MODEL FOR DETERMINING THE EFFECTIVE THERMAL CONDUCTIVITY OF PARTICLE BEDS WITH HIGH SOLID-TO-GAS THERMAL CONDUCTIVITY RATIO

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Abstract

A Be packed bed between the high temperature breeder and low temperature coolant has been proposed for an ITER solid breeder base blanket. A particularly attractive feature of such a design is the possibility of adjusting the solid breeder temperature through active control of the packed bed effective conductivity. Such control can potentially be achieved by varying the pressure or flow rate of the helium purge flowing through the Be packed bed. This paper describes a modeling effort directed at estimating the effective thermal conductivity of pebble beds with high solid-to-gas conductivity ratio (such as Be and He). The model has the capability of accounting for different particle sizes and surface contact characteristics, which are particularly important in determining the extent to which the bed effective thermal conductivity can be controlled through pressure variation for high ratios of solid-to-gas conductivity.

Introduction

A Be/He packed bed has been proposed as the mechanism to provide the required temperature drop between the breeder and coolant of a ceramic breeding blanket for ITER.[1] The breeder must be kept at a high temperature for adequate tritium release while the coolant is kept at low temperature based on safety and reliability considerations. One of the advantages of such a concept is the possibility of actively controlling the thermal resistance of the packed bed region through purge gas pressure, composition and/or flow rate changes. To better explore the performance of such a mechanism, experiments were performed for measuring the effective thermal conductivity, k_{eff}, of high conductivity metallic particle beds with both single-size and binary particle distributions under different gas pressures. The reference materials were Al to simulate Be and He. Copper and nitrogen were also included as alternate materials. The results of these experiments are summarized in Ref. [2].

In parallel with the experiments, a modeling effort was initiated to better understand the thermal behavior of particle beds with high solid-to-gas thermal conductivity ratios. This paper summarizes this modeling effort.

Model Features

In order to accurately model the thermal behavior of metal packed beds under conditions relevant to ITER, several key parameters must be included in the model.

(1) Sizes of particles: The gas conductivity is markedly affected by pressure changes in the Knudsen (molecular) region. The local characteristic dimension determining the gas conduction regime (i.e. molecular, regular or transition) varies in proportion to the particle size. It is expected that the effect of pressure changes on the effective thermal conductivity are more important for a packed bed with smaller particle sizes.

(2) Contact area between particles: The contact area between particles plays an increasingly important role in determining the heat flow path as the solid-to-gas conductivity ratio, k_s/k_g, increases. The combination of the contact area, nature of the contact and k_s/k_g value determines the fraction of the total heat transfer flowing through the contact. If this fraction is high, there is correspondingly only a small fraction of heat transferred through the gas and any change in the gas thermal conductivity through pressure variation would have a small effect on the overall packed bed effective thermal conductivity.

(3) Roughness characteristics: Both the roughness height and density are important in particular for characterizing the nature of the contact. Over the interfacial area, the roughness density determines the actual solid-to-solid contact with gas trapped in between the roughnesses over a thickness determined by the roughness height.

(4) Multiple-size mixtures: In order to achieve the packing fractions necessary for good breeding performance, binary or even tertnary size distributions are necessary. Thus, the model should also have the capability of accounting for single-size or multiple-size mixtures.

Note, however, that since the experimental metallic packed bed of Ref. [2] and the Be/He packed bed in an ITER ceramic blanket would operate at relatively low temperature, radiation effects are small and do not need to be incorporated in the k_{eff} model.

Two possible modeling approaches are the deterministic and statistical approaches. The deterministic approach assumes that the particle bed consists of a number of regular geometric configurations (or unit cells) and calculates k_{eff} based on that geometry. The statistical approach can be applied to random packed bed configurations, and the influence of various microstructural formations is treated statistically.

Based on the relatively good agreement of available deterministic models (e.g. [3] and [4]) with experimental data for different types of packed bed and on the ability of such models to account for gas pressure effects, a deterministic approach is chosen. For packed beds with a high k_s/k_g ratio, it is believed that the isotherms will be curved within the particles, in particular for cases with larger contact areas, which result in most of the heat flowing through the solids and contacts. In order to better account for the curvature of the isotherms, it is desirable that the model be at least two-dimensional which would require a computational approach because of the complexity of the 2-D solution.

