Simulation of Flow in an Alveolated Duct within the Human Lung with Application to Porous Media

Christopher T. DeGroot and Anthony G. Straatman

Department of Mechanical and Materials Engineering
The University of Western Ontario, London, ON, N6A 5B9, Canada

Email: cdegroo@uwo.ca

ABSTRACT

In the human lung, gas exchange occurs by passive diffusion through the walls of small sacs known as alveoli. These sacs surround small airways, which, together are known as alveolated ducts. In this work, a numerical study of flow in an alveolated duct has been conducted to explore the flow patterns and to determine its permeability by considering it as a representative element of a porous medium. The permeability is obtained using a mathematically rigorous closure method based on the use of constitutive equations to express the unknown pore-level quantities in terms of volume-averaged quantities. One key finding of this work is that the closure problem can be considered as quasi-steady such that the expansion and contraction of the alveoli does not need to be considered directly in the solution of the closure problem. As a result, the dimensionless permeability is a constant throughout the breathing cycle and changes in the dimensional permeability can be simply accounted for based on the changing alveolar length scale. It is also found that the permeability of an alveolated duct is nearly 5 times lower than that of a smooth tube, which may have significant impacts on modelling of the pressure drop in the human airway tree.

1 INTRODUCTION

Simulation of flow in the human lung using computational fluid dynamics is of interest because it can provide details of the flow that can not be measured in vivo. Knowledge of the flow patterns within the lung are of practical importance because of the potential impacts on respiratory drug delivery, particle deposition, and our general understanding of lung function. The human lungs serve the purpose of providing oxygen from the atmosphere to the bloodstream, while removing excess carbon dioxide from the blood and expelling it from the body. The internal structure of the lung consists of a network of bifurcating airways that become smaller in both length and diameter and larger in number with each subsequent bifurcation (or ‘generation’). This poses an interesting challenge when attempting to simulate flow within the lungs because of the large number of possible flow paths. In general, the airway tree must be truncated at some point in order for the problem to be of manageable size.

As computational power has increased over the years, researchers have been able to simulate the flow in more and more airway generations. In 2000, Comer et al. [1] were among the first to attempt three-dimensional simulations of flow in an idealized bifurcating airway geometry. In this work, they were able to consider an airway tree with two bifurcations. By 2005, simulations were being conducted on airway trees with up to seven generations with subject-specific spatial features obtained from medical imaging [2]. Gemci et al. [3], in 2008, attempted simulations in a partially-resolved 17-generation airway tree containing 1453 individual branches. Their results were not, however, grid independent due to limitations in the maximum number of control volumes that could be considered. Recently, Walters and Luke [4] proposed a novel method of simulating flow in many generations by truncating most of the branches and using the flow fields in fully-resolved branches to stochastically apply boundary conditions where the tree has been truncated.

Since fully-resolved simulations in all 23 airway generations is well beyond the capabilities of current and foreseeable computing resources, one would expect to see a continual increase in the number of airway generations simulated as computational power increases. While this is certainly valuable, it is also interesting to note that as the airways become smaller, they be-
gin to appear as a porous medium, especially as the ducts become covered in alveoli (shown in Fig. 1). Note that alveoli are small sacs surrounding the small airway branches that are primarily responsible for gas exchange. On this basis, we propose that the small airways within the human lung can be represented as a porous medium and the flow can be solved using volume-averaged transport equations [5]. Further, we propose that flow in larger airways can be computed by numerically solving the Navier-Stokes equations, coupled with the porous media model of the smaller airways using a model such as that of DeGroot and Straatman [6].

The outline of this work is to first present the problem under consideration, followed by relevant theory pertaining to the volume-averaging of transport equations and their closure. Subsequently, the method by which the permeability tensor is obtained will be shown, followed by results for the flow field and the permeability tensor for the alveolated duct geometry.

## 2 Problem Definition

In this work we focus on flow in a fully alveolated duct, corresponding to the 20th-22nd generations of the human lung. The geometric idealization of the alveolar shape is based on the space-filling model used by Kumar et al. [7, 8], in which the shape of each alveolus is a truncated octahedron fitted to a central duct with a dodecagonal cross-section. Figure 2(a) shows this geometric idealization of a duct surrounded by three rows of alveoli. Here we assume that there are many rows of alveoli, such that we can exploit the periodicity of the flow and simulate only one periodic unit cell. Additionally, since the geometry is symmetric, we simulate only half of the domain, as shown in Fig. 2(b).

Under normal breathing conditions, the Reynolds number in alveolated airways is very low (approximately 0.01 in the terminal sacs and up to 2 in the transitional region beyond the terminal bronchus). The flow field results that are to be presented are obtained at a Reynolds number of 1 using the hydraulic diameter of the duct as the length scale. The permeability is obtained using a closure method which requires the solution of additional transport equations that are independent of the flow field. Thus, the selection of the Reynolds number has no impact on the computed value of the permeability. The development of this closure method and its connection to the theory of porous media is discussed next.
3 Theory

3.1 The method of volume-averaging

The method of volume-averaging is a procedure by which the partial differential equations describing the flow and thermal fields in a general medium are integral-averaged over many pores of a porous medium to obtain a new set of governing equations in terms of quantities averaged over many pores. In the paragraphs to follow, the basics of volume-averaging are briefly described. Further details are readily available in the literature [5, 9, 10, 11].

Consider the flow in a porous medium composed of both fluid and solid constituents, as shown in Fig. 3. Let the length scale of the medium be $L$ and let $V$ define an averaging volume with length scale $\ell$. Provided $V$ is sufficiently large compared to the pore size and $\ell \ll L$, the extrinsic volume-average of a quantity $\phi_k$ is given by

$$\langle \phi_k \rangle = \frac{1}{V} \int_{V_k} \phi_k dV,$$

where $k \in \{f, s\}$ denotes the phase in which the quantity $\phi_k$ is defined with ‘$f$’ and ‘$s$’ indicating the fluid and solid phases, respectively. Alternatively, the intrinsic average is defined as

$$\langle \phi_k \rangle^k = \frac{1}{V_k} \int_{V_k} \phi_k dV,$$

which is an average over a single phase only. The two types of averages are related through the porosity, $\varepsilon = V_f / V$, according to

$$\langle \phi_k \rangle = \begin{cases} \varepsilon \langle \phi_f \rangle^f & \text{if } k = f \\ (1 - \varepsilon) \langle \phi_s \rangle^s & \text{if } k = s \end{cases}.$$  

In addition to these basic definitions, we require the ‘spatial averaging theorem’ [9, 5] to complete the derivation of the volume-averaged governing equations. For the gradient operator, this theorem is stated as

$$\langle \nabla \phi_k \rangle = \nabla \langle \phi_k \rangle + \frac{1}{V} \int_{A_{kl}} \phi_k \mathbf{n}_{kl} dA,$$

where $k, l \in \{f, s\}$, $k \neq l$, and the unit normal vector $\mathbf{n}_{kl}$ is oriented from the $k$-phase to the $l$-phase. $A_{kl}$ is the area contained within $V$ forming the intersection of $V_k$ and $V_l$. Analogous to Eq. 4, the spatial averaging theorem for the divergence of a vector or second-rank tensor, $\mathbf{a}_k$, is given as

$$\langle \nabla \cdot \mathbf{a}_k \rangle = \nabla \cdot \langle \mathbf{a}_k \rangle + \frac{1}{V} \int_{A_{kl}} \mathbf{a}_k \cdot \mathbf{n}_{kl} dA.$$

Figure 3: An illustration of a typical averaging volume, $V$, for an arbitrary porous medium containing fluid and solid volumes $V_f$ and $V_s$, respectively [11].

Note that in Eqs. 4 and 5 the subscripts denote either the fluid or solid phase, thus no summation is implied over repeated indices.

To simplify volume-averages of products of variables a quantity $\phi_k$ may be decomposed into its intrinsic volume-average and a pore-level spatial deviation $\tilde{\phi}_k$. The quantity $\phi_k$ is then expressed as

$$\phi_k = \langle \phi_k \rangle^k + \tilde{\phi}_k,$$

leading to the volume-average of a product of variables, $\phi_{k,1}$ and $\phi_{k,2}$, being defined as

$$\langle \phi_{k,1} \phi_{k,2} \rangle = \frac{1}{\varepsilon_k} \langle \phi_{k,1} \rangle \langle \phi_{k,2} \rangle + \langle \phi_{k,1} \tilde{\phi}_{k,2} \rangle.$$

