A Review of Acoustic Absorption Mechanisms of Nanoscopic Fibres

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ABSTRACT

Advances in nanotechnology have provided acoustic researchers with a number of new materials with nanofibres and nanopores that can potentially be implemented as an acoustic porous absorber. The molecular behaviour of these new nanoscopic materials may have a significant influence on their sound absorption; in addition, their properties could play an important role in reducing the absorber thickness compared to the currently available materials. However, the absorption mechanisms of nanoscopic fibres are not fully understood and the application of numerical and analytical modelling methods to this problem is still at an early stage. This paper presents a review of numerical methods which have been implemented for various micro- and nano-scale analyses of relevance to the acoustics of nanofibres. The review is focused mainly on the application of non-continuum particle based approaches such as the Lattice Boltzmann Method (LBM) and the Direct Simulation Monte Carlo (DSMC) method, since it is expected that the flow behaviour for nanoscopic fibres will be in transition regime (where molecular mean free path is comparable to characteristic dimension) due to the high Knudsen number. The acoustic absorption mechanisms are thus likely to deviate from the continuum phenomena and modelling approaches applicable to flow associated with larger scale fibres. It is intended that this review will provide an overview of the potentially applicable approaches for the exploration of acoustic absorption mechanisms of nanoscopic fibres.

INTRODUCTION

A fundamental understanding of the physical mechanisms associated with the use of nanotubes acting as acoustic absorbers and their potential benefits has not as yet been developed. Development of this understanding will advance the knowledge base of the discipline, and will also allow a number of novel arrangements for acoustic absorbers to be investigated. In this paper, a review is presented which provides details on the problems that may be encountered during the numerical simulation of nanoscopic fibres and the potential simulation techniques that can be applied for acoustic flow behaviour considering possible nonlinear behaviour of nanoscopic fibres and deviation from continuum assumptions.

Currently, three different kinds of nanotube are available which could form the nanoscopic fibres: carbon nanotube (CNT) (Iijima, 1991; Koziol et al., 2007), boron nitride nanotube (BNT) (Cohen & Zettl, 2010) and titania nanotube (TNA) (Peng et al., 2005). Although carbon nanotube is the most widely studied materials for the nano fibres and composite foams (Ajayan et al., 2006), other nanotubes have also similar potential characteristics to form the nanocopic fibres and composites (Yuan & Su, 2004; Cohen & Zettl, 2010). However, no one has described the acoustic propagation mechanisms for the range of characteristic dimensions of nanoscopic fibres, although a few researchers have attempted to demonstrate the fluidic behaviour in the micro scale range (Beskok & Karniadakis 1999; Niu et al., 2004; Karniadakis et al., 2005; Ansumali et al., 2006; Zhang, 2011). Moreover, most of the flow simulations in microscale range, modelled were for monatomic, or at most, for diatomic gases with the simulation of employing rigid spheres as gas molecules (Danforth & Long, 2004a). Conversely, for the case of nanotubes, the acoustic wave propagating media would be air, which is a polyatomic gas; hence, the method must have the capability to model polyatomic molecules. Furthermore, no measurements of the acoustic properties of nano-materials have been reported.

Mechanisms of sound absorption for conventional porous acoustic materials have been described by a number of researchers (Mechel & Ver, 1992; Ingard, 1994; Bies & Hansen, 2003), and are associated with the propagation of air molecules within the pores or interstices in the material, and the interaction of the sound with the structure of the material. Viscous losses are associated with the frictional losses of the air molecule oscillations within the pores, as well as the loss of momentum caused by the changes in flow direction and expansion and contractions of the air as it passes through the irregular arrangement of pores in the material. Heat conduction from the air to the absorber material is also responsible for thermal losses. The forced mechanical oscillation of the frame or structure of the porous material is also responsible for losses in some instances. While the various mechanisms of sound absorption are currently well understood for conventional porous acoustic materials having particle diameters or pores in the microscale (down to 1 μm), the relative influence of the various mechanisms are expected to change for materials with pores or fibres at the smaller nanoscale (down to 1 nm), while other mechanisms and non-linear effects may also have a significant influence.

