Optimum Bifurcating-Tube Tree for Gas Transport

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This paper describes optimality principles for the design of an engineering bifurcating-tube tree consisting of the convection and diffusion zones to attain the most effective gas transport. An optimality principle is formulated for the diffusion zone to maximize the total diffusion mass-transfer rate of gas across tube walls under a constant total-volume constraint. This optimality principle produces a new diameter distribution for the diffusion zone in contrast to the classical distribution for the convection zone. In addition. this paper gives a length distribution for an engineering tree based on an optimality principle for minimizing the total weight of the tree under constraints of a finite surface and elastic criteria for structural stability. Furthermore, the optimum branching angles are evaluated based on local optimality principles for a single bifurcating-tube branch. [DOI: 10.1115/1.1899168]

Introduction

A biological respiratory system for gas transport can be considered as a bifurcating-tube tree (bronchial tree) consisting of a number of branching generations of tubes [1,2]. Hence, a bifurcating-tube tree can served as a biologically inspired model for gas transport in engineering applications. Here, we want to devise an engineering bifurcating-tube tree for the most effective gas transport based on optimality principles and scaling analyses. As shown in Fig. 1, the diameter, length, and wall thickness of a bifurcating tube are three basic metric quantities, and the branching angle is an angular quantity characterizing the geometric structure of a bifurcating-tube tree. Since trees are not necessarily planar to avoid intersection with each other, another parameter is the azimuthal rotational angle of a tube branch relative to the preceding branch. The biggest tube is designated as the generation 0. The successive left and right branches are designated as the first generation, and so on. Therefore, the total number of tubes in the nth generation is 2^n. Consider an engineering bifurcating-tube tree in which tubes are circular and tree bifurcation is symmetrical, and steady flow through it is driven by a constant pressure difference between the generation 0 and the end generation (unlike periodic flow in bronchial trees). An engineering tube tree is distinctly divided into the convection and diffusion zones. Tubes are bigger in the convection zone where the generation number is lower than a critical value for division. Since the Péclet number is large, the dominant physical process is convection while diffusion is negligible. For simplicity, it is assumed that tube walls in the convection zone are impermeable. As the generation number exceeds a certain critical value for division, diffusion becomes a dominant physical mechanism in the diffusion zone (higher generations) where tubes are fine and highly permeable. Separation of a tree into two distinct zones where different physical mechanisms prevail is convenient for an engineering analysis. The critical number for division between the two zones depends on the Péclet number indicating the relative importance of convection to diffusion. The core problem is to determine the diameter, length, wall thickness, and branching angle of tubes as a function of the generation number.

Strikingly, a diameter distribution in the convection zone has been obtained based on simple optimality principles without considering hydrodynamic details [3–9]. An optimality principle for the minimum power gives a classical diameter-generation relation [3]

$$d_n \propto 2^{-n/3}, \tag{1}$$

where d_n is the tube diameter in the nth generation and n is the generation number. This result has also been derived based on similar optimality principles for the minimum volume [4], minimum entropy production [7], and minimum resistance [10–12]. In fact, Eq. (1) is an asymptotic distribution in the convection zone where resistance (entropy production or work) is a legitimate target for minimization. Naturally, a question is whether we can derive another asymptotic distribution of the diameter in the diffusion zone based on appropriate optimality principles.

The objective of this work is to formulate appropriate optimality principles for designing an engineering bifurcating-tube tree for gas transport rather than providing a teleological explanation for the architecture of bronchial trees. Based on these optimality principles, we deduce a diameter distribution for the diffusion zone of a tube tree and a length distribution for the entire tree. Moreover, the optimum branching angles are determined for both the convection and diffusion zones.

Diameter Distribution and Maximum Gas Diffusion

An optimality principle for the diffusion zone of an engineering bifurcating-tube tree is formulated based on scaling analyses of surface, volume, and gas concentration. We consider the ad hoc solutions $d_n \propto 2^{-pn}$ and $l_n \propto 2^{-qn}$ for the diameter and length, respectively, and $V_n \propto 2^{\beta n}$ for the total volume of the nth generation, where the parameter β is defined as $\beta = 1-2p-q$. Clearly, the main task is to determine the parameters p and q.

