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Pore-scale analysis of Newtonian flow in the explicit geometry of vertebral trabecular bones using lattice Boltzmann simulation

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Abstract: The geometric and transport properties of trabecular bone are of particular interest for medical engineers active in orthopaedic applications and more specifically in hard tissue implantations. This article resorts to computational methods to provide some understanding of the geometric and transport properties of vertebral trabecular bone. A fuzzy distance transform algorithm was used for geometric analysis on the pore scale, and a lattice Boltzmann method (LBM) for the simulation of flow on the same scale. The transport properties of bone including the pressure drop, elongation, and shear component of dissipated energy, and the tortuosity of the bone geometry were extracted from the results of the LBM flow simulations. Whenever suitable, dimensionless numbers were used for the analysis of the data. The average pore size and distribution of the bone were found to be $746\mu\text{m}$ and between 75 and $2940\mu\text{m}$, respectively. The permeability of the flow in the cavities of the specific bone sample was found to be $5.05 \times 10^{-8} \text{ m}^2$ for the superior–inferior direction which was by a factor of 1.5–1.7 higher than the permeability in the other two anatomical directions (anterior–posterior). These findings are consistent with experimental results found 3 years prior independently. Tortuosity values approached 1.05 for the superior–inferior direction, and 1.13 and 1.11 for the other two perpendicular directions. The low tortuosities result mainly from the large bone porosity of 0.92. The flow on the pore scale seems to be shear dominated but 30 per cent of the energy dissipation was because of elongational effects. The converging and diverging geometry of the bone explains the significant elongation and deformation of the fluid elements. The transition from creeping flow (the Darcy regime), which is of interest to vertebral augmentation and this study, to the laminar region with significant inertia effects took place at a Reynolds number of about 1–10, as usual for porous media. Finally, the authors wish to advise the readers on the significant computational requirements to be allocated to such a virtual test bench.

Keywords: trabecular bone permeability and tortuosity, vertebroplasty, lattice Boltzmann computational fluid dynamics simulation, virtual experiment

1 INTRODUCTION

Flow simulation is of interest to a wide range of engineering disciplines. In medical engineering, there is a keen interest in understanding the flow of medical cements in trabecular bone cavities, which is an emerging medical procedure to treat

spinal insufficiency fractures. In this procedure, medical cements are injected through a long cannula into the bone. Cement, once hardened *in situ*, strengthens the insufficient bone [1, 2].

Because of the recent nature of this spinal procedure, techniques for cement delivery into the bone, thus far, are based on physicians' experience and preferences, often leading to adverse effects. In the medical literature [3], two complications are frequently reported: firstly, excessive pressure required to deliver cements; secondly, extraosseous

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cement leakage into adjacent fractures through defects, and into the cardiovascular system through blood vessels. Medical engineers are interested in designing adequate delivery tools and techniques that are based on a thorough understanding of the pressure drop and cement–bone interaction during the cement injection process.

The trabecular bone structure is particularly complicated. Researchers have treated bone, thus far, as a macroscopically uniform continuum. On this scale, transport in bone is described by its permeability. Respective reports describing fluid transport in trabecular bone are limited in number and to experimental studies. Specifically, reports exist on the permeabilities of tibial [4], calcaneal [5], femoral [6], and vertebral trabecular bone [6–8]. However, these studies which are based on Darcy's law derived in the nineteenth century, do not provide a mechanistic or pore-scale understanding of fluid transport in the trabecular bone skeleton and do not provide explanations for the unusual variation in the reported bone permeabilities.

