

A new method for accurate estimation of diatom biovolume and surface area

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INTRODUCTION

Micro algae biovolumes (BV) and surface areas (SA) are used in many ecological studies. Many water quality indices are based on micro algae biovolumes. Biovolumes are converted to concentration of organic carbon or chlorophyll a. Surface to volume ratio allows evaluating cell physiological status and estimating matter fluxes through cell walls.

The traditional approach to calculation of micro algae BV and SA is based on the approximation of cell shape by similar geometric figures (Hillebrand et al. 1999). The main drawback of this method is the discrepancy between figures and the real cell shape. Complex shaped micro algae are approximated by combinations of geometric figures. The more complex a cell is, the more figures should be included into the combination which complicates mathematical equations used for cell BV and SA estimates. Instead of geometric figures, we propose to use 3D-models that allow simulating complex micro algae with different degrees of accuracy.

3D modeling of many groups of micro algae (Dinoflagellates, Desmids) can be time-consuming; geometric figures remain the best alternative for them. Diatom shapes are simpler; their frustules are clear cut and can be easily imitated by 3D models. A technique for 3D diatom model construction has been described and the results of the comparison of the two methods (similar geometric shapes and 3D modeling) are being presented in the paper.

MATERIAL & METHODS

A 3D diatom model was constructed from digitized projections of a diatom cell (cell outline) in valvar, apical and transapical planes. Valvar and apical outlines were considered as pivots and were placed orthogonal to each other with the valvar-outline-plane corresponding to the xy-plane of a coordinate system and the apical-outline-plane to the orthogonal zx-plane. The pivot outlines were aligned as such that their centers were located in the coordinate system's origin. The transapical outline was placed orthogonal to the pivots. It was discretely moved along them and scaled as such that on every step its length and width fitted the breadths of pivot outlines in the current point. As a result, the 3D skeleton formed by the consequence of scaled transapical outlines (skeleton sections) was created.

To form 3D model, the skeleton was covered by 3D surface. Every adjacent section of the skeleton was connected by oriented triangles using the following algorithm. Let p_i , p_{i+1} were two neighbor points on one section and p_k , p_{k+1} were neighbor points on another one. They were linked by two oriented triangles consisting of points (p_i, p_k, p_{k+1}) and (p_i, p_{k+1}, p_{i+1}) . This operation was repeated for all points on every section. After the procedure finished, the created model had only two open ends – the first and the last sections, which were covered by a surface, using triangulation algorithm (O'Rourke 1994).

The 3D model surface area was calculated as the sum of all triangle areas. The model volume was the sum of the volumes of all triangular pyramids constructed in the following manner: the model triangles served as pyramid bases and an arbitrary selected point served

as the top for all pyramids. The pyramids volumes had a sign, therefore when they were summarized, superfluous ones were mutually annihilated and only the model volume remained. Triangular pyramid volume was calculated as

$$V_{pyramid} = \frac{1}{6} \begin{vmatrix} x_1 & y_1 & z_1 \\ x_2 & y_2 & z_2 \\ x_3 & y_3 & z_3 \end{vmatrix}, \quad (1)$$

where (x_k, y_k, z_k) were coordinates of vectors directed from pyramid top to pyramid base vertices; $||$ meant a determinant.

The constructed model simulates only those cells, which outlines had been digitized. To imitate cells with slightly different morphology (frustule proportions) the model should be deformed or reconstructed. The method for deformation of created 3D microalgae was proposed by Lyakh (2002). Another new approach is based on the reconstruction of 3D models from initial contours, which are fit to the studied cell outlines.

The model of cell contour consisted of joined cubic Bezier curves. The shape of cubic Bezier curve is determined by the positions of four control points P_0, \dots, P_3 (Bourke 1996):

$$Bz(t) = \sum_{k=0}^N \frac{N!}{k!(N-k)!} \cdot t^k \cdot (1-t)^{N-k} \cdot P_k, \quad 0 \leq t \leq 1. \quad (2)$$

The first and the last curve points were named *key-points*; the second and the third were *control points*. Two vectors directed from the first to the second and from the last to the third points were tangent vectors. The Bezier curve had some advantages over the other curves: (1) the local deformation of curve shape was fulfilled only by the displacement of control points; (2) to smoothly join two Bezier curves, their tangent vectors should be collinear in the point of connection.