3.2 Volume-averaged mass and momentum equations

At the pore-level, the flow field is governed by the standard mass and momentum equations for a general continuum. The continuity and Navier-Stokes equations are given by

$$\nabla \cdot \mathbf{u} = 0$$

and

$$\rho_f \left( \frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} \right) = -\nabla p + \mu_f \nabla^2 \mathbf{u},$$

where $\mathbf{u}$ is the velocity vector, $p$ is the pressure, $\rho_f$ is the density of the fluid, $\mu_f$ is the dynamic viscosity of the fluid, and $t$ is time. Assuming the porosity may vary in both space and time, extrinsically averaging Eqs. 8 and 9 results in

$$\nabla \cdot \langle \mathbf{u} \rangle = -\frac{\partial \varepsilon}{\partial t}$$

(10)
and

\[
\rho_f \left[ \frac{\partial (u)}{\partial t} + \nabla \cdot \left( \frac{1}{\varepsilon} (u) \right) \right] = -\varepsilon \nabla \langle p \rangle / \varepsilon + \mu_f \nabla^2 (u) \\
+ \frac{1}{V} \int_{A_{f_s}(t)} (-\bar{p} \mathbf{n}_{f_s} + \mu_f \nabla \bar{u} \cdot \mathbf{n}_{f_s}) \, dA \\
- \rho_f \nabla \cdot \langle \bar{u} \rangle, \quad (11)
\]

where \( A_{f_s}(t) \) represents the area where \( V_f \) and \( V_c \) intersect. Note that the spatial averaging theorem as well as the spatial decomposition given in Eq. 7 are required to arrive at Eq. 11. Since Eq. 11 remains in terms of the unknown pore-level spatial deviations \( \bar{p} \) and \( \bar{u} \), it cannot be solved in its present form. Thus, the closure of the volume-averaged momentum equation, which involves characterization of these unknown terms will be discussed next.

### 3.3 Closure of volume-averaged equations

To close Eq. 11, we follow the general approach of Whitaker [13] in which transport equations for the spatial deviations are derived by subtracting Eq. 10, divided by \( \varepsilon \), from Eq. 8 and subtracting Eq. 11, divided by \( \varepsilon \), from Eq. 9. In this case, however, there are additional terms arising from the fact that we have not assumed a constant porosity in space and time. The transport equation for the velocity deviations arising from the continuity equation is given as

\[
\nabla \cdot \bar{u} = \frac{1}{\varepsilon} \frac{\partial \varepsilon}{\partial t} - \frac{1}{\varepsilon^2} \nabla \varepsilon \cdot \langle u \rangle. \quad (12)
\]

Compared to the equation of Whitaker [13], Eq. 12 is quite complicated, however we can show through various scaling arguments that it can be simplified substantially, such that it is equivalent to that of [13]. First we assume that \( \bar{u} \) and \( \langle u \rangle \) are of the same order (call this characteristic velocity \( U \)), which is reasonable based on the spatial decomposition given in Eq. 6. Additionally, we note that variations in \( \bar{u} \) occur at the length scale of the averaging volume, \( \ell \), while variations in \( \varepsilon \) occur at the length scale of the porous domain, \( L \). In the human lung, more than 90% of the space is occupied by air, so it can be assumed \( \varepsilon \sim O(1) \). On this basis, it can be said that \( \nabla \cdot \bar{u} \) is of the order \( U/\ell^2 \) and that \( \nabla \varepsilon \cdot \langle u \rangle / \varepsilon^2 \) is of the order \( U/L \), such that the second term on the right side of Eq. 12 can be neglected in comparison to the term on the left side. The first term on the right side of Eq. 12 can also be neglected in comparison to the term on the left side, provided the timescale, \( t^\ast \), over which \( \varepsilon \) varies is much larger than \( \ell/U \). For flow in an alveolar duct, an appropriate length scale is the size of an alveolus, which is of the order of 100 \( \mu \)m. The peak velocity, according to Kumar et al. [8] is of the order \( 10^{-2} \) m/s. Thus, \( \ell/U \sim O \left( 10^{-2} \right) \). Since a reasonable breathing rate is 12-20 breaths/min, the timescale \( t^\ast \sim O \left( 1 \right) \), so the first term on the right side of Eq. 12 can be neglected since it is about two orders of magnitude less than the term on the left for normal breathing conditions. Thus, the simplified transport equation for the velocity deviations, arising from the continuity equations is

\[
\nabla \cdot \bar{u} = 0, \quad (13)
\]
as in the analysis of Whitaker [13]. Subtracting Eq. 11, divided by \( \varepsilon \), from Eq. 9 results in