The size of the thermal and viscous boundary layers relative to the diameter of the nanotubes and the wavelength of the sound of interest will be significantly different for the nanoscale acoustic absorber structures. In addition, nanotubes have been shown to be highly flexible (see for example CSIRO, 2005), so interaction of sound waves with the nanotubes is expected to be significantly different to the interaction with the relatively rigid glass and mineral fibres commonly used in conventional absorber materials, requiring models that account for these effects (Beltman, 1999).

The controlling parameters of acoustic absorption for structures at the nanoscale will differ from those of conventional absorber materials. Developing an applicable analytical framework will involve extending the application of the current theory for fibrous acoustic materials from the microscale

(for example, synthetic fibres diameter: 2~25 μm and natural fibres diameter: 8~38 μm; Arenas & Crocker, 2010) to the nanoscale. Because the length scales of the nanotubes (CNT: diameter 10 to 50 nm; BNT: diameter 10 to 80 nm; TNA: diameter 20 to 100 nm) are of the same order as the mean free path (65 nm) of particles in air at ambient temperature and pressure, the commonly used acoustic assumptions, such as continuity, are invalid. In addition, the viscous effects which are assumed negligible in deriving the wave equation for acoustics will be important for the nanotube acoustic absorbers. Modelling the flow and acoustic propagation within a nanotube acoustic absorber will thus require the application of analytical or numerical approaches appropriate to the nano-scale such as the Lattice Boltzmann Method (Karniadakis et al., 2005) or Direct Simulation Monte Carlo (Bird, 1994). The methods have successfully been applied to modelling nonlinear acoustic wave propagation (Hadjiconstantinou & Garcia, 2001; Danforth & Long, 2004b; Hanford & Long, 2007). It is likely that the thermal interactions between the nanotubes and the fluid will also need to be considered.

In continuum models, internal flow properties such as density, velocity, pressure and temperature are usually considered to be constant or follow a linear relation and change accordingly with well-defined theoretical and empirical relations. However, such assumptions are not always valid in the case of real gases confined in a small channel at the nanoscale (Czerwinska, 2009). Quantification of the validity of continuum models and deviation from this behaviour can be established by a non-dimensional parameter known as the Knudsen number, $Kn = \lambda/H$, which is a ratio of the molecular mean free path (λ) and characteristic length scale (H). For $Kn = 0$ to 0.001 the medium is considered to be in a continuum region, however, in general, for $Kn \geq 0.1$ the continuum approximation is considered to be invalid (Czerwinska 2009, Hadjiconstantinou 2002). Flows can also be classified more specifically according to their Knudsen number using the different features of the flow regimes. For instance, in $0.1 < Kn < 1.0$, the regime is known as slip flow regime (Karniadakis and Beskok 2005); and for $Kn < 10$, the regime is regarded as the transition regime which represents transition between diffusive and ballistic free molecular behavior (Hadjiconstantinou 2001, 2002). For the nanoscale structures considered in this research, acoustic waves are propagating in air (a polyatomic gaseous media), and the flow is through cylindrical channel nanotubes. Hence, the average molecular free path of air at STP, which is 65 nm (Karniadakis and Beskok 2005) and the average diameter of the tube, which is between 50 to 100 nm (maximum values considered), should be considered for the relative values of Knudsen number. It turns out that the characteristic scale is comparable to the molecular mean free path which places them in a transition flow regime, since the value of Kn will be in the range of 0.1 to 10 (for CNT: $Kn = 65/50 = 1.3$) as exhibited in Figure 1. It also means that molecules have the possibility to collide with the nanotube walls more frequently than between themselves (Czerwinska 2009). Therefore, the surface effects will be dominant and depending on the wall boundary condition, the flow behaviour will be varied with the flow interactions between the molecules and wall, and rarefaction behaviour of the medium, and hence tend to exhibit large flow disturbances and complex physical effects; thus continuum phenomenon will be invalid (Czerwinska 2009, Prasanth & Kakkassery 2006). In this case, the Boltzmann equation of kinetic theory would be applicable, and in order to solve this equation, particle collision simulation techniques should be considered. In other words, the larger value of Knudsen number for the case of air flow in nanoscopic fibres indicates that particle based non-continuum approaches such as Lattice Boltzmann Method (LBM) and Direct Simulation Monte Carlo Method (DSMC) should be implemented for the investigation of the flow behaviour.

