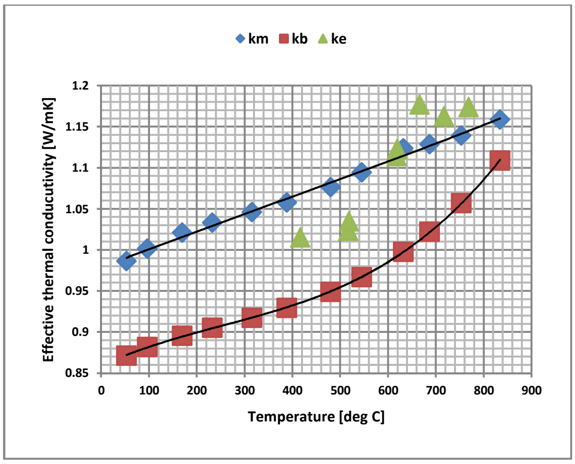

Figure 11. Comparison of theoretical kb, modelling km and experimental ke results

4. Discussion

It can be seen from the modelling and theoretical results of 2D pebble bed (with packing factor of 78.5%), 3D mono-sized (with packing factor of 52.3%) and 3D binary sized pebble bed (with packing factor of 65.8 %) that the packing fraction is an important design parameter for enhancing the value of effective thermal conductivity in pebble bed design of TBM. The theoretical results of effective thermal conductivity is obtained by using very simplified and regular calculation models so the theoretical results is limited for the reality model of pebble bed which will be always irregular and complex in geometry. Fig. 11 shows the modelling km results is different from experimentally ke results, this is possible because of the experimental ke results is always based on very complex and irregular geometrical arrangements of pebble bed while the modelling km results is obtained by using very simple and regular configuration of pebble bed. The other modes of heat transfer may also present in experimental ke results while modelling km results is obtained by using the steady state heat conduction equation only. Therefore, the better modelling work is required. These will be carried out in next work.

5. Conclusions

In this work, the effective thermal conductivity of Li_2TiO_3 pebble bed is obtained by theoretical calculations and modelling analysis approach. The approximate estimation of pebble bed thermal conductivity is possible by this work which will be very helpful to design an experimental test facility. This is a simple thermal conduction model with regular geometry of pebble bed, so the result gives preliminary and approximate response for the effective thermal conductivity of Li_2TiO_3 pebble bed. So, further work is needed.

6. References

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