In this paper, computational fluid dynamics (CFD) are employed. In particular, a lattice Boltzmann method (LBM) [9, 10] is applied to simulate the flow of a Newtonian fluid on the pore-scale level of the explicit trabecular bone geometry acquired using a microcomputed tomography technique. In principle, such investigations based on a marker-and-cell representation of the explicit geometry could be carried out with any CFD approach but LBM proved to be particularly useful and efficient for directly simulating flow in complex porous geometries [10]. Because of the complex and anisotropic bone geometry and the not fully understood rheology of real bone cements, a Newtonian fluid was chosen to validate the lattice Boltzmann approach for the particular area of application and to demonstrate its potential. With the simulations applied to mainly the creeping flow regime, a description of the flow velocities and pressure drop on the pore scale is first sought and then attempts were made to relate them to the bulk transport properties. Further, the aim is to provide a more detailed analysis of the dissipated energy resulting from both shear and elongational and deformational components. Both components are responsible for the pressure drop and owing to the contracting bone geometry a significant amount can be attributed to elongation and deformation. In addition, the tortuosity of trabecular bone is determined. Because of the novelty of this approach and limited number of pages designated to this article, this study is restricted to one bone sample and the

focus is on the establishment of this approach and potential results rendered.

This short article is organized as follows. In the subsequent methodological section, the applied LBM is briefly described, followed by the division of dissipated energy in the two components; the dimensionless numbers used in this study, and sample preparation. A short description of LBM is warranted because it is novel for medical engineering. The results section is laid out in a linear fashion and will be followed by a short discussion.

2 METHODS

2.1 Description of the LBM

The LBM [9, 10] is a recent method from CFD which has its roots in a highly simplified gas-kinetic description, i.e. a velocity-discrete Boltzmann equation with appropriate collision term. When properly applied, the results of LBM simulations satisfy the Navier–Stokes equations in the macroscopic limit with second order of accuracy [9, 10].

The lattice Boltzmann equation with Bhatnagar–Gross–Krook (BGK) [11] collision operator

$$f_i(\mathbf{x} + \mathbf{e}_i \Delta t, t + \Delta t) - f_i(\mathbf{x}, t) = -\frac{1}{\tau} [f_i(\mathbf{x}, t) - f_i^{\text{eq}}(\mathbf{x}, t)], \quad i=0, \dots, 18 \quad (1)$$

with

$$f_i^{\text{eq}}(\rho(\mathbf{x}, t), \mathbf{u}(\mathbf{x}, t)) = \rho(\mathbf{x}, t) w_i \left[1 + \frac{3}{c^2} \mathbf{e}_i \cdot \mathbf{u}(\mathbf{x}, t) + \frac{9}{2c^4} (\mathbf{e}_i \cdot \mathbf{u}(\mathbf{x}, t))^2 - \frac{3}{2c^2} \mathbf{u}(\mathbf{x}, t) \cdot \mathbf{u}(\mathbf{x}, t) \right] \quad (2)$$

describes the evolution of the single-particle distribution function f_i . The macroscopic quantities, density ρ and velocity $\mathbf{u}$, are obtained as zeroth- or first-order moments of f_i , and f_i^{eq} is a Taylor-expanded version of the Maxwell–Boltzmann equilibrium distribution function [12, 13], w_i are direction-dependent constants, and $c = \Delta x / \Delta t$ with the lattice spacing Δx and lattice time step Δt . The kinematic viscosity of the fluid is determined by the dimensionless collision frequency $1/\tau$ according to $\nu = \frac{1}{6}(2\tau - 1) \Delta x c$ with $\tau > 0.5$ owing to stability reasons [9, 10]. For the present simulations, a slightly modified equilibrium distribution function was used to enhance the incompressibility of the fluid [14]. The pressure, however, could nevertheless be obtained locally by the equation of state of an ideal gas.

Solid wall boundary conditions are realized by the bounce-back rule [9, 10] and information about the geometric pore-scale structure is directly taken from segmented X-ray microcomputed tomography images [15] as typical for a Cartesian marker-and-cell approach. From a computational point of view, the explicit lattice Boltzmann algorithm is very efficient [16–19]. A single simulation of the flow in the bone structure described in the present work consisted of about 50×10^6 voxels using the D3Q19 lattice, or about 1×10^9 degrees of freedom and took some hours of elapsed time on one symmetric multi-processor node of the NEC SX-8 vector-parallel system located at the Höchstleistungsrechenzentrum Stuttgart (HLRS) to reach a converged steady state solution. On a typical personal computer (PC) cluster such simulations easily take several days despite the good parallel speed-up of the LBM [17, 20].