Based on the above disucssion, a strategy was adopted to develop two models: a 1-D analytical zone model with a correction for 2-D effects, and a 2-D computational approach based on the progressive unit cell method of Ref. [5]. The 1-D model would be used for initial calculations and would provide a basis for future comparison between the 1-D and 2-D approaches.

In the 1-D model, the unit cell is defined by the number of contacts and the bed porosity. The unit cell is then divided into zones based on the gas conduction heat transfer mechanism (molecular, transition, regular) determined by the local Knudsen number. This results in a matrix of thermal resistances, which can be expressed in equation form and solved to obtain the effective thermal conductivity of the bed unit cell. The model is described in details in Ref. [6]. Benchmarking of the model with past experimental data was carried out satisfactorily using this model and is discussed in Ref. [7]. However, due mainly to space limitations, the remainder of the paper will cover only the 2-D model.

2-D Model

The 2-D model, described more fully in Ref. [8], assumes that the packed bed arrangement is essentially orthorhombic. Typically, a single-size packed bed has a porosity of 0.36 to 0.4 and the arrangement is about 80% orthorhombic (with a corresponding porosity of 0.395) on the average, with the rest being probably double nested, thus accounting for the lower porosities [9,2].

A 3-D othorhombic unit cell can be converted to a 2-D one, as shown in Fig. 1, by setting r_f so as to reproduce the desired porosity. In order to overcome the large temperature jump condition at the solid/gas interface, a spherical grid was used. The advantage of using a spherical grid is the ability to form a very fine mesh at the solid/gas interface and in the gas where large temperature drops occur and a coarse mesh in the solid where temperatures do not vary as much. The following 2-D heat condition equation in spherical coordinates was expressed in finite difference form and solved using a successive over-relaxation (SOR) scheme for given boundary conditions (adiabatic on each side of the unit cell due to symmetry and fixed temperatures T_1 and T_2 on the upper and lower boundary of the unit cell respectively).

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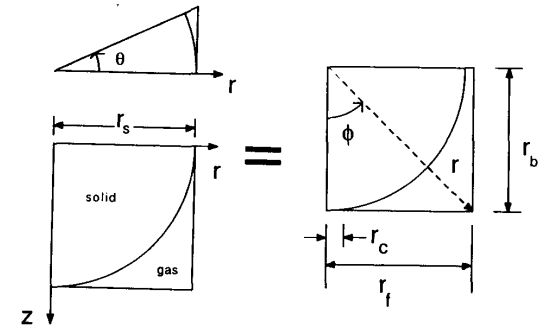


Fig. 1: Orthorhombic Unit Cell Rearrangement from 3-D (r, θ, z) to 2-D (r, ϕ)

$$\frac{\partial}{\partial r}\left(kr^2\frac{\partial T}{\partial r}\right)+\frac{1}{\sin\phi}\frac{\partial}{\partial\phi}\left(k\sin\phi\frac{\partial T}{\partial\phi}\right)=-qr^2 \qquad (1)$$

The thermal conductivity is specified at each node inside the grid. To account for pressure variation is the molecular regime, the gas conductivity was expressed as a function of the local characteristic dimension, accomodation coefficient and local gas mean free path.[10] Once the temperature field is obtained for the unit cell, the local heat flux, q_{uc} at the upper boundary is calculated from the local thermal conductivities and temperature gradients of the finite difference grid. Since the sides are adiabatic, the heat flux entering the unit cell at the upper boundary (at temperature T_2) must be the same as the heat flux leaving at the lower boundary (at temperature T_1). The effective thermal conductivity is then calculated from:

$$k_{eff} = q_{uc} r_b / A_{uc}(T_1 - T_2) \qquad (2)$$

where A_{uc} is the unit cell area.

Surface Roughness

The particles in a packed bed are not perfectly smooth. There will always be microscopic surface roughness whose characteristics depend on the porosity and manufacturing techniques. Previously developed models seldom account for these surface characteristics because of a lack of surface property data and difficulty in modeling. For the case of high k_s/k_g ratios, especially in the interfacial region (defined by r_c in Fig. 1), roughness effects on the heat transfer can be important. Roughness is incorporated in the model in a simple way based on Ref. [11]. Basically, surface roughnesses are modeled as cylindrical elements of radius, R_1, and height, δ, with a density of one roughness per cylindrical surface unit area corresponding to a radius R_2, as illustrated in Fig. 2. Thus, in effect actual contact occurs over a fraction $(R_1/R_2)^2$ of the interfacial area. The magnitudes of parameters R_1/R_2 and δ are estimated roughly from available particle surface examination data and are fine-tuned so as to best fit the experimental data.

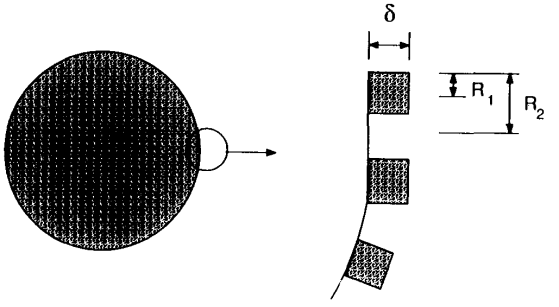


Fig. 2: Modeling of Surface Roughness

Binary Mixture

The modeling of a binary mixture is based on the progressive filling method of Ref. [5]. In this case the gas in Fig. 1 is replaced by the fine particle packing and the solid represents one of the large spheres. In the lower left corner, there is a void space between the two large spheres where the smaller particles cannot fit. This void space is determined by the diameter of the fine particles. Thus, there are effectively three regions, the large sphere which is pure solid, the void which is pure gas, and the fine particle region whose porosity is determined from the porosity of the single large particle bed, the binary bed porosity and the void area. The calculation proceeds by first estimating k_{eff} for the fine single-size mixture and then using this k_{eff} (fine) to determine the overall k_{eff} for the three-region binary mixture unit cell.

3-D Effect

To determine the effect of 3-D heat transfer, a fully 3-D orthorhombic unit cell, as shown on the left side of Fig. 1, was also modeled. The 3-D heat conduction equation in cylindrical coordinates was expressed in finite difference form and then solved using a SOR scheme for given boundary conditions (adiabatic at r = 0, r = r_s, θ = 0, and θ = 30°, fixed temperatures T_1 and T_2 at z = 0 and z = r_b).

Good agreement with available experimental data was obtained up to a ratio k_s/k_g of about 150. Beyond this, the temperature drop across the solid/gas interface becomes much larger than that in the solid creating computational difficulty. Solutions could only be obtained then for extremely fine, tailored grid, which would be expensive computationally and impractical for repeated calculations. At the same time, the nodal temperatures inside the 3-D unit cell for the lower values of k_s/k_g were virtually independent of the third dimension (θ), and k_{eff} results from the 3-D model were essentially the same as those from the 2-D model. Thus, since the solution appears to be sufficiently accurate with a 2-D model with much lower computational effort, the 2-D model has been adopted for most calculations.

Model Benchmarking

The 2-D model was benchmarked against data from a companion experiment[2] using Al/He beds, and also cross-checked with available data from the literature. Of all the different experimental data found in the literature, those of Swift cited in Ref. [12] correspond to k_s/k_g ratios closest to the ratios applicable for ITER. Swift's experimental data includes k_{eff} of single-size particle bed as a function of pressure for U/He (k_s/k_g = 170) and Ur/Ar (k_s/k_g = 1400).

Figures 3 and 4 show the effective thermal conductivity normalized to the gas standard thermal conductivity, k_{eff}/k_g, as a function of pressure for the U/He and U/Ar cases, respectively, obtained from the 2-D model. The average particle diameter, d, is 0.19 mm and the porosity 0.4. The model is seen to agree quite well with experimental data for R_1/R_2 = 0.25 and δ = 5 microns. These sets of numbers are not unreasonable since the roughness height is about 2.6% of the particle diameter while the resulting roughness area fraction of 6.25% is expected to be in this low range.[10] Note that the same values for R_1/R_2 and δ were used for both cases since the U powder is the same. The interfacial area $(r_c/r_s)^2$ is chosen to be 0.4 x 10^{-4} in both cases in order to obtain the best fit. An important observation, though, is the insensitivity of the results at higher pressures (>10^{-3}-10^{-2} atm) to this parameter as illustrated in Figures 3 and 4 by the results assuming zero contact area.

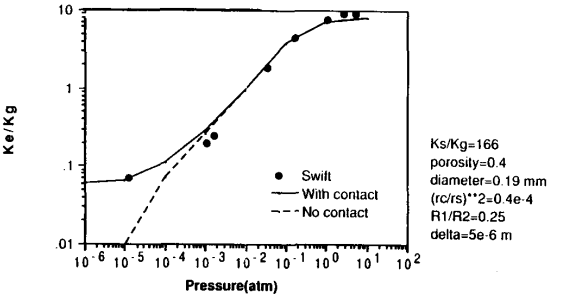
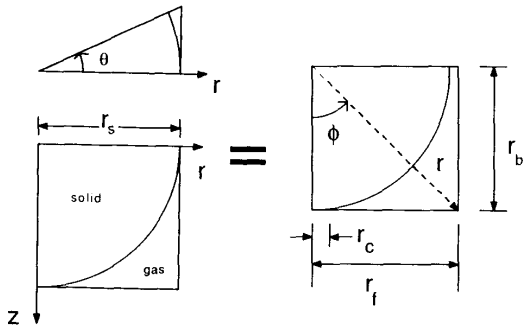


Fig. 3: U/He Packed Bed Effective Thermal Conductivity as a Function of Pressure



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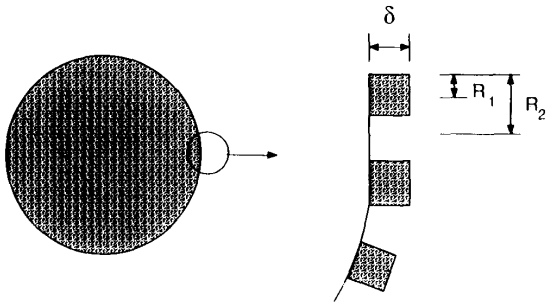

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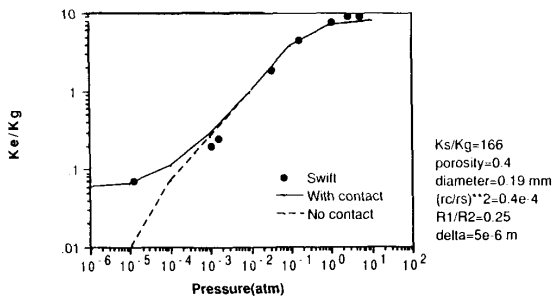

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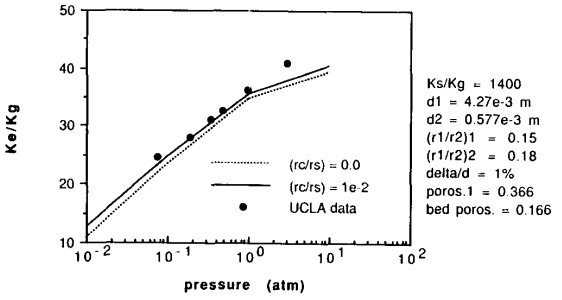

Fig. 8: Effective Thermal Conductivity of Al/He Binary Packed Bed as a Function of Pressure

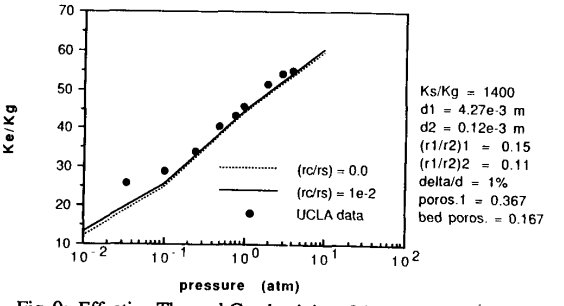

Fig. 9: Effective Thermal Conductivity of Al/He Binary Packed Bed as a Function of Pressure