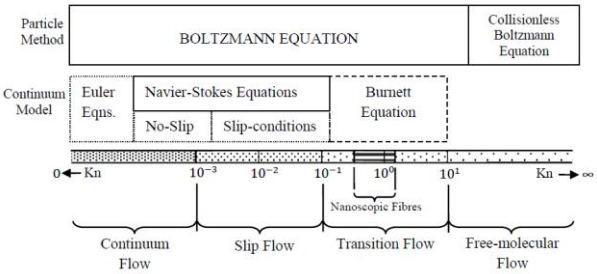

Figure 1. Applicability range of the models based on Knudsen number (Adapted from Ivanov et al. 2007 & Hanford 2008).

ACOUSTIC ABSORPTION IN NANOSCOPIC FIBRES

Wave propagation in micro- and nano-scale flows are usually characterised by the confinement of the fluid environment (Czerwinska 2009). The hierarchy of the mathematical models available to solve such types of fluid dynamics problem can be categorised in two groups; continuum and non-continuum methods, despite the varying degrees of approximation (Hanford, 2008). Continuum models consider the fluid as a continuous medium which allows description of the average bulk properties of the fluid domain at the macroscopic level using physical quantities such as velocity, density, temperature and viscosity (Czerwinska, 2009). The validity of the continuum assumption remains as long as the characteristic length of the problem is much larger than the molecular spacing between fluid particles, which can also be characterised by the dimensionless Knudsen number 'Kn', as mentioned earlier (Hanford, 2008). It is also a scale which defines the nonequilibrium or viscous effect of the gas and if the system has a lower value of Kn, continuity assumption of the models can be applicable (Hanford, 2008). Several engineering applications including acoustics have used this continuum approximation with the implementation of Euler or Navier-Stokes equations for the simulation of flow behavior and found it to be adequate for successful results. However, continuum models have limitations for the approximation of thermal equilibrium, as it considers negligible deviation from equilibrium, which is generally only applicable for the macro scale (Hanford, 2008). In the case of nano- or micro-scale modelling, the molecules might not even have sufficient time to obtain equilibrium for momentum and energy transport of solid-fluid interaction (Czerwinska, 2009). Moreover, for such complex physics, additional equations need to be included to consider those factors of non-equilibrium and nonlinearity which make the simulation complicated and computationally costly (Czerwinska, 2009). Therefore, there is a need to apply non-continuum methods, preferably via a molecular approach, to understand and consider the uncertainty of the molecules.

In non-continuum methods, which are developed based on molecular models, the state of the gas at the microscopic level is realised by the particle nature of the gas and described by the particle position and velocity in 3D space (Hanford, 2008; Czerwinska, 2009). A comparison between the continuum and molecular approaches is presented in Ta-