For thin and permeable tube walls in the diffusion zone, according to Fick's law, the diffusion mass-transfer rate of gas from the inside to the outside of tubes in the nth generation is

$$\dot{m}_n = D_{diff}(A_{eff})_n \Delta C_n / h_n, \tag{2}$$

where D_{diff} is the gas diffusion coefficient of wall material, h_n is the wall thickness, $(A_{eff})_n$ is the effective diffusion area, ΔC_n is a change in the gas concentration across a tube wall, and the subscript n denotes the nth generation. For simplicity, it is assumed that the gas concentration outside tubes is zero; i.e., $\Delta C_n = C_n$. Generally, to consider nonhomogeneous diffusion surfaces, the effective diffusion area is expressed as a power-law function of the total surface of tubes, i.e., $(A_{eff})_n \propto A_n{}^{\alpha}$, where A_n is the total surface area in the nth generation. The positive exponent $\alpha = A_n (A_{eff})_n^{-1} [d(A_{eff})_n / dn]/(dA_n/dn)$ represents the increasing rate

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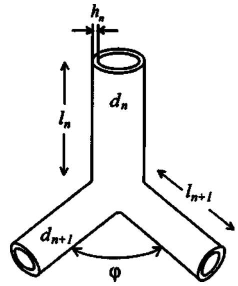

Fig. 1 Geometry of tube bifurcation

of the effective diffusion area relative to that of the total surface area in the nth generation. For homogeneous permeable surfaces, the exponent is simply $\alpha=1$.

In addition. we generally consider the fractal surface of tubes; hence, an area-volume relation is $A_n \propto V_n^{D_2/3}$ [13], where D_2 is the fractal dimension of the surface of tubes and V_n is the total volume of tubes in the nth generation. The non-fractal surface is treated as a special case of $D_2=2$. Therefore, the effective diffusion area is $(A_{eff})_n \propto V_n^{\alpha D_2/3}$. According to structural stability criteria for a tube described in the subsequent section, the tube wall thickness should be proportional to the tube diameter; i.e., $h_n \propto d_n$. Furthermore, using a length distribution $l_n \propto 2^{-n/4}(q=1/4)$ derived in the subsequent section, we have a relation between the total volume V_n of tubes in the nth generation and the wall thickness h_n; i.e., $V_n \propto 2^n d_n^2 l_n \propto 2^{3n/4} d_n^2 \propto 2^{3n/4} h_n^2$.

Using the estimates $(A_{eff})_n \propto V_n^{\alpha D_2/3}, h_n \propto 2^{-3n/8} V_n^{1/2}$, and $C_n \propto V_n^{-\gamma}$ given in Appendix A for the concentration distribution, we have a power-law relation between the total diffusion mass-transfer rate and the total volume of tubes in the nth generation

$$\dot{m}_n = B_1 2^{3n/8} V_n^{1/s}, \tag{3}$$

where the parameter s is defined as $s=(\alpha D_2/3-\gamma-1/2)^{-1}$ and B_1 is a positive proportional constant. Setting $x_n=V_n^{1/s}$, we have the total diffusion mass-transfer rate of gas across tube walls in the diffusion zone

$$\dot{m}_T = \sum \dot{m}_n = \sum w_n x_n, \tag{4}$$

where the weight coefficients are $w_n=B_1 2^{3n/8}$. Thus, an optimization problem is to maximize the cost function $\dot{m}_T$ subjected by a total volume constraint

$$\sum V_n = \sum x_n^s = B_2, \tag{5}$$

where B_2 is a positive constant.