2.2 Pressure drop and energy dissipation

The investigation of flows in porous media has attracted many researchers since the beginning of the nineteenth century and Darcy derived for the creeping flow regime a linear relation between the pressure drop $\partial p / \partial x$ and the superficial flow velocity u_0 , given by

$$\frac{\partial p}{\partial x} = -\frac{\mu}{\kappa} u_0 \quad (3)$$

with the permeability κ and the dynamic viscosity μ . Beyond creeping flow, a second quadratic velocity term has to be added, resulting in the well-known Ergun equation.

To generalize the observations, dimensionless numbers should be used. The Reynolds number

$$Re = \frac{ul}{\nu} = \frac{\rho ul}{\mu} \quad (4)$$

describes the flow regime (with the kinematic viscosity ν or the density ρ and dynamic viscosity μ). The density of acrylic bone cements is in the region of 1200 kg/m^3 , with a viscosity of 500 to 2000 Pa.s. The infiltration velocity is less than 1 mm/s , while the characteristic length of the trabecular bone is expected to be in the region of 1 mm . Assuming this scaling, which is characteristic for vertebroplasty application, the Reynold number characteristic for the process is expected to be in the region of 10^{-6} [21].

It should be noted, however, that the choice of the characteristic velocity u and length l are not unique, but the superficial velocity u_0 and the mean pore size are intuitive for the present application. The friction coefficient λ and friction factor f are dimensionless versions of the pressure drop or the permeability [22, 23]. With these dimensionless quantities, the Ergun equation for example can be written as $f = 150 / Re + 1.75$. No general relation exists between the pressure drop or the permeability κ and the geometry of the porous media. Most theoretical models (e.g. capillary theories [22]) assume that the pressure drop is caused only by shear forces. However, a more rigorous description is possible, which is based on the mechanical energy balance equation [23], and the total energy dissipation Φ can be expressed as a sum of two parts, namely the dissipation caused by shear forces and the dissipation caused by deformational strain owing to elongation [24–26], according to

$$\Phi = -\mu \left\{ \underbrace{2 \left[\left(\frac{\partial u_\alpha}{\partial x_\alpha} \right)^2 \right]}_{\text{elongation}} + \underbrace{\left[\left(\frac{\partial u_\alpha}{\partial x_\beta} + \frac{\partial u_\beta}{\partial x_\alpha} \right)^2 \right]}_{\text{shear}} \right\}, \quad \alpha, \beta = 1, 2, 3 \quad (5)$$

and implied Einstein summation over repeated Greek indexes. By a carefully designed experiment of the flow of a non-Newtonian fluid in glass beads, Durst *et al.* [24] could show that the elongation of fluid elements is not negligible and that the usually geometrically motivated tortuosity (i.e. the ratio of the actual flow path to the length of the straight line between its starting point and end point) with values between 2 and 4 is mainly a fudge factor in capillary theory models owing to an inappropriate description of the actual physical processes. The lattice Boltzmann simulations made by Bernsdorf *et al.* [25] and Zeiser *et al.* [26] confirmed this physical effect for the flow of Newtonian fluids in different kinds of porous structure.

2.3 Microcomputed tomography

The images used in this study were acquired using a SkyScan medical microcomputed tomography scanner at a spatial resolution of $18.2 \mu\text{m} \times 18.2 \mu\text{m} \times 36.4 \mu\text{m}$. Biopsies were performed on each vertebra extracting each time two cores (cylindrical trabecular bone excisions) of 16 mm height and 16.45 mm diameter and from the usual site of injection of bone

cement during vertebroplasty. Details on the samples excision may be found in reference [8].

Just one three-dimensional data set was used in the present study for all simulations. Results for the superior-inferior (SI) and the two anterior-posterior (AP) directions were obtained by changing the orientation of the flow. If nothing else is explicitly noted, results for the main flow in SI direction are visualized.