ble 1, adopted from the literature (Bernsdorf, 2008; Hanford, 2008; Czerwinska, 2009). The limitations and disadvantages of continuum methods as stated in Table 1 suggest that continuum models do not have the necessary features for the simulation of the phenomena likely to be required to accurately model the acoustic absorption of nanoscale fibres, whereas the non-continuum particle based simulation approach provides the required capabilites. The comparison indicates that application of particle based simulation shows the favourable attributes to solve this kind of flow problem. There are several simulation techniques for computational modelling based on molecular approximation such as Molecular Dynamics (MD), Stochastic Rotational Dynamics (SRD), Dissipative Particle Dynamics (DPD), Cellular Automata, Lattice Boltzmann Method (LBM) and Direct Simulation Monte Carlo method (DSMC) (Czerwinska, 2009). In the last two decades, the most popular and successfully implemented simulation methods in acoustics and fluid dynamics for similar types of channel flow behaviour at the micro- and nano-scale are LBM and DSMC. The LBM has been applied more frequently for solving the computational problems due to its simplicity, despite some deficiencies for the results, especially in the case of the higher Knudsen number transition flow regime. On the other hand, DSMC has been used for the simulation of gaseous media more frequently because it overcomes the errors related to compressibility issues. Nevertheless, in general, LBM is preferable over DSMC, when both methods are capable of simulating the problem, mainly because of LBM's simple collision rules and numerical efficiency; and conversely, DSMC's large computation time. A general overview and origin of the various models can be found in these papers by Benzi et al. (1992), Chen & Doolan (1998), Succi (2001), Bird (1994) and Oran et al. (1998).

Table 1. Comparison of Continuum and Non-continuum particle based approaches.

Approach	Continuum Approach (Euler and Navier-Stokes Equations)	Molecular Particle based Approach (LBM, DSMC etc.)
Features	• Assumes properties from other theories or experiments and only the motion is simulated (Czerwinska, 2009).	• Has to provide bulk properties as well as the motion at the same time and simulate molecular behaviours in a more realistic way (Czerwinska, 2009).
Advantages	• Continuum models of fluidic systems are very well developed and therefore computational methods applied for such configurations expected to give relatively fast, accurate and predictable results (Czerwinska, 2009). • Flow properties follow simple well defined theoretical and empirical relations which makes it easier to develop bulk properties during the simulation.	• Applicable for any kind of flow regime. • Flow properties defined by the molecular behaviour, hence it can be extended beyond the continuum range. • Simple implementation of boundary conditions.
Disadvantages	• Additional equations need to be incorporated to simulate the complex flow behaviour which makes it complicated (Czerwinska, 2009). • Require considerable computational resources during simulation (Hanford, 2008). • Numerical instability (Hanford, 2008).	• High computational cost. • Difficulty during the simulation of multidimensional flows as it requires large memory intensive program. • Simulation domain has to be kept to a limited characteristic length in order to maintain a reasonable computational time and cost.
Limitations	• Inability to simultaneously model following conditions (Hanford, 2008): ➢ Non-equilibrium condition ➢ Diatomic or polyatomic molecules or gas ➢ Nonlinearity ➢ Relaxation effect • Based on continuum assumptions. • Limited in the range of validity indicated by Knudsen number. • Infinitesimally short time of solid-fluid interaction which rules out the capability of simulating thermal transportation created by the solid-fluid interaction (Czerwinska, 2009).	• Limited to predefined collision rules. • Limited to particular collision grid or domain.

Lattice Boltzmann Method (LBM)

The Lattice Boltzmann Method is a mesoscopic approach developed based on the theory of cellular automata model with the Boltzmann equation approximation, which considers the particle distribution in a lattice divided into solid and fluid points (Aaltosalmi, 2005; Hanford, 2008). During one lattice time step, idealised particles move from one node to another with unit speed and propagate to adjacent lattice points, subsequently redistributing their momentum with predefined simple collision rules for succeeding collisions, which also involves boundary conditions and external forces (if any) at the solid-fluid interfaces (Aaltosalmi, 2005; Hanford, 2008). The particle collision rules are replaced by a relaxation term known as collision operator which produces the new particle distributions after the collisions (Bernsdorf, 2008). The Lattice-Boltzmann equation for particle density f_i can be written as (Aaltosalmi, 2005; Bernsdorf, 2008)

$$f_i(r + \lambda c_i, t + \eta) = f_i\,(r + t) + \Omega_i(r, t) \qquad (1)$$

where, $f_i\,(r, t)$ is the particle density distribution in a lattice site r at time t with a velocity c_i pointing in the lattice direction i; and λ and η are denoted for the lattice spacing and lattice time interval, respectively. $\Omega_i(r, t)$ represents the collision operator which is a model-dependent term described by the employed model such as in lattice-BGK model