As shown in Appendix B, for $s>1$, there is an optimum solution to maximize the total mass-transfer rate $\dot{m}_T$ in the diffusion zone

$$(V_n)_{op}^{1/s} = B_2^{1/s} w_n^{1/(s-1)} \left(\sum w_n^{s/(s-1)}\right)^{-1/s}. \tag{6}$$

Substitution of Eq. (6) into Eq. (3) gives an optimum solution for $\dot{m}_n$

$$(\dot{m}_n)_{op} = B_1 B_2^{1/s} 2^{3n/8} w_n^{1/(s-1)} \left(\sum w_n^{s/(s-1)}\right)^{-1/s}. \tag{7}$$

Because of $\dot{m}_n=(\dot{m}_n)_{op}$ at the optimum state, we know the consequences of $s \to +\infty$ and $\gamma=\alpha D_2/3-1/2$. For $s \to +\infty$, the condition $s>1$ for the maximum value is always satisfied. Therefore, at the optimum state, the total volume of tubes in the nth generation is $(V_n)_{op} \propto 2^{3n/8}$. Using the relation $V_n \propto 2^n d_n^2 l_n \propto 2^{3n/4} d_n^2$, we obtain a diameter distribution at the optimum state for the diffusion zone

$$d_n \propto 2^{-3n/16}. \tag{8}$$

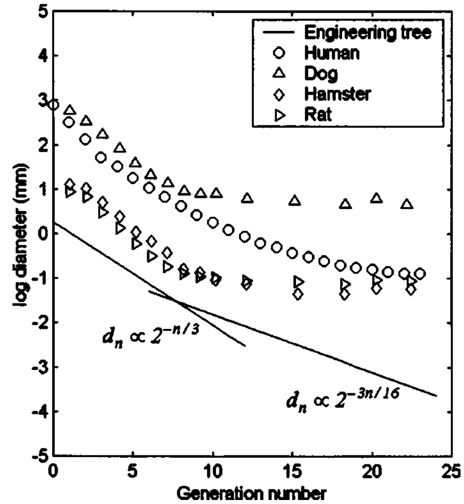

Fig. 2 The theoretical diameter distributions for an engineering bifurcating-tube tree along with measured data for bronchial trees

Interestingly, this result does not depend on the intermediate parameters introduced in the analyses. Figure 2 show the diameter distributions $d_n \propto 2^{-n/3}$ for the convection zone and $d_n \propto 2^{-3n/16}$ for the diffusion zone in an engineering tree along with measured data for the bronchial trees of human, dog, hamster, and rat [2,8]. Obviously, unlike the human's bronchial tree, the bronchial trees of dog, hamster, and rat do not follow the theoretical distribution for the diffusion zone in an optimal engineering tree.

We should examine the underlying assumptions made in the above analyses. First, we assume the ad hoc exponential distributions for the diameter and length ($d_n \propto 2^{-pn}$ and $l_n \propto 2^{-qn}$) in the diffusion zone. From a viewpoint of engineering design, these distributions enjoy simplicity that makes analytical solutions possible. However, we cannot exclude the existence of more complicated solutions for the same optimization problems; therefore, the uniqueness problem of solution is worth further investigation. In Appendix A, to estimate the concentration distribution, a bifurcating-tube tree is considered as a discrete system in which the cross-section-area-averaged concentration is constant in each generation. Further, using an approximation $C_n \approx (C_{n-1}+C_{n+1})/2$, we find that the diffusion mass-transfer fluxes into and out a tube along the axial direction are approximately equal; i.e., $\Delta f_{n,ax} \approx 0$. These results are reasonable as first-order approximations. A power-law estimate $C_n \propto V_n^{-\gamma}$ for the gas concentration in the diffusion zone is another major approximation (see Appendix A). This is based on an exponential function approximation for the asymptotic behavior of a complicated product function in higher generations ($n \in [0.5N, N]$). The fitting error is typically 1–4% in a semi-log plot.