Most diatoms have the shape of a cylinder. Their valves correspond to cylinder bases; girdles form cylinder lateral surfaces. For calculation BV and SA of those species, it is not a necessity to create 3D models, only the models of cell valves are needed. In this paper only those cylindrical diatom models are considered.

Modeled valves were divided into two or four equal sectors depending on their symmetry and only one sector of each valve was used for modeling. Key-points were located on those parts of the sector, whose sizes were changed during cell life-cycle. We did not consider small morphological changes in valve outline because they had no significant influence on the resulted volume and surface area. Key-points were connected by cubic Bezier curves that followed sector shape. Two control-points were linked with every key-point, so when a key-point was moved its linked control-points were also moved to the same distance that allowed to hold a curve shape.

Created sector was symmetrically mirrored to form the resulting valve model. Some of the corresponding key-points (the same on each mirrored sector) were grouped in dimensional pairs and linked by straight segments. The distance between key-points of one pair determined the size of a cell local part. When pair distance was changed, key-points and linked control-points moved which changed the shape of the adjacent Bezier curves and, consequently, the shape and size of a model part. To fit the model to a real cell, the distances between key-points should be set equal to the measured cell dimensions. Once created, the valve model can be used for many diatom species because of their similar shapes.

The volume V_{cyl} and surface area A_{cyl} of a diatom cylindrical model were calculated as:

$$\begin{aligned} V_{cyl} &= h \cdot A_{base}, \\ A_{cyl} &= 2 \cdot A_{base} + h \cdot P_{base}, \end{aligned} \quad (3)$$

where h – cell height; A_{base} – valve area; P_{base} – valve perimeter. To find A_{base} and P_{base} , smooth Bezier curves were transformed into closed polylines (polygons) consisting of points (x_i, y_i) . Their areas and perimeters were calculated by the following equations (Weisstein 2004):

$$P_{base} = \sum_{i=1}^{N-1} \sqrt{(x_{i+1} - x_i)^2 + (y_{i+1} - y_i)^2},$$

$$A_{base} = \frac{1}{2} \left| x_N y_1 - x_1 y_N + \sum_{i=1}^{N-1} (x_i y_{i+1} - x_{i+1} y_i) \right|. \quad (4)$$

As it is difficult to measure cell height (Agbeti 1997), in the comparison of the two methods we assumed that model's heights were equal.

Calculated model volumes and surface areas were compared with parameters of similar geometric shapes recommended for the studied species (Hillebrand et al. 1999). Differences between the two groups of results were found. When they did not exceed 5 %, we can say that the geometric shapes can be used for the cell approximation. When differences were between 5–15 %, we can say that geometric figures are only a rough approximation of diatom shapes and preferably 3D models should be used. When differences exceed 15 % the 3D models were considered as the best alternative for diatom BV and SA estimation. Model construction and all calculations were done with the software developed by the author (see www.3d-diatoms.awardspace.info for more information).

RESULTS

A parametric model of the valve of *Petroneis humerosa* (Bréb. ex W.Sm.) Stickle & D.G. Mann and *P. monilifera* (Cleve) Stickle & D.G.Mann was created from photographs and description published by Jones et al. (2005). Model shape and sizes were controlled by six parameters (Fig. 1): a – the breadth of central constriction; b – maximal valve breadth; c – rostrate pole breadth; e – rostrate pole length; l – length of valve without poles; w – full length of valve (not shown).

