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Comparative Analysis of Geometric Models for Predicting the Dynamic Specific Surface of Foamlike Media

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COMPARATIVE ANALYSIS OF GEOMETRIC MODELS FOR PREDICTING THE DYNAMIC SPECIFIC SURFACE OF FOAMLIKE MEDIA

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ABSTRACT
An adaptable geometric pore-scale model is proposed for predicting the specific surface area of actual foams. The proposed model, based on rectangular geometry, is compared to a cubic unit cell model from the literature based on cylindrical struts, a tetrakaidecahedron model as well as a dodecahedron model (both based on either cylindrical of triangular struts). The predicted specific surface areas of the proposed model are of the same order of magnitude as the other model predictions from the literature. The relative percentage errors in the predicted values are at most equal to the relative percentage errors associated with the measured diameter values. This is satisfactory, given the uncertainty in measuring the average pore-scale linear dimensions and also taking into consideration that the possibility of hollow struts, pore blockage and surface roughness are not accounted for in the model. The advantage of the proposed model is that only the solid width or the channel width needs to be known a priori to predict the specific surface area, and that it is physically adaptable.

INTRODUCTION
Specific surface areas of foamlike porous media are of special interest in the performance and design of reactors and/or heat exchangers which due to their high values enhance heat and mass transfer ([5]). The definition most widely used for the specific surface area of foam structures is the total external surface of the struts per bulk volume of foam subject to the assumption that the surfaces of the struts are perfectly smooth ([7, 8]). If the method of permeametry is used to obtain values for the dynamic specific surface, it cannot at the same time be employed to predict pressure drops, since it uses the latter values to determine the former. In this instance an independent method is required to provide values for the dynamic specific surface. In such a case one has to rely on direct measuring techniques (e.g. volume imaging techniques such as X-ray computer tomography and magnetic resonance imaging) or make use of theoretical correlations based on geometric models. This study will be attributed to a comparative analysis on the predictive capability of such analytical models based on various geometries available in the literature.

NOMENCLATURE
d	=	RUC cell size
d_s	=	Strut diameter
d_c	=	Cell diameter
d_p	=	Pore diameter
e	=	Analytical compression function
S_{fs}	=	Total fluid-solid interface in RUC
S_v	=	Specific surface area
U_o	=	Total RUC volume

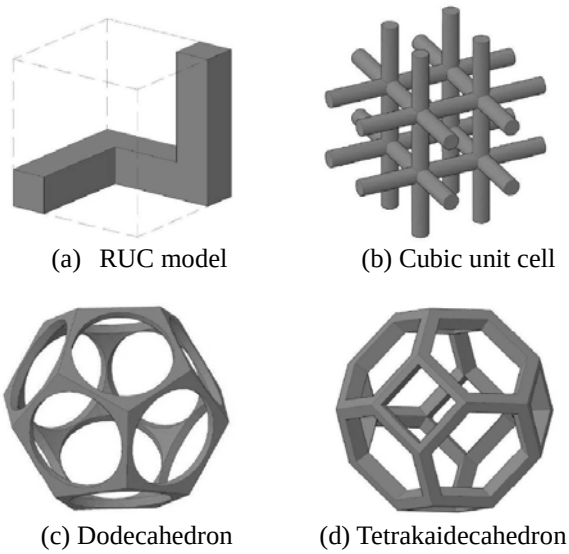
Greek Symbols

ϵ	=	Porosity
ψ	=	Geometric factor in RUC model

Subscripts

exp	=	Experimental
f	=	Fuid
s	=	Solid
$\parallel$	=	Parallel
$\perp$	=	Perpendicular

1 Existing geometric models
Four well recognized geometric pore-scale models used in the literature for approximating the intricate solid geometry of foamlike media, are the (i) representative unit cell (RUC) model (ii) cubic unit cell model (iii) pentagonal dodecahedron model and (iv) tetrakaideca-hedron model. Schematic representations of the models are shown in Fig. 1 (a) to (d), respectively. The shaded volumes represent the solid struts of the foam structure. The cubic unit cell model of [3] consists of a cubic unit cell with cylindrical struts on the edges. The dodecahedron model of [6] consists of 12 pentagonal faces with triangular struts (in the case of high porosity and cylindrical struts lower porosities. [6] represented this accumulation of solid material in the latter case by a tetrahedron. The tetrakaidecahedron model of [8] and [7]



(a) RUC model (b) Cubic unit cell

(c) Dodecahedron (d) Tetrakaidecahedron

Figure 1: Available geometric models

consists of 14 faces of which six faces are squares and the remaining eight hexagons. This paper provides a comparative study on the predictive capability of the relatively simple geometric RUC model as opposed to the more complex dodecahedron and tetrekaidecahedron geometries. The reason for this is that the simple rectangular geometry provides mathematical simplicity without the need to compromise for a loss in accuracy, as will be illustrated in this study. The physical adaptability of the model will also be outlined by presenting predictive equations for the specific surface area that accounts for anisotropy due to one-dimensional compression.

1.1 RUC model

The rectangular foam RUC model presented in Figure 1 was originally introduced by [2]. The shaded volumes represent the *average strut geometry* in the three-principle directions of a rectangular Cartesian coordinate system. The RUC should not be regarded as a building block of the exact geometry of a foam structure but rather an average representation of the porous structure.

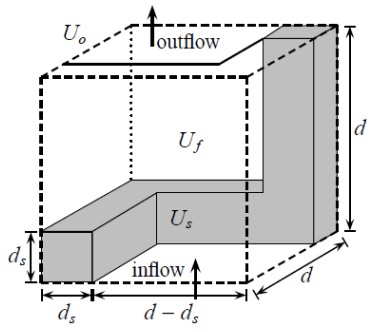


Figure 2: Foam RUC model

The specific surface area in terms of the pore diameter d_p=d-d_s is given by

$$S_v = \frac{S_{fs}}{U_o} = \frac{3(3-\psi)^2(\psi-1)}{2d_p}, \quad (1)$$

where S_{fs} is the total fluid-solid interface in the RUC model and U_o is the total volume of the RUC. The geometric factor ψ which is equal to the geometric tortuosity and a function of porosity ϵ is given by

$$\psi = 2 + 2\cos\left[\frac{4\pi}{3} + \frac{1}{3}\cos^{-1}(2\epsilon - 1)\right]. \quad (2)$$

2 Specific surface area predictions

Table 1 gives a number of analytical predictions and empirical correlations for specific surface areas of foams in terms of the strut diameter d_s and the pore diameter d_p. In RUC notation d=d_c. [6] proposed a slim and fat pentagonal dodecahedron model corresponding to high and low porosities, respectively. For both slim and fat dodecahedron models predictive equations are proposed for triangular and cylindrical struts. For all four model predictions of [6] given in Table 1 for the specific surface area, the parameter k is a second degree polynomial function. The latter polynomials are dependent on the porosity but cannot be expressed as explicit functions of porosity. For the low and high porosity model predictions for triangular and cylindrical struts, different second degree polynomials need to be solved to obtain the values of k corresponding to different porosity values. [7] made use of the tetrakaidehedron geometry to derive three correlations for the specific surface areas of ceramic foams for three different strut morphologies (cylindrical, triangular and triangular concave), depending on the porosity. They support the view of [6] that for porosities less than 0.9 the struts are cylindrical and for values greater than 0.9 the struts take on triangular prismatic or triangular concave geometries.

3 Model validation

Figure 3 shows the specific surface area S_v dimensionalized with the pore diameter, i.e. $S_v d_p$, as a function of porosity. The RUC model prediction is compared to the model predictions from the literature based on cylindrical strut geometry. The experimental data presented in Figure 3 are labelled as follows: □:[3], o:[8], △:[4], *:[5], ◁:[1] Figure 4, on the other hand, provides a comparison between the RUC model and the models involving triangular struts. The data of [4] presented in Figures 3 and 4 was obtained by application of the tetrakaidecahedron model. Measured mean strut diameters obtained through image analysis were used as input to the model. The data of [3] has also not been obtained through direct measurement. The mean strut diameter and porosity values were measured and the cubic unit cell geometry applied to predict the specific surface area. [8] observed an over-prediction by the

TABLE 1. Model predictions for the specific surface area of foams from the literature.

Specific surface area, S_v	Model description	Strut shape
[3]: $\frac{4(1-\epsilon)}{d_p\left[\frac{4}{3\pi}(1-\epsilon)\right]^{1/2}}$	Cubic unit cell	Cylindrical
[6] – low ϵ: $\frac{F}{d_p}\left[\frac{12\pi k(1-k/2\sqrt{2/3})}{\sqrt{5}\phi\sqrt{3-\phi}}+\frac{\sqrt{15}\left(1-k/2\sqrt{2/3}\right)^2 sin^2(\pi/5)}{2(3-\phi)}\right]$ with $\phi = 1.6180$ and $F=\left(1-{}^{k}/_{2}\sqrt{2/3}\right)/(\phi\sqrt{3-\phi})$	Dodecahedron	Triangular & Cylindrical
[6] – high ϵ: $\frac{F}{d_p\sqrt{5}\phi^2}60k\left(1-{}^{1}/_{2}\sqrt{{}^{2}/_{3}\,k}\right)$	Dodecahedron	Triangular
[6] – high ϵ: $\frac{F}{d_p\sqrt{5}\phi^2}20\pi k\left(1-{}^{1}/_{2}\sqrt{{}^{2}/_{3}\,k}\right)$	Dodecahedron	Cylindrical
[7]: $5.62\frac{\left[1-0.971\sqrt{1-\epsilon}\right]}{d_p\sqrt{1-\epsilon}}(1-\epsilon)$	Tetrakaidecahedron	Triangular
[7]: $4.867\frac{\left[1-0.971\sqrt{1-\epsilon}\right]}{d_p\sqrt{1-\epsilon}}(1-\epsilon)$	Tetrakaidecahedron	Cylindrical
[7]: $6.49\frac{\left[1-0.971\sqrt{1-\epsilon}\right]}{d_p\sqrt{1-\epsilon}}(1-\epsilon)$	Tetrakaidecahedron	Triangular concave

cubic unit cell model of [3], which is also evident in the lower porosity range (i.e. for ϵ <0.9) in Figure 3. For ϵ <0.9 the data in Figure 3 is more or less bounded by the RUC and tertrakaidecahedron models with the docedahedron model prediction lying in between. [8] attributed the over-prediction of the cubic unit cell model of [3] to (i) the uniform strut diameter assumed in the (ii) the accumulation of solid material at the intersection of struts which is not accounted for in the model and (iii) the influence of closed pores. It is unclear what the effect of uncertainty is in the measurement techniques employed to obtain the experimental data of [1] as well as the data shown in Figures 3 and 4, since, as already

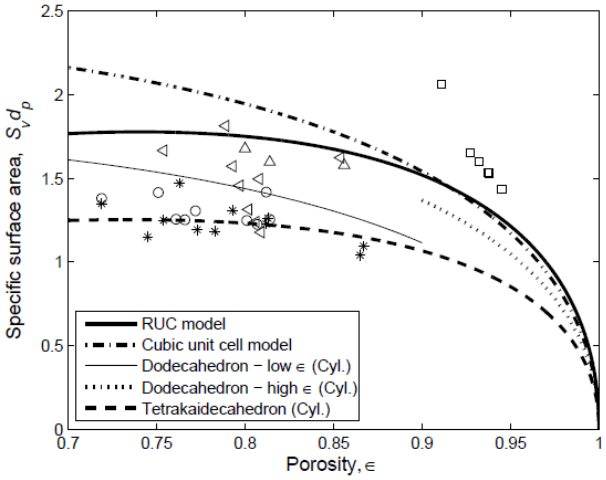


Figure 3: RUC model compared to models based on cylindrical geometry

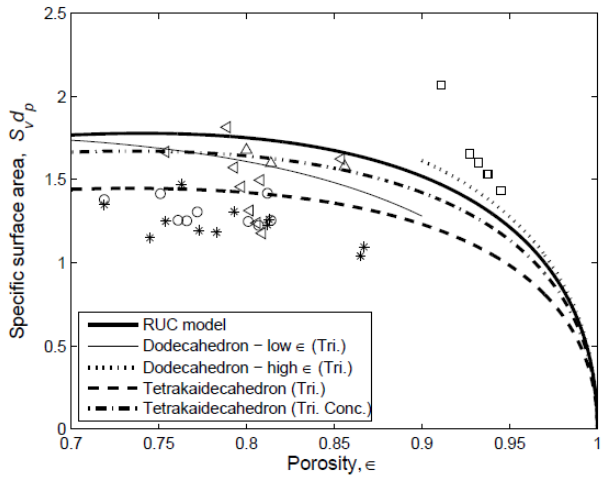


Figure 4: RUC model compared to models based on triangular geometry

mentioned, the measuring technique affects the accuracy of the experimental data. This should be kept in mind when evaluating the various models.

4 Effect of model geometry

[7] obtained the most accurate prediction with their analytical models (based on the tetrakaidecahedron geometry) compared to other analytical models. They state that their analytical models contain no empirical coefficients. On this basis of accuracy and no empiricism they conclude that the tetrakaidecahedron geometry represents the actual foam structure better than the cubic, Weaire-Phelan and pentagonal dodecahedron geometries. A few authors in the literature (e.g. [8]) are of opinion that the tetrakaidecahedron model geometry provides the best representation of open-cell foams. [6] found both the dodecahedron and tetrakaidecahedron models to be superior to the other model geometries.

[3] on the other hand, argues that the increased complexity of the tetrakaidecahedron model above that of the simple cubic unit cell is not worth the relative inaccuracy of its model predictions for the specific surface area. The same can be said about the simple RUC model. Based on an acceptable level of accuracy, simplicity and adaptive capabilities towards anisotropy, [3] chose to work with the cubic unit cell model. In Figure 5 the RUC model predictions are compared to the predictions for S_v based on the dodecahedron and tetrakaidecahedron model geometries. The absolute relative percentage difference is shown as a function of porosity.

It is evident from Figure 5 that the RUC model shows closer correspondence to the predictions based on triangular struts than cylindrical struts. The absolute relative percentage difference of the RUC model with respect to the dodecahedron and tetrakaidecahedron models based on triangular struts is less than 25.0%. The absolute relative percentage difference between the

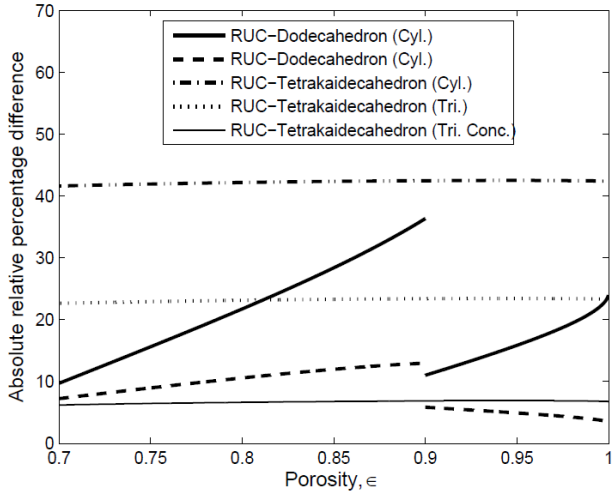


Figure 5: Percentage difference between RUC model and dodecahedron and tetrakaidecahedron models

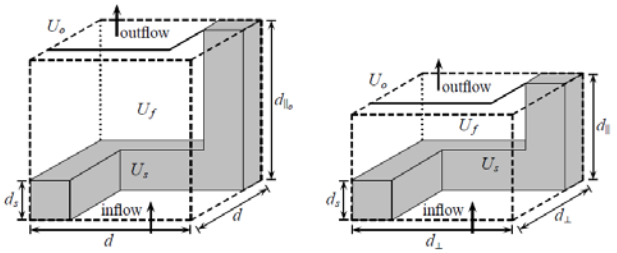
tetrakaidecahedron models based on cylindrical and triangular struts is 13.4%. The same percentage difference is obtained between the tetrakaidecahedron models based on triangular and triangular concave struts.The absolute relative percentage difference between the dodecahedron models based on cylindrical and triangular struts ranges between $15.1< \epsilon <22.1\%$ for high porosities (i.e $0.9< \epsilon <1.0$) and between $7.2< \epsilon <15.0\%$ for the lower porosities (i.e $0.7< \epsilon <0.9$). [8] report relative deviations for their measured pore size distribution ranging between 36% and 47%. These errors are manifested in the model predictions for the specific surface area. [9] reported deviations of up to 40% and that their mean projected pore diameter and cell size measurements deviated significantly from the values supplied by the manufacturer of the foams. [9] furthermore states that the latter measured values in addition depend on how the pore diameter is defined. The maximum relative percentage difference between the RUC and that of the dodecahedron and tetrakaidecahedron models (i.e. 43% according to Figure 5) is less than the measured relative pore size deviation of 47% given by [8]. In view of this, the question is now raised whether the increased complexity of the tetrakaidecahedron and dodecahedron models are worth the slight increase in accuracy and whether the relatively simple geometry of the cubic unit cell and RUC models are not sufficient for first order predictions of the specific surface area. The latter models in addition do not contain any empirical coefficients. In evaluating the different geometric models, the authors (e.g. [6, 7, 8]) assumed that the experimental data to which the models was compared is exact whereas in reality, as mentioned above and also in the Introduction section, the measured specific surface area values strongly depend on the measuring technique used. The average geometry of the RUC model is therefore regarded as sufficient in providing correct order-of-magnitude estimates for the specific surface area of various foam structures. In the next section it will furthermore be illustrated that the RUC model is physically adaptable to account for the effect of anisotropy on the predicted S_v-values.

5 Anisotropic RUC model

The anisotropic RUC model given in Figure 6(b) is used to investigate the effect of one-dimensional compression on the permeability of a foam. The streamwise strut is shortened to $d_{||}$ which introduced the anisotropy effect. The dimension of the RUC in both transverse directions is $d_{\perp}$. The anisotropic RUC model will be applied in this study to account for the effect of anisotropy on the specific surface area prediction. The specific surface area predicted by the anisotropic foam model is given by

$$S_v = \frac{8(d_{\perp}-d_s)d_s+4(d_{||}-d_s)d_s}{d_{\perp}^2 d_{||}}. \qquad (3)$$

Should experimental values for the compression ratio e_{exp} be provided as well as the corresponding ε values, the



(a) Isotropic model (b) anisotropic model

Figure 6: Anisotropic foam RUC model

pore-scale linear dimensions required to determine the specific surface area, i.e. $d_\perp$ and $d_{||}$ can be determined. The compression-porosity relationship is assumed to take on the following form e = C/(1- ϵ), where e is the analytical compression function. The coefficient C is determined by substituting the corresponding values for e_{exp} and ϵ into the latter equation, solving for C, and determining the average value. The RUC thickness in the streamwise direction can then be expressed as

$$d_{||} = d_{||_o} \mathrm{e}\,, \tag{4}$$

where $d_{||_o}$ is the short strut length in the uncompressed state, as indicated in Figure 6(a). In order to determine the value of $d_{||_o}$ measured mean hydraulic pore diameter values D_h should be provided and set equal to $d_\perp$-d_s which is the linear dimension of the cross-sectional area $(d_\perp$-$d_s)^2$ through which the fluid enters the RUC in the streamwise direction. From the expression for the porosity of the anisotropic model, i.e.

$$\epsilon = \frac{d_\perp^2 d_{||} - d_s^2(2d_\perp - 2d_s + d_{||})}{d_\perp^2 d_{||}}, \tag{5}$$

it then follows that

$$d_{||exp} = \frac{2d_s^2 D_h}{(D_h + d_s)^2(1-\epsilon) - d_s^2}\,. \tag{6}$$

By using Eq. (4) for $d_{||}$ in the relation: $d_{||_o} = d_{||exp}/\mathrm{e}_{exp}$ values for $d_{||_o}$ can be obtained for the different states of compression. The transverse RUC dimension $d_\perp$ can be obtained from Eq. (5), yielding

$$d_\perp = \frac{d_s\left(d_s + \sqrt{d_s^2 + (1-\epsilon)d_{||}(d_{||} - 2d_s)}\right)}{(1-\epsilon)d_{||}}. \tag{7}$$

Eqs. (4) and (7) should be used in Eq. (3) to predict the specific surface area of foamlike porous media. Eq. (3) can only be used should *all* the following values be available: e_{exp}, ϵ, D_h and d_s since they are required as input parameters to the model prediction. Experimental data on compressed foams containing all the latter values could not be found in the literature. As a result the anisotropic model could not be validated. Should these values be provided in future by authors in the literature, the model prediction for S_v presented by Eq. (3) can be evaluated.

CONCLUSIONS

There are several factors that influence the accuracy of experimental specific surface area data. A crucial factor that can have a significant effect on the specific surface area predictions is the assessment of the pore-scale linear dimensions, i.e. the pore diameter, strut diameter and cell size. The manufactured foams used as test samples may also contain imperfections such as hollow struts and pore blockage in the morphology of actual foams. Each measuring technique is subject to its own margin of uncertainty. Care should thus be taken when comparing different geometric models to such data due to the risk involved in drawing incorrect conclusions on the predictive capability of the models. The relative percentage errors in the predicted values were at most equal to the relative percentage errors associated with the measured diameter values. This is satisfactory in view of the uncertainties involved in the measured diameter values as well as the pore structure imperfections. The RUC model produced predicted specific surface values of the same order of magnitude as the actual foams and other analytical models. The model provides a first order approach but maintains a balance between accuracy and simplicity. The advantages of the RUC model is its simple rectangular geometry and that either the strut diameter or pore diameter needs to be known to predict the specific surface. The model also contains no empirical coefficients. It is furthermore illustrated that the model is physically adaptable to account for the effect of anisotropy in the specific surface area.

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