Length Distribution, Minimum Weight, and Structural Stability

From the viewpoint of structural mechanics, a bifurcating-tube tree can be modeled as an elastic tree on which a single segment is idealized as an elastic tube. Similar to McMahon's analysis of a botanical tree [14], we suppose that an elastic tube must satisfy two necessary elastic criteria to form a stable tree structure under the gravitational force. One criterion is that a tube should be stable when its outer wall is pressed by a certain amount of force. This requires the wall thickness h of a tube proportional to the tube diameter d, i.e., $h \propto d$, where the prefactor is related to the critical pressure [15]. Another criterion is that a cantilever tube on a tree cannot exceed a critical length beyond which the tube no longer extends further due to the bending force by its own weight. The

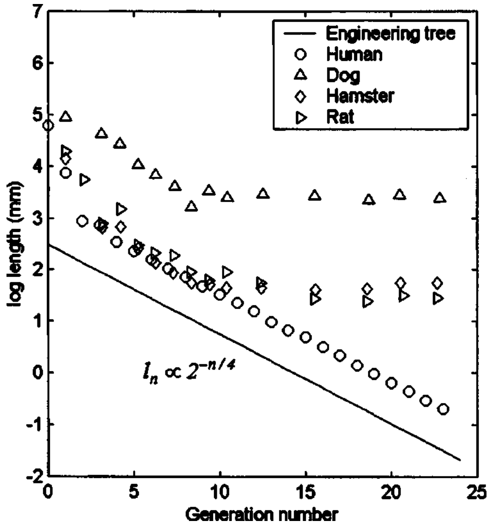

Fig. 3 The theoretical length distribution for an engineering bifurcating-tube tree along with measured data for bronchial trees

critical length for bending obeys a power-law relation $l_{cr} \propto h^{2/3}$ [14]. If tubes in a tree tend to achieve the maximum length to occupy as large space as possible, a combination of these criteria leads to a length-diameter relation for a single tube $l \propto l_{cr} \propto h^{2/3} \propto d^{2/3}$. Furthermore, since the weight of a single tube is $W \propto ld^2$, a length-weight relation for a single tube is $l \propto W^{1/4}$, which is valid for tubes in all the generations.

An appropriate optimization problem is to minimize the total weight of a tree

$$W_T = \sum (W_T)_n, \tag{9}$$

while the total surface area remains constant, where $(W_T)_n$ is the net weight of tubes in the nth generation. According to a area-weight relation $A_n \propto V_n^{D_2/3} \propto (W_T)_n^{D_2/3}$, the total surface constraint can be written as

$$\sum (W_T)_n^{D_2/3} = \text{const}, \tag{10}$$

where D_2 is the fractal dimension of the surface. This weight minimization problem is the same max-min problem discussed in B. Because of $D_2/3 < 1$, there is an optimum solution to minimize the total weight W_T, i.e.,

$$[(W_T)_n]_{op} = 2^n W_n = \text{const} \tag{11}$$

where W_n is the weight of a single tube in the nth generation. Combination of Eq. (11) with a length-weight relation $l_n \propto W_n^{1/4}$ for structural stability yields a length distribution for a bifurcating-tube tree

$$l_n \propto 2^{-n/4}. \tag{12}$$

Figure 3 show a length distribution $l_n \propto 2^{-n/4}$ for an engineering tree along with measured data for bronchial trees (human, dog, hamster, and rat) [2,8]. Equation (12) is in good agreement with data for the human branchial tree, but deviates significantly from data for dog, hamster, and rat.