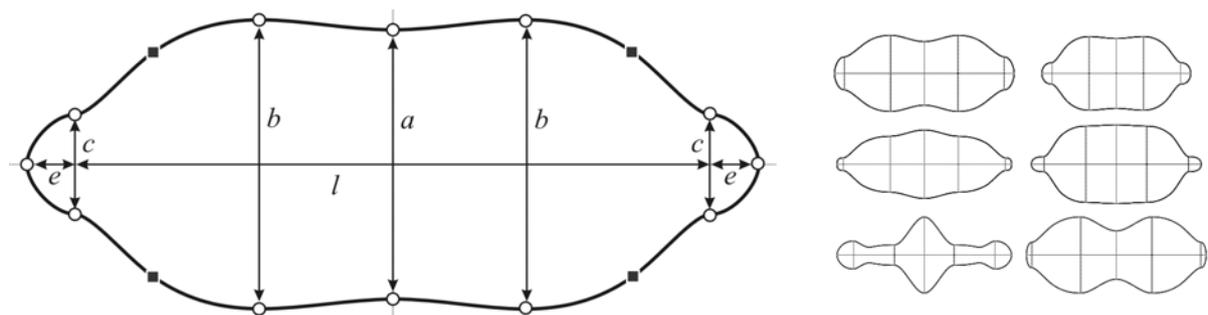


Fig. 1. The model of *Petroneis humerosa* valve. *Left.* The model of valve consists of cubic Bezier curves: white circles are key-points (control-points linked with them are not shown); arrows indicate dimensional pairs; black squares are key-points that do not group into pairs (they are used for a preserve model shape). *Right.* Valve outlines generated by means of dimension pair sizes changing.

The perimeter and area of the constructed model were compared to an ellipse that was recommended for the approximation of *Petroneis* (Hillebrand et al. 1999). Two tests were performed:

1. In the first test, l -parameter was decreased from $2b$ to b and a -parameter was decreased from b to $0.8b$. Results showed that the ellipse area exceeded the model area and the difference between them increased until 15 %, when both the length of valve without poles (l) and the valve middle breadth (a) were decreased (Table 1).

2. In the second test, the pole sizes (c and e) were decreased jointly with the l and a , proportionally to l . When l was equal to $2b$, c was equal to $b/3$ and e was equal to $b/6$. When l decreased to b , c decreased to $b/4$ and e decreased to $b/12$. Results showed the same as the previous test, but the differences between areas were lower (Table 1). In both tests, ellipse perimeter was lower than the model one, but the differences between perimeters were not exceeding 5 % and are not shown in the table.

Table 2. Results of two tests. The differences between ellipses and model areas are shown.

		$l = 2.0 b$	$l = 1.8 b$	$l = 1.6 b$	$l = 1.4 b$	$l = 1.2 b$	$l = 1.0 b$
Test 1	$a = 1.0 b$	1.1 %	2.2 %	3.5 %	5.2 %	7.3 %	10.3 %
	$a = 0.9 b$	3.6 %	4.5 %	5.8 %	7.5 %	9.6 %	12.5 %
	$a = 0.8 b$	6.1 %	7.2 %	8.5 %	10.2 %	12.4 %	15.4 %
Test 2	$a = 1.0 b$	1.1 %	1.6 %	2.0 %	2.4 %	2.9 %	3.3 %
	$a = 0.9 b$	3.6 %	4.0 %	4.5 %	4.9 %	5.4 %	5.9 %
	$a = 0.8 b$	6.1 %	6.6 %	7.1 %	7.5 %	8.0 %	8.5 %

In the second test, the size reduction of *P. humerosa* and *P. monilifera* during cell-cycle was simulated. When $a = 0.8b$, it means a deep central constriction, which is not typical for modeled species (Jones 2005); so, these results are presented only for comparison.

DISCUSSION

Constructed models can be used for simulating diatom species, because many of them have similar shapes. The results of comparing 3D models with similar geometric figures allow the division of diatom species into two groups – simple-shaped and complex-shaped. The first ones can be well approximated by geometric figures; the second only by 3D models. *P. humerosa* and *P. monilifera* can be placed in the group of simple-shaped species.

Besides the precise approximation of diatom shapes and the calculation of cell biovolumes and surface areas, the proposed models can also be used for imitating and studying cell cycles.

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