(Bhatnagar et al., 1954), it is expressed as (Aaltosalmi, 2005)

$$\Omega_i(r,t) = \frac{1}{\xi}\left[f_i^{(0)}(r,t) - f_i(r,t)\right] \quad (2)$$

where, ξ is the relaxation time and $f_i^{(0)}$ is the equilibrium distribution of particles which can be chosen to produce the required behaviour of the particle. Details of this method along with the derivation of the afore-mentioned equations can be found in the literature (Bernsdorf, 2008; Aaltosalmi, 2005; Viggen, 2009).

Applications of LBM in Micro Channel and Acoustics Problems

Numerous researchers have conducted molecular simulations using Lattice Boltzmann Method (LBM) with applications in acoustics (Buick et al., 1998, 2000; Viggen, 2009) for different aspects. For instance, in the study of LBM conducted by Viggen (2009), a point acoustic source method was proposed to perform a lattice Boltzmann simulation of viscously damped cylindrical and plane waves. Good approximation was exhibited with the numerical results for the simulation of the Doppler effect, diffractions and damped standing waves. However, application of LBM was only feasible in the ultrasound frequency range and small spatial scales; and would take long computation times for lower frequencies or larger scales (Viggen 2009). Buick et al. (1998) applied LBM to simulate the linear sound waves, propagating in an unbound region and in a tube, in situations where the density variation is small compared to the mean density. Good agreements with the analytical expression were obtained. Even for a nonlinear sound wave simulation at higher intensity, expected features were observed using LBM simulation. They showed that LBM can successfully be employed for sound wave propagation and accordingly they extended their study for nonlinear acoustic wave propagation to simulating the developments of a shock front from a high-amplitude sinusoidal source (Buick et al., 2000). Although, it was found to be a useful approach, they suggested a progressive model for the consideration of wall boundary layer influences.

Many computational studies in micro flows (Niu et al., 2004), gas flows (Niu et al., 2007; Tang et al., 2008), micro channel (Aminfar & Mohammadpourfard, 2008) or nano channel (Suga et al., 2010), have investigated the implementation of LBM in transition regimes at Knudsen number ranging between 0.01 to 1. Niu et al. (2004) applied a new approach of the lattice Boltzmann BGK model developed based on the entropic LBM (Ansumali & Karlin, 2002), that uses the modified relaxation time in terms of Knudsen number for the simulation of planar Coquette flow and pressure driven micro channel flows. They studied the flow behaviour in the *Kn* range between 0.01 to 0.5 and found that the proposed model can predict the micro fluidic behaviours well. They extended the study (Niu et al., 2007) using the same method to address the issues related to boundary condition, relaxation time and regularisation for the micro-scale gas flows; and suggested that a range of Knudsen number flows can be modelled using LBM by introducing the effective mean free path with boundary effects and a regularisation procedure to ensure the presence of nonequilibrium moments of LBM within the defined Hermite space. Suga et al. (2010) also used the modified expression for effective relaxation time in conjunction with the bounce back/specular reflection (BSBC) and the diffuse scattering (DSBC) wall boundary conditions to evaluate the force driven flow behaviour in a combined nano channel which consists of a narrow channel with $Kn = 1.1$ inserted in another large channel with $Kn = 0.14$. Satisfactory results were obtained for the wider channel flow region, whereas the flow rate was over predicted for the narrower channel region, as $Kn > 0.5$. Tang et al. (2008) showed that current high-order and modified LBM are not yet able to capture the nonlinear flow behaviour in the Knudsen layer (i.e. evaporation layer) for the nonequilbrium gas flows. They proposed a wall function approach for the standard lattice BGK model, which can predict the nonlinear velocity profile accurately. However, they identified the need for an improved model for the quantitatively accurate prediction of the transition regime gas flows. Aminfar & Mohammadpourfard (2008) employed LBM to study the flow behaviour of isothermal pressure driven micro channel flow within the transition region $0.1 < Kn < 0.5$ and low Reynolds number $Re < 1$, using an expression for the complete momentum accommodation coefficient based on outlet Knudsen number and relaxation time based on the Knudsen number. They showed that the modified method could improve the results and reduce the number of iterations significantly for the large aspect ratio channel investigated, leading to reduced CPU time, which is very sensitive and important for large lattice sizes.