Branching Angles

An optimization problem for the branching angle φ is generally formulated for a single bifurcation branch [16–18]; in this sense, the optimum branching angle can be determined independently when the diameter distribution is given a priori. In a study of arterial branching geometry, Zamir [16] proposed four local optimality principles that minimize surface, volume, power, and drag, respectively. For a symmetrical bifurcation, the optimum branching angles given by the four principles are, respectively,

$$\cos(\varphi) = R_A^{-1} - 1, \quad (\text{min. surface}), \tag{13}$$

$$\cos(\varphi) = 2R_A^{-2} - 1, \quad (\text{min. volume}), \tag{14}$$

$$\cos(\varphi) = R_A^{4}/2 - 1, \quad (\text{min. power}), \tag{15}$$

$$\cos(\varphi) = R_A^{2}/2 - 1, \quad (\text{min. drag}), \tag{16}$$

where $R_A = 2d_{n+1}^2/d_n^2$ is a ratio of the total cross-sectional areas between successive generations. In the convection zone ($d_n \propto 2^{-n/3}$ and $R_A \approx 1.26$) where all the four principles are plausible, Eqs. (13) and (16) predict the same optimum branching angle $\varphi \approx 102°$, while both Eqs. (14) and (15) give $\varphi \approx 75°$. For simplicity of design, a single branching angle, such as the average value of the branching angles $\varphi \approx (75° + 102°)/2 \approx 89°$, could be used for the convection zone in an engineering bifurcating-tube tree.

For the diffusion zone in which gas diffusion is the dominant physical process, three of the four principles can be excluded. The optimality principles for the minimum power and drag are not strong constraints for the diffusion zone where the Reynolds number (as well as the Péclet number) is small. In addition, the optimality principle for the minimum surface is clearly inapplicable to the diffusion zone where the total mass-transfer rate of gas across tube surfaces should be maximized. Hence, the optimality principle for the minimum volume is the remaining one that seems plausible; in the diffusion zone ($d_n \propto 2^{-3n/16}$ and $R_A \approx 1.54$), the optimum branching angle given by Eq. (14) is $\varphi \approx 99°$.

At the branching angle of 89°, tree branches may intersect with each other after some bifurcations if a tree is strictly two dimensional. Therefore, to avoid such intersections, a tree must be constructed in three-dimensional space by choosing a suitable distribution of the azimuthal rotational angle of a branch with respect to the preceding branch. Since no physical mechanism constrains the azimuthal angle, the determination of a distribution of this angle in a tree can be considered as a pure geometric problem to construct the most compact tree without intersections. This nontrivial problem will be investigated in the future.

Conclusions

A biologically inspired engineering bifurcating-tube tree, which is divided into the convection and diffusion zones, is designed based on the proposed optimality principles to achieve the most effective gas transport. In the convection zone, the classical diameter distribution $d_n \propto 2^{-n/3}$ holds for minimizing the energy expenditure of gas transport. In the diffusion zone, the diameter distribution $d_n \propto 2^{-3n/16}$ is derived based on the optimality principle for maximizing the total diffusion mass-transfer rate of gas across tube walls under a constant total-volume constraint. In addition, the length distribution $l_n \propto 2^{-n/4}$ is given for the whole tree based on the optimality principle for minimizing the total weight of a tree under a constant total-surface constraint while the elastic criteria for structural stability are satisfied. The estimated optimum branching angles for the convection and diffusion zones are *89°* and *99°*, respectively.

Appendix A: Gas Concentration in Bifurcating-Tube Tree

To estimate the gas concentration C_n in the nth generation, we consider an ideal cascade process in which a bulk of gas mass sequentially distributes from a lower generation into a higher generation of tubes. From the continuity equation $\nabla \cdot \boldsymbol{u} = 0$ for steady incompressible flow, we give a relation for the cross-section-area-averaged axial velocity u_n in the nth generation

$$u_n/u_0 = 2^{-n}(d_0/d_n)^2, \quad \text{(A1)}$$

where d_n denotes the tube diameter in the nth generation. Integrating the mass-transfer equation $\nabla\cdot(\boldsymbol{u}C) = -\nabla\cdot\boldsymbol{f}$ over a volume of a tube in the nth generation, and applying Gauss theorem and a zero-normal-velocity condition on the periphery wall, we obtain the diffusion mass-transfer flux across the periphery wall for a single tube

$$f_{n,peri} = (d_n/4l_n)\{u_n(C_{n-1} - C_{n+1}) + \Delta f_{n,ax}\}, \quad \text{(A2)}$$

where $\Delta f_{n,ax}$ is a difference between the diffusion mass-transfer fluxes into and out a tube along the axial direction. Here, the flux $\boldsymbol{f} = -D_{diff}\nabla C$ is the diffusion mass transfer rate per unit area. When a tube tree is considered as a discrete system in which the cross-section-area-averaged concentration is constant in each generation, an estimate is $\Delta f_{n,ax} \propto (C_{n-1} - C_n) - (C_n - C_{n+1})$. Using an approximation $C_n \approx (C_{n-1} + C_{n+1})/2$, we know $\Delta f_{n,ax} \approx 0$. This means that the diffusion mass-transfer fluxes into and out a tube along the axial direction are approximately equal. Therefore, we have the mass-transfer rate across the effective diffusion surface of tube walls in the nth generation (2^n tubes)

$$\dot{m}_n \propto (A_{eff})_n(d_n/l_n)u_n(C_{n-1} - C_n). \quad \text{(A3)}$$

As pointed out in the main text, the diffusion mass-transfer rate across tube walls in the nth generation is also $\dot{m}_n \propto (A_{eff})_n C_n/h_n \propto (A_{eff})_n C_n V_n^{-1/2} 2^{3n/8}$. Using the exponential relations $d_n \propto 2^{-pn}$ and $l_n \propto 2^{-qn}$ for the diameter and length and $V_n \propto 2^{\beta n}$ for the total volume of the nth generation, we have a relation $C_{n-1} = \varepsilon^{-1}(V_n^{\gamma} + \varepsilon)C_n$, where the parameters are $\lambda = (11/8 - p - q)/\beta - 1/2$ and $\beta = 1 - 2p - q$, and ε is a positive constant. The parameters p and q are to be determined in optimization problems. Furthermore, we have a relation

$$C_0 = \varepsilon^{-n}\prod_{k=1}^{n}(V_k^{\lambda} + \varepsilon)C_n, \quad \text{(A4)}$$

which describes a cascade process of mass transfer through successive generations of a bifurcating-tube tree. We calculate the function $\varepsilon^{-n}\Pi_{k=1}^{n}(V_k^{\lambda} + \varepsilon)$ over a range of generations $(n \in [0, N])$ for different values of the parameters λ and ε, and find that the asymptotic behavior of this function for sufficiently higher generations $(n \in [0.5N, N])$ can be reasonably approximated by an exponential function of the generation number n. The fitting error is typically 1–4% in a semi-log plot. Hence, we have an estimate for the gas concentration in the diffusion zone

$$C_n \propto V_n^{-\gamma}, \quad \text{(A5)}$$

where γ is an empirical constant.

Appendix B: Max-Min Problem

The optimality of an engineering bifurcating-tube tree is related to the following max-min problem. Consider a cost function (performance measure) $P = \Sigma_{n=1}^{N} w_n x_n$ for a system that is characterized by a set of the positive quantities $\{x_n\}(n = 1, 2, \ldots, N)$, where $\{w_n\}$ are the positive weight coefficients. We want to find the optimum state to maxmize or minimize the cost function P subject to a constraint $\Sigma_{n=1}^{N} x_n^s = B$, where B is a positive constant and s is a positive exponent. For $s \neq 1$, the use of the Lagrange-multiplier method gives an optimum solution

$$(x_n)_{op} = B^{1/s} w_n^{1/(s-1)}\left(\sum_{n=1}^{N} w_n^{s/(s-1)}\right)^{-1/s}, \quad (n = 1, 2, \ldots, N). \quad \text{(B1)}$$

When $s > 1$, Eq. (B1) gives the optimum state maximizing the cost function P, while it minimizes P when $s < 1$. Particularly, for $w_n = 1$, the optimum solution is simply $(x_n)_{op} = B^{1/s}N^{-1/s} = \text{const}$. The consequence of the above analysis is used to formulate the optimality principles for the design of an engineering bifurcating-tube tree.

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