Conclusion

A modeling effort for predicting the k_{eff} for single-size and binary packed beds with high conductivity for ITER gap conductance application has resulted in two models which could reasonably well reproduce experimental data: a 1-D zone model and a 2-D computational model. Key parameters affecting k_{eff} that were included in the modeling include the particle size, porosity, contact area and surface characteristics.

Analysis of experimental results using the 2-D model discussed in this paper, indicate that there is a threshold level for the contact area, dependent on k_s/k_g, above which the variation of k_{eff} with pressure is reduced.

For cases with k_s/k_g ratios of the order of 1000, the following observations can be made:

- For a typical R_1/R_2 value of 0.11, the k_{eff} variation with pressure in the range of 0.2 atm to 2 atm is not affected by the actual contact area for solid-to-solid interfacial radius of up to 2.5% of the particle radius.
- Such an interfacial area can only be produced by fully constrained thermal expansion of Be over a temperature rise of 800°C. Thus, for the low temperature and low fluence conditions of ITER (hence, negligible Be swelling), the expected contact area is not likely to significantly affect the controllability of a Be/He packed bed through pressure variation.

Acknowledgement

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References:

[1] A.R. Raffray, et al, "Tritium-Producing Blanket for Fusion Engineering Facility," Fusion Engineering and Design, 8 (1989), 101-107, North Holland, Amsterdam.

[2] M. S. Tillack, et al., "Experimental Study of the Effective Thermal Conductivity of a Packed Bed Temperature Control Mechanism for ITER Ceramic Breeder Blanket Design," to be presented at the IEEE 13th Symposium on Fusion Engineering, Knoxville, Tennessee, October 1989.

[3] D. Kunii and J.M. Smith, "Heat Transfer Characteristics of Porous Rocks," A.I. Ch. Journal, 6, (1960), 1,71.

[4] R.O.A. Hall and D.G. Martin, "The Thermal Conductivity of Powder Beds. A Model, Some Measurements on UO_2 Vibro-Compacted Microspheres, and their Correlation," Journal of Nuclear Materials, 101, (1981) 172-183, North Holland Publishing Company.

[5] M.J. Ades and K.I. Peddicord, "A Model for Effective Thermal Conductivity of Unrestructured Sphere-Pac Fuel," Nuclear Science and Engineering, 81, (1982), 540-550.

[6] Z. R. Gorbis, et al., "Zone Model for Packed Bed Effective Thermal Conductivity," UCLA-FNT-28, University of California, Los Angeles, October 1989.

[7] Z.R. Gorbis, et al., "Parametric Analysis of Packed Bed Effective Thermal Conductivity using Zone Model," UCLA-FNT-30, University of California, Los Angeles, November 1989.

[8] P. Adnani, et al., "Modeling of Effective Thermal Conductivity for a Packed Bed," UCLA-FNT-29, University of California, Los Angeles, November 1989.

[9] R.K. McGeary, "Mechanical Packing of Spherical Particles," Journal of the American Ceramic Society, 44, 10, P513, October 1961.

[10] A. Ullman, et al., "Thermal Accomodatin Coefficients of Inert Gasses on Stainless Steel and UO_2," Journal of Nuclear Materials, 51 (1974), 277-279, North Holland Publishing Company.

[11] D. R. Olander, "Fundamental Aspects of Nuclear Reactor Fuel Elements," Technical Information Center, Office of Public Affaira, Energy Research and Devleopment Administration, TID-26711-P1, 1976, P137.

[12] R. Bauer and E.U. Schliinder, "Effective Radial Thermal Conductivity of Packings in Gas Flow. Part II. Thermal Conductivity of the Packing Fraction without Gas Flow," International Chemical Engineering, 18 (April 1978) 2, 189.