As described above, most of the cases evaluated the transitional flow regime at higher Knudsen number only in canonical flows such as gaseous flow in long micro channel, pressure driven micro channels, isothermal Coquette and Poiseuille flow, and combined nano channels (Suga et al. 2010). Although accuracy was only in the range of $Kn < 1$, very good prediction obtained for the range within $Kn \leq 0.5$; which indicates a clear research gap in the case of nano flows at the range of $Kn \geq 1$ using LBM. However, LBM shows promising results for those cases in that Knudsen range considering the comparison of outcomes with other molecular simulations. Beyond this range ($Kn \geq 1$), it seems that the relaxation time model needs to have more sensitivity to *Kn*, as suggested by the work in Suga et al. (2010). This implies that for solving the current case of acoustic propagation within nanoscopic fibres in air, there is a necessity of developing effective relaxation time model which can simulate the flow behaviour without any over-prediction caused by the sensitivity issues for high Knudsen number flows.

Direct Simulation Monte Carlo Method (DSMC)

DSMC is a particle based simulation method which describes the bulk properties of gas using the physical modelling of particle motion and collisions based on kinetic theory (Oran et al., 1998; Hanford, 2008). The distinct attribute of this model is that the particle motions and collisions are treated separately. The particle motions are modelled deterministically, while the collisions are modelled statistically (or probabilistically) (Oran et al., 1998; Hanford, 2008). Due to the employment of a probabilistic procedure for the computation of collisions, the computing requirement in this model becomes manageable and it gives flexibility during the simulation (Prasanth & Kakkassery 2006). The DSMC approach, like a CFD calculation, proceeds from a set of prescribed initial conditions and consists of four essential routine processes for each time step as described in the following (Oran et al., 1998; Hanford, 2008):

I. *Moving simulated particles and apply the boundary conditions*: In this stage, a computational domain is defined and the initial state of the molecules are specified in the domain of physical space, which is initialised by their molecular weight, diameter, number of internal degrees of freedom, internal energy, location in space and velocity. During the particle movement for each time step, appropriate boundary conditions are applied for

each molecule that can include: diffuse boundaries, specular boundaries, periodic boundaries, in-flow/outflow boundaries, and moving boundaries such as a piston boundary condition.

II. *Sorting, indexing and tracking particles*: In this stage of the simulation, particles are sorted to determine their cell location, which is a prerequisite for the next two steps: modelling collisions and sampling the flow field.

III. *Simulating collisions*: Collisions are simulated stochastically in this step. Several collisional modelling techniques have been employed successfully between randomly selected pairs of molecules within each cell. However, the currently preferred model is a no-time-counter technique (Bird, 1994), used along with the sub-cell technique, which enhances accuracy by ensuring that collisions occur only between near neighbours (Oran et al., 1998).

IV. *Sampling macroscopic properties*: Macroscopic flow properties are sampled in this final process which is performed by using the spatial coordinates and velocity components in a particular cell.

Applications of DSMC in Micro Channel and Acoustics Problems

Various applications in the field of nonlinear acoustics have been examined using DSMC such as molecular relaxation effects in monatomic and diatomic gas (Danforth & Long, 2004a; Danforth & Long, 2004b; Hanford et al., 2006), and numerical simulation of acoustics problems in planetary environments (Hanford 2008). It was observed that the deviation from continuum prediction for high Knudsen number flows can be distinguished with the use of DSMC. In addition, application of DSMC in various acoustic problems indicated that for the large range of *Kn* flows, all physical properties of wave propagation at molecular level such as absorption, dispersion, nonlinearities and molecular relaxation can be simulated without any modification in the model (Hanford 2008). Moreover, DSMC can be expected to be useful for efficient modelling of other acoustical phenomena related to boundary layer problems and boundary interactions, despite some imposed limitations in the wavelengths and sound source, which is usually restricted during the simulation with the target of low computational cost and time (Hanford 2008). This prior research gives an insight and aspiration for the possible implementation of DSMC for the nonlinear boundary interactions in the case of sound propagation through nano tubes.

Extensive simulation for sound wave propagation using DSMC was conducted by Hadjiconstantinou et al. (2001; 2002; 2003) in micro- and nano-channels and in simple gases at transitional flow regime, for continuum and noncontinuum transport conditions (Hadjiconstantinou & Garcia, 2001; Hadjiconstantinou, 2002; Hadjiconstantinou & Simek, 2003). During the molecular simulation of sound wave propagation at high Knudsen number flows (Hadjiconstantinou & Garcia 2001), DSMC was implemented to predict the variation of wave speed and attenuation constant as a function of oscillating frequency in the gaseous medium argon which was modelled as a dilute hard sphere particle for small amplitude oscillations. The acoustic wavelength was considered as the characteristic length for the comparison with molecular mean free path. Simulations were performed for those factors when the behaviour deviates substantially from the classical phenomena. For instance, the speed of sound deviates from classical adiabatic constant when the period of oscillation is comparable to the molecular collision time, and similarly, at high frequencies the attenuation rate seems to show significantly different non-classical behaviour in the low attenuation limit. For both of those cases DSMC produced a good agreement with the experimental data and approximate solutions of the Boltzmann equation. Moreover, their simulation (Hadjiconstantinou & Garcia 2001) by DSMC offered significantly accurate and consistent results for the variation of sound speed and attenuation constant over the whole frequency range, whereas, classical theories and molecular kinetic formulations based on Boltzmann equation could not capture the variation appropriately, especially at high frequencies, as reported in the surveys done by Cercignani (1988). In other simulations of acoustic wave propagation in micro- and nano-channels (Hadjiconstantinou 2002, Hadjiconstantinou & Simek 2003), where channel height was considered as the characteristic length, DSMC was used for the simulation of a dilute monatomic gas to verify the theoretical results produced by their presented extended theory of existing continuum wave phenomena devised by Lamb. Characteristics of axial plane waves, such as wave propagation and complex propagation constant, were investigated in two-dimensional narrow channels where the height is much smaller than the characteristic diffusion length based on the wave frequency, placing this case in the transition regime. Again, in this case, DSMC was able to capture the physics fairly accurately and showed consistent agreement with theoretical results. Further investigations in channel flow with non-continuum conditions have been conducted by these researchers using DSMC (Hadjiconstantinou 2006). This continued research work for channel flow at transitional regime indicates that DSMC has the potential attributes to simulate the wave propagation in nanoscopic fibres.

Comparison between LBM and DSMC

As discussed in earlier sections, both LBM and DSMC have been implemented successfully for the flow simulation in acoustics problems and in different size ranges of micro channel. However, simulations using LBM were conducted mostly for flow behaviour in channels with low Knudsen numbers and partly in acoustics, whereas DSMC has been employed frequently for sound wave propagation in acoustic problems with small scale channels. Nevertheless, it cannot be judged which method would be more suitable for the flow simulation with nanoscopic fibres based only on the application range of the methods. It would be more reasonable and practical if the method is chosen considering the limitations, capability, advantages and disadvantages associated with any particular problem. A comparison between LBM and DSMC is presented in Table 2 based on the literature review of the application of LBM and DSMC in fluid dynamics and acoustics. The table lists the advantages and disadvantages of both methods along with their limitations that constrain those models to be selected for a particular problem, which can also be a selection criterion for a phenomenon to be simulated. In the case of nanotubes, the selected method must have the ability to simulate the following mechanisms:

- