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A non-iterative mathematical description of three-dimensional bifurcation geometry for biofluid simulations

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ABSTRACT

We propose a mathematical model to describe the three-dimensional bifurcation geometry for airway flow simulations. The numerical scheme is explicit, non-iterative, and therefore stable and efficient. In addition, our model successfully reproduces the characteristic cross-sectional shape transition (from circular, to flattened elliptical, and then to 8-like shapes) across a bifurcation as observed in anatomical examinations. Several examples with various bifurcation parameters are presented, and these examples demonstrate the capacity and usefulness of our work in airway flow and transport simulations. The model developed here may also be useful for blood flow simulations and experimental model design.

1. Introduction

Bifurcations are the fundamental structure of the human and animal respiratory system, where an airway splits into two smaller daughter branches [1,2]. To investigate the complicated flow and transport processes in such bifurcation regions, numerical simulations have been proven to be useful [3–10]. Thanks to the advanced computational facilities and technologies, patient-specific calculations are possible with system geometry reconstructed from CT (Computed tomography) or MRI (magnetic resonance imaging) images [11,6,12,13]. However, information obtained from such simulations is limited to that particular situation. For general and fundamental studies aiming at a better understanding of the mechanisms and effects of various parameters on the flow and transport behaviors, an analytical description based on anatomical observations of these flow passages is more desirable [14]. While the straight segments between two consecutive bifurcations can be approximately considered as circular tubes, it is not a trivial task to construct a mathematical formulation for the three-dimensional (3D) bifurcation surface, which connects the parent and daughter branches smoothly.

Efforts in this direction can be traced back to the work by Gradon and Orlicki [15], where three types of rational functions were employed to describe a sequence of inter-penetrating cylindroids to construct the bifurcation geometry. In addition to the mathematical complexity, this model is limited to symmetric bifurcations, while asymmetric branching is very common in pulmonary architecture [2]. The *narrow* and *wide* models were then developed by Balashazy and Hofmann [16] to incorporate the branching asymmetry, where the carina is modeled as a sharp wedge and the side surfaces of the transition zone

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Nomenclature

D_{DL}	diameter of the straight part of the left branch
D_{DR}	diameter of the straight part of the right branch
D_P	diameter of the parent airway
L_{DL}	length of the straight part of the left branch
L_{DR}	length of the straight part of the right branch
L_P	length of the parent airway
R_L	local tube radius along the left branch
R_L^*	curvature radius of the left branch
R_{LR}	local tube radius along the transition arc between two branches
R_{LR}^*	curvature radius of the transition arc between two branches
R_R	local tube radius along the right branch
R_R^*	curvature radius of the right branch
r_c	carinal curvature radius
s_L	curvilinear coordinate along the left branch axis
s_{LR}	curvilinear coordinate along the transition arc between two branches
s_R	curvilinear coordinate along the right branch axis
w_L	weight factor to the left branch axis
w_{LR}	weight factor to the transition arc between two branches
w_R	weight factor to the right branch axis
δ	cut-off value for the surface height calculation at central zone corners
ϵ	gradient transition function
ϵ_0'	spatial gradient of local tube radius at the intersection point of the left branch axis and the transition arc
ϵ_1'	spatial gradient of local tube radius at the intersection point of the right branch axis and the transition arc
σ	sigmoidal transition function
Φ_L	left branching angle
Φ_R	right branching angle
ϕ_L	left sagittal angle
ϕ_L^c	left sagittal angle where the branch diameter becomes constant
ϕ_L^*	left sagittal angle where the branch separates from the bifurcation
ϕ_{LR}	sagittal angle along the transition arc between two branches
ϕ_R	right sagittal angle
ϕ_R^c	right sagittal angle where the branch diameter becomes constant
ϕ_R^*	right sagittal angle where the branch separates from the bifurcation

are not smooth either. In 1995, Heistracher and Hofmann proposed to describe the carinal region with rounding circles to smoothly connect the two daughter branches [17]. As noticed later by Hegedus et al. [14], the mathematical descriptions in Ref. [17] were rather sketchy and the two-parameter iteration is numerically sensitive and hard to reproduce. They therefore improved this rounding-circle approach with more rigorous formulations for the carinal region, and the problematic two-parameter iteration was replaced by a one-parameter root-finding process. Even with this improvement, numerical instability may still be encountered in the carina rounding process, depending on the control geometric parameters and the transition functions utilized [14]. To avoid the numerical difficulty associated with the rounding-circle approach, which works in planes parallel to the bifurcation plane (the plane where the axes of the parent and daughter branches lie), Lee et al. [18] suggested to construct the bifurcation shape in the vertical cross-sections perpendicular to the bifurcation plane. In place of the iteration or root-finding process in the rounding-circle methods [17,14], a six-order polynomial fitting is necessary to smoothly connect the branch circular arcs across the bifurcation [18]. Such a high-order polynomial fitting is still iterative and sensitive to initial guess of the coefficients, and could be computationally unstable. A nonlinear equation also needs to be solved to determine the separating line (called the boundary curve there) location. Although this method might be attractive for highly asymmetric bifurcations, the symmetric bifurcation from this model has a deep indentation groove up to the very parental end (see Figs. 8a and 10a in Ref. [18]). This is different from the physiological observations, which indicate that the transition section consists of two regions: an elliptical region where the circular parent tube gradually changes to an elliptical shape with flattened top and bottom sides; and the carinal region where two indentations appear and grow in the middle of the top and bottom surfaces, leading to an 8-like cross-sectional shape and eventually two separate circles [2,19,17]. A similar problem also exists with the rounding-circle methods due to the non-zero rounding radius near the parental end.

In this paper, other than constructing the two-dimensional cross-sectional shapes in planes parallel [17,14] or perpendicular [18] to the bifurcation plane, we look the transition region as a 3D surface, and propose an explicit, robust, and non-iterative mathematical description for the bifurcation geometry. No iteration process of root-finding or nonlinear fitting is