\[
\rho_f \left( \frac{\partial \bar{u}}{\partial t} - \frac{1}{\varepsilon} \frac{\partial \varepsilon}{\partial t} \langle u \rangle \right) + \bar{u} \cdot \nabla \bar{u} + \bar{u} \cdot \nabla \langle u \rangle / \varepsilon \]

\[
- \frac{\nabla \varepsilon}{\varepsilon} \cdot \langle u \rangle / \varepsilon = -\nabla \bar{p} + \mu_f \nabla^2 \bar{u} \\
- \mu_f (\langle u \rangle / \varepsilon - 2 \nabla \varepsilon \cdot \nabla \langle u \rangle / \varepsilon^2) - \mu_f \langle u \rangle / \varepsilon \nabla \langle u \rangle \\
- \frac{1}{\varepsilon} \int_{A_{f_s}(t)} (-\bar{p} \mathbf{n}_{f_s} + \mu_f \nabla \bar{u} \cdot \mathbf{n}_{f_s}) \, dA \\
+ \frac{\partial \bar{p}}{\partial t} \nabla \cdot \langle \bar{u} \rangle \quad (14)
\]
after much algebraic simplification. The final two terms on the left side of Eq. 14 are both of the order \( \rho_f U^2 / L \) since changes in \( \varepsilon \) and \( \langle u \rangle \) occur over the macroscopic length scale \( L \). Since the third last term on the left side of Eq. 14 is of the order \( \rho_f U^2 / \ell \), the last two terms can be considered negligible in comparison to this term. Also, since the first two terms on the left side of Eq. 14 are of the order \( \rho_f U^2 / \ell^2 \) and it has been shown that \( t^\ast \gg \ell/U \), these terms can also be neglected in comparison to the third term. Since the final term on the right side of Eq. 14 is of the order \( \rho_f U^2 / L \), this term can also be neglected in comparison to the third term on the left side. The additional viscous terms, arising from the fact that the porosity is assumed to be spatially varying, can also be simplified. Since we have \( \nabla^2 \bar{u} \sim U/\ell^2 \), \( \langle u \rangle \nabla^2 \varepsilon / \varepsilon \sim U^2 / L^2 \), \( \langle u \rangle \nabla \varepsilon \cdot \nabla / \varepsilon^2 \sim U^2 / L^2 \), and \( \nabla \varepsilon / \varepsilon \sim U / L^2 \) we can neglect all but the first viscous term. This results in the recovery of the transport equation for the velocity and pressure deviations given by Whitaker [13]:

\[
\rho_f \bar{u} \cdot \nabla \bar{u} = -\nabla \bar{p} + \mu_f \nabla^2 \bar{u} \\
- \frac{1}{\varepsilon} \int_{A_{f_s}(t)} (-\bar{p} \mathbf{n}_{f_s} + \mu_f \nabla \bar{u} \cdot \mathbf{n}_{f_s}) \, dA. \quad (15)
\]

Thus we have shown that under normal breathing conditions, where the timescale of the breath is much
longer than the timescale for a parcel of air to travel through a typical averaging volume, that all transient terms in the closure problem can be neglected. Additionally, provided the length scale over which the porosity changes is much larger than the pore length scale, any porosity gradient terms can be neglected in the development of the closure equations. This is very advantageous since these additional terms would be quite challenging to deal with. Fortunately, under these limiting conditions, the transport equations for the spatial deviations reduce to those of Whitaker [13] and we may use the closure method proposed in that work.

To derive closure problems, which are to be solved on the appropriate periodic unit-cell, we first redefine the additional integral term remaining in Eq. 11 in terms of the permeability tensor $K$ according to:

$$\frac{1}{V} \int_{A_{fs}} (-\tilde{p} n_f + \mu_f \nabla \tilde{u} \cdot n_f) dA = \varepsilon \mu_f K^{-1} \cdot (u)$$

(16)

Then we use the following constitutive equations, proposed by Whitaker [13] for $\tilde{u}$ and $\tilde{p}$:

$$\tilde{u} = M \cdot (u)/f + v$$

(17a)

$$\tilde{p} = \mu_f m \cdot (u)/f + \xi,$$  

(17b)

where $M$ is a second-rank tensor and $m$ is a vector, both of which are functions of position. Whitaker [13] has shown that $v$ is zero and $\xi$ is constant, such that it does not pass through any integrals and is therefore inconsequential to the solution of the closure problem. Whitaker [13] then made substitutions to separate the problem into a part which depends only on pore geometry and a part which depends on the flow field. In this work, since we are concerned with very low Reynolds number flows, this step is not necessary. Instead, we simply drop the inertial terms on the left side of Eq. 15. To eliminate the integral terms from the closure problems, we follow an approach similar to Whitaker [13], which is summarized by the substitutions below:

$$d = \varepsilon^{-1} m \cdot K$$

(18a)

$$\mathbf{D} = \varepsilon^{-1} (M + I) \cdot K.$$  

(18b)

Substituting and substituting Eqs. 18a,b into Eqs. 17a,b and substituting the result into Eq. 15 results in the closure problem

$$\nabla \cdot \mathbf{D} = 0$$

(19a)

$$-\nabla d + \nabla^2 \mathbf{D} + I = 0$$

(19b)

subject to the boundary conditions

$$\mathbf{D} = 0,$$ on $A_{fs}$

(20a)

$$\mathbf{D}(x_n + \Delta x) = \mathbf{D}(x_n),$$ on $A_{fe}$

(20b)

$$\mathbf{d}(x_n + \Delta x) = \mathbf{d}(x_n),$$ on $A_{fe}$

(20c)

where $A_{fe}$ refers to the periodic inflow/outflow faces, $x_n$ is the position vector of a point along the flow path, and $\Delta x$ is a displacement vector from $x_n$ to the corresponding periodic location on the outflow face. Equations 19a and 19b may then be solved along with the conditions listed in Eqs. 20a–20c to determine the permeability tensor as

$$K = \varepsilon \langle \mathbf{D} \rangle /\varepsilon.$$  

(21)

The closed form of the volume-averaged momentum equation is then given by

$$\rho_f \left[ \frac{\partial (u)}{\partial t} + \nabla \cdot \left( \frac{1}{\varepsilon} \langle u \rangle \langle u \rangle \right) \right] = -\varepsilon \nabla \langle p \rangle /\varepsilon + \mu_f \nabla^2 \langle u \rangle$$

$$-\varepsilon \mu_f K^{-1} \cdot (u),$$

(22)

where the final term in Eq. 11 has been neglected due to periodicity.

## 4 RESULTS AND DISCUSSION

To obtain the flow field and solve the closure problem, an in-house finite-volume method [6] is used.

A grid resolution study was conducted to ensure that the presented results are independent of the particular grid employed. This study showed that a grid containing 120,058 control volumes was sufficient to achieve grid-independent results.

### 4.1 Flow field

A plot of the streamlines on the centre plane of the alveolated duct is given in Fig. 4 for a Reynolds number based on the hydraulic diameter of the duct, $D_H$, of $Re_{D_H} = 1$. This figure shows the expected flow pattern in which the fluid flows in well-defined, straight streamlines through most of the duct. Within the cavities corresponding to the alveoli, there is a large recirculation zone that serves to mix the air within the alveolus, promoting gas exchange.

### 4.2 Permeability

The dimensionless permeability of the alveolated duct structure is found to be $K/D_H^2 = 6.68 \times 10^{-3}$. Comparing this to the dimensionless permeability of a circular tube without alveoli ($K/D^2 = 1/32 = 0.03125$) it is found that the pressure drop in an alveolated duct is
almost 5 times higher than that for a smooth tube. This finding is of relevance to those using bifurcating tube networks to estimate the total pressure drop through the airway tree, as in Kuwahara et al. [14].

Note that as the lung inhales and exhales, the alveoli will expand and contract. In the development of the closure model, it was found that this process can be considered as quasi-steady and transient terms did not have to be considered as part of the closure process. When using this result in a volume-averaged model, however, it is desirable to be able to account for changes in permeability as the state of the lung changes. This can be accomplished quite simply with the current model since the result is presented in dimensionless form. Regardless of the inflation state, the dimensionless permeability is constant, but the diameter of the duct will change. Thus the dimensional permeability is obtained simply by adjusting the hydraulic diameter.

5 SUMMARY

In summary, we have computed low Reynolds number flow in an alveolated duct geometry and determined the permeability of this flow structure using a mathematically rigorous closure model. The computed results will be useful in applications where the pressure drop in the airway tree is obtained by modelling the flow as a bifurcating network of tubes as in Kuwahara et al. [14]. Additionally, results may be applied in studies considering the lung as a porous medium at an organ level.

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REFERENCES