To have an isotropic resolution for the simulation, 2×2 pixels within each plane have been combined to one voxel. The resulting change in porosity was less than 0.5 per cent and thus negligible.

2.4 Geometric analysis

The aim of the geometric analysis was to segment the gray-scale computed tomography images into binary data as required for the subsequent LBM flow simulation and to provide a measure of the characteristic length scale of the void space.

The geometric analysis on the pore scale used the fuzzy distance transform (FDT) algorithm initially reported in reference [27] and recently further developed in reference [28]. Specifically, this algorithm consists of three steps:

- (a) FDT computations;
- (b) skeletonization;
- (c) analysis of the pore size of the bone cavities.

The first two steps are rather preprocessing of the microcomputed tomography images. The pore size is calculated by combining their results.

In the FDT algorithm, the distance of each voxel of the bone cavity to the background, which in this case is the trabecular bone, is calculated on the basis of the expressions

$$L_P = \sum_{k=1}^{l-1} \frac{1}{2} [\mu_{\text{BVF}}(p_k) + \mu_{\text{BVF}}(p_{k+1})] \|p_k - p_{k+1}\| \quad (6)$$

$$D_f(p) = \min_{P \in \text{paths}(p,q)} L_P \quad (7)$$

where L_P is the length of the path P and $\|p_k - p_{k+1}\|$ is the Euclidian distance between two adjacent points or pixels p_k and p_{k+1} . There are many paths between an object point p and background point q . The fuzzy distance D_f is defined by equation (7) and results in the shortest path length for all object points from background. Finally, $\mu_{\text{BVF}}(p)$ is the membership, which is a measure of the grey value, of pixel p [27, 28].

This computation leads to the FDT map, wherein the shortest distance of each voxel to the background is depicted. The calculation of the FDT map usually includes the fuzzification process [27]. Once the FDT map has been obtained, the focus shifts to obtaining its ridge points, representing the voxels with the maximum distance to the background. Extracting the voxels with the maximum distance to the background is obtained by the so-called skeletonization process of the cavities. In this study, the skeleton of the cavity structures has been extracted using ridge-based detection methods [28]. In this, the second derivative of the distance map (Hessian matrix) is calculated using

$$\nabla D_f \cdot v_1 = 0 \quad \text{and} \quad \lambda_1 < 0 \quad (8)$$

$$\nabla D_f \cdot v_2 = 0 \quad \text{and} \quad \lambda_2 < 0 \quad (9)$$

$$\nabla D_f \cdot v_3 = 0 \quad \text{and} \quad \lambda_3 < 0 \quad (10)$$

where λ_1 , λ_2 and λ_3 are eigenvalues and v_1 , v_2 , and v_3 are eigenvectors of the Hessian matrix.

This computation makes the local maxima in the bone cavity or distance map visible. Once obtained, an uphill climbing method is used to connect the local maxima and to obtain the skeleton.

In the final analysis step, the FDT of the pore voxels, coinciding with those of the skeleton are extracted and tabulated with respect to their occurrence frequency, which can be depicted graphically in the form of a histogram. The average thickness value is obtained arithmetically. Additionally, the median value is calculated because of the unsymmetrical nature of the distribution.

For the flow simulations, the FDT values and the skeleton are not used as the lattice Boltzmann simulations operate on the pore-scale level, directly using the segmented or reconstructed images. However, to convert to flow results during post-processing and analysis to a dimensionless number, a measure of the average pore size or the equivalent capillary tube is required. Information obtained from the FDT is helpful for that.

3 RESULTS

To calculate non-dimensional values, the superficial velocity u_0 and the mean pore size are used as characteristic quantities.

3.1 Morphology and geometric structure

Figure 1 depicts in three dimensions the trabecular bone geometry, the distance map, and the histogram count of pore size in both differential and cumulative manner. The porosity of the bone sample (bone mineral density, 0.52 g/cm^2 ; age, 72 years) was 0.92. The distance map reveals characteristic pores larger than 80 pixels ($2912 \mu\text{m}$), with the maximum being coloured red. The pores range between approximately 75 and $2940 \mu\text{m}$, with the average being approximately 0.75 mm and a median value of 0.72 mm .

