Comparison of Interparticle Phase Morphology Characterization Methods Using Covariance- and Fitzgibbon-Based Analyses

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1. Introduction

The thermal performance of composite nuclear fuels is often governed not only by the intrinsic properties of the constituent phases, but also by the microstructural configuration at the microstructural scale. A high-conductivity phase frequently resides along particle boundaries, forming continuous networks that significantly affect heat conduction. To optimize such composites, it is crucial to characterize the morphology and alignment of these interparticle phases. For example, cermet fuels (Fig. 1a) [1], such as microcell fuel pellets (Fig. 1b) [2], consist of UO_2 granules encapsulated by a highly conductive metallic phase. Two key descriptors of these structures are the aspect ratio (AR) of the boundary region and the orientation angle of elongated features relative to the heat transfer direction, which in a reactor is typically radial. In previous studies, AR was defined as the ratio of the length parallel to the primary heat transfer direction to that perpendicular to it [3]. However, in real cross-sectional images, it is often difficult and confusing to apply this definition directly. This study therefore compares two representative approaches—the covariance-based method and the Fitzgibbon ellipse-fitting method—to assess their applicability and limitations.

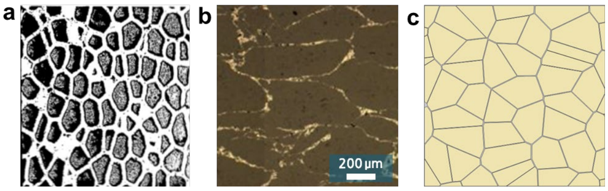

Figure 1. Cross-sectional images of (a) UO_2-W cermet [1], (b) UO_2-metal microcell pellet [2], and (c) schematic connective network structure generated by Voronoi diagram.

2. Methods

To present a representative composite microstructure, a set of seed points was randomly distributed within a two-dimensional domain. A Voronoi diagram was then performed, producing polygonal cells that represent granules (Fig. 1c). The boundaries of these polygons were regarded as the regions occupied by a high-conductivity interparticle phase, thereby mimicking the encapsulated structure observed in real composite fuels. The resulting Voronoi image served as the input data for morphological analysis. The geometry of each Voronoi polygon was analyzed using two different approaches: the covariance-based method and the Fitzgibbon ellipse-fitting method. In the covariance approach, the spatial coordinates of the polygon vertices (x_i, y_i) were used to construct the covariance matrix (Eq(1)).

$$C = \begin{bmatrix} \sigma_{xx} & \sigma_{xy} \\ \sigma_{xy} & \sigma_{yy} \end{bmatrix} \quad (1)$$

where σ_{xx} and σ_{yy} are the variances along the *x*- and *y*-directions, respectively, and σ_{xy} is the covariance between *x* and *y*. The eigenvalues λ_{max} and λ_{min} of *C* correspond to the variances along the principal axes. The shape factor (SF) was then defined as Eq (2)

$$SF = \sqrt{\frac{\lambda_{max}}{\lambda_{min}}} \quad (2)$$

and the orientation angle (θ) was determined from the eigenvector associated with λ_{max}. Here, θ represents the angle between the major axis of the polygon and the horizontal heat transfer direction.

In the Fitzgibbon method, an ellipse was fitted to the polygon boundary using a least-squares fitting algorithm. The fitted ellipse yielded the major axis length *a*, the minor axis length *b*, and the orientation angle θ. The SF in this case was calculated as Eq (3).

$$SF = \frac{a}{b} \quad (3)$$

The orientation angle (θ) was again measured as the angle of the major axis relative to the horizontal reference direction. Overall, these two methods provide complementary perspectives. The covariance approach emphasizes statistical robustness across ensembles of polygons, while the Fitzgibbon method provides a more intuitive geometric description of individual particle boundaries.

3. Results and Discussion

For the simulated UO_2–5 vol% Mo composite material represented by Voronoi polygons (Fig. 1c), the morphology was analyzed using the covariance-based method and the Fitzgibbon ellipse-fitting method. The average shape factor (SF) and average orientation angle were obtained, and the effective thermal conductivity of the structure was also evaluated using a finite element method (FEM) calculation [3]. Here, the average SF represents the mean ratio of the major to minor axes obtained from approximating each polygon with an ellipse, while the average orientation angle corresponds to the angle between the major axis and the x-direction (which, in practice, is the radial direction in the reactor).

A slight difference was observed between the two methods. The covariance-based method yielded an average SF of 2.41 and an average orientation angle of 44.12°, whereas the Fitzgibbon method gave 2.11 and 44.96°, respectively (Table 1).

In addition, the effective thermal conductivity was calculated using the thermal resistance circuit model [5], in which the average SF information and Mo content were used as input parameters (Fig. 2a). Since both FEM- and thermal resistance–based approaches are well-established and provide nearly identical results [5], the direct use of SF values derived from image analysis for conductivity prediction was found to overestimate the effective thermal conductivity. Specifically, predictions based on image-derived SF values resulted in an effective conductivity approximately 1 W/mK higher than FEM results, with a relative error approaching 20%. This confirms that directly using image-analyzed SF as AR is problematic. To incorporate the influence of orientation relative to the heat-transfer direction, the SF values were multiplied by the cosine of the measured orientation angle and treated as a changed AR (Table 1). Although this adjustment reduced the predicted conductivity compared with the unmodified SF case, significant discrepancies with FEM-calculated values remained (Fig. 2b).

Table 1. Morphological parameters obtained by the covariance-based method and the Fitzgibbon method

	Covariance-based method	Fitzgibbon method
Shape factor	2.41	2.11
Orientation angle	44.12°	44.96°
Changed aspect ratio	1.73	1.50

4. Conclusion

In this study, the morphology of interparticle phases in Voronoi-simulated UO_2–Mo composite structures was analyzed using two approaches, namely the covariance-based method and the Fitzgibbon ellipse-fitting method. Both methods provided reasonable evaluations of SF and orientation angle, although small differences were observed between them. The effective thermal conductivity of the composite was estimated using the thermal resistance circuit model [5] with input values derived from image analysis. Direct use of SF values obtained from morphological analysis led to an overestimation of effective conductivity, and the relative error reached nearly twenty percent when compared with FEM results. This finding demonstrates the limitation of applying SF directly as an aspect ratio descriptor in thermal transport modeling. To reduce this discrepancy, the orientation information was incorporated by multiplying the SF by the cosine of the orientation angle, which was treated as a changed AR. Although this adjustment lowered the difference relative to FEM predictions, a considerable deviation remained. The overall results suggest that accurate prediction of thermal conductivity in such composites requires a more refined descriptor that considers both particle morphology and directional alignment. The concept of a modified aspect ratio will be further investigated in future studies in order to establish a more consistent and physically meaningful measure for structure–property correlations in composite nuclear fuels.

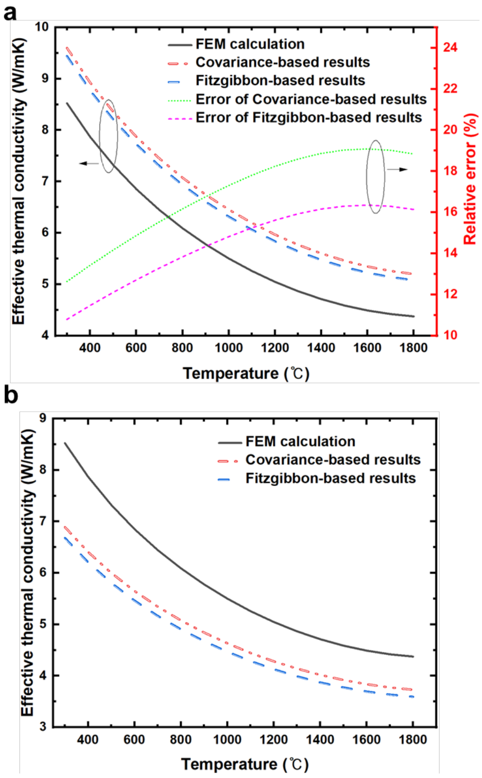

Figure 2. Comparison of effective thermal conductivity for simulated UO_2 – 5 vol% Mo composite materials using Voronoi polygons. Results of (a) based on SF value, and (b) based on the changed AR values.

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