3.2 Flow field

The kinematics of the flow (Fig. 2) seem non-uniform with local velocities of up to sevenfold compared with the superficial velocity applied at the inlet of the bone sample. A velocity map, with the maximum being in red, in two sections of the X direction (i.e. normal to the main flow direction), and in addition a velocity map in the Y direction (i.e. parallel to the chosen main flow direction) are depicted in Fig. 2. The histogram counts of the two maps in the X direction show variable velocity distributions depending on the location of the slides, which is not surprising because of the different local geometries. Two-dimensional cross-correlation of FDT and local velocities values showed that the FDT explains roughly 73.7 per cent of the velocity field.

3.3 Pressure drop and energy dissipation

The pressure graduation shown in Fig. 3 equally demonstrates a non-uniform distribution. The respective permeability values in three anatomical directions are listed in Table 1. These values are valid for the creeping-flow regime which extends up to a Reynolds number of about 1 and correspond to those shown in Fig. 3. Further, the friction coefficient versus Reynolds number relation is plotted in Fig. 3. The typical shape of a quadratic pressure drop correlation can be seen, as known for example from the Ergun equation. The permeability values are highest in the SI direction.

Detailed analysis of dissipation underlying the pressure drop, in accordance with equation (5) shows that the flow is shear dominated in the SI direction with the shear contribution to the pressure drop being 70 per cent. Surprisingly, the shear contribution reduces to 55 per cent in the other

Fig. 1 Geometric structure, distance map, and pore size histogram of the examined bone sample. The dimensions of the investigated bone sample are $400 \times 300 \times 300$ voxels or $14.5 \text{ mm} \times 11 \text{ mm} \times 11 \text{ mm}$, i.e. the resolution of one voxel is $(36.4 \mu\text{m})^3$

Fig. 2 Velocity maps on the local pore scale. The first two show the cross-sections normal to the chosen main flow direction and correspond to planes of the investigated sample with average local mean porosity (section A, left) and low local mean porosity (section B, right). The third map is in the Y direction (i.e. parallel to the chosen main flow direction). This histogram of the local velocity quantifies the non-uniformity of the flow field shown in the top two maps. The superficial velocity u_0 was always used to normalize the local velocity u

Fig. 3 Pressure map corresponding to the velocity map in the Y direction (i.e. parallel to the chosen main flow direction) of Fig. 2. Overall, there is a linear pressure drop but, locally, significant deviations occur owing to the complex geometric structure. The second and third graphs depict the permeability and the friction coefficient versus the Reynolds number respectively

two directions, indicating a stronger geometrical contraction, which is plausible because of the directionality of trabecular bone. These ratios did not depend on the Reynolds number.

3.4 Tortuosity of flow paths

Figure 4 depicts various flow paths in the trabecular geometry studied. Path lengths were determined by integrating the streamlines from the inlet to the outlet of the sample. The colours depict the absolute locale flow velocities that a fluid element locally experiences. The tortuosity histograms show an increased length of maximum 15 per cent in the X direction, and of maximum 35 per cent in both the Y and the Z directions. The average tortuosities are listed in Table 1. The distribution shifts, as shown in Fig. 4 for the SI direction, slightly to the left for an increased Reynolds number.

4 DISCUSSION AND CONCLUSION

The article addresses both the geometric and the transport properties of vertebral trabecular bone. More specifically, the average pore size and distribution have been determined using the FDT algorithm. The LBM delivered the transport properties of the bone. Integrating both methods on the pore scale is particularly novel to the medical engineering of orthopaedics.

Flow analyses were conducted for a creeping-flow protocol characteristic for the kinematics of the infiltration process of vertebroplasty [3, 7, 29]. The analysis has been further extended into the early laminar regime where inertial forces start to dominate. The transition occurs at a Reynolds number in the range 1–10. This transition is typical for consolidated porous media.

The specific value of directional permeability calculated using this virtual environment compares well with already existing permeability values that were obtained experimentally in 2002 [6, 8]. The persons conducting the numerical experiments in 2006 had no prior knowledge that these permeability values were available for this specific bone sample, which were made available once the computations were complete. Specifically, experimental permeability in the SI anatomical direction, corresponding to the X direction in this study was found to be $4.83 \times 10^{-8} \text{ m}^2$, while the numerical value is $5.05 \times 10^{-8} \text{ m}^2$. The slight difference can be explained by the different sample sizes and shapes used in the

Fig. 4 Tortuosity map with the colours indicating local velocities followed by the differential and cumulative tortuosity distribution with the Reynolds number. In the analysis, the magnitude of the local velocity was normalized with the superficial velocity

numerical and virtual experiments. Also, the relatively low permeabilities in the other anatomical direction is consistent with the experimental findings [6, 8]. This consistency in the results increases the confidence of a medical engineer in this virtual experiment.

The tortuosity values approached roughly 1.05 for the X direction and increased in the other two directions. These low tortuosities are conceivable because of the large porosity of the trabecular bone. Also, the relatively low tortuosity value in the Y and Z directions results from the orientation of vertebral trabecular bone in this direction. There seems to be a strong correlation between the directional permeability and tortuosity. It is not feasible, however, to make any conclusive remarks based on this study. The average tortuosity and its distribution seem to shift to the left with an increasing Reynolds number. Further examination will bring some clarity to this subject and its relation to the reduced permeability.

The reader should note the extensive computational requirements of the simulation described in this article and the larger amount of data produced mainly because of the complicated trabecular bone. The results shown in the paper were calculated on a NEC SX-8 vector parallel computer using eight central processing units (CPUs). It took 3.5 h of elapsed time or equivalently 28 h of CPU time. The update rate was roughly 300×10^6 lattice cells/s.

A formal conversion study was not carried out in this investigation. From the experience of the lattice Boltzmann community and previous conversion studies by the first author [25, 26], the present authors are confident that the results presented in this study are both qualitatively and quantitatively correct. A general problem of conversion studies with such small geometry is that the computed tomography images are only available for a specific spatial resolution. Choosing adequate threshold values for segmentation, in spite of the advanced fuzzy distance methods being used in this study, remains a technical challenge. If additional subsampling and supersampling are used, a non-negligible error may be introduced. Therefore, it is not surprising that a formal conversion study may fail [30]. However, in this preliminary investigation of the explicit bone geometry, the volume of the sample was chosen to be sufficiently large for a

Table 1 Summary of the permeability values, ratios, and shear versus elongational dissipation

Orientation	Porosity (%)	Permeability (m ²)	Permeability ratio (%)	Shear contribution (%)	Tortuosity
SI	92.3	5.05×10^{-8}	Reference	70	1.05
AP	92.3	2.98×10^{-8}	60	56	1.13
AP	92.3	3.43×10^{-8}	68	57	1.11

representative volume of the trabecular bone. Interested readers are recommended to consult references [25] and [26] for more details on this topic.

This article has been limited to Newtonian flow. Medical-grade cements will show an even more complex non-linear interaction with the geometry. However, the principle of the work flow and analysis would be similar. Thus, the limitation to Newtonian fluid in the present work does not conflict with the potential of the approach. Future work will focus on the derivation of an appropriate rheological model for polymeric bone cements and consider the non-Newtonian fluid rheology in the simulation.

Discussion among the authors led to the conclusion that this analysis should be extended to more samples in future work. The data bank currently contains 35 samples excised from vertebrae with a bone mineral density value ranging from 0.38 to 1.20 g/cm², which represents highly osteoporotic bone to healthy bone.

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All flow simulations reported in this work have been carried out on the NEC SX-8 vector-parallel computer located at the HLRS within the LBA_diff project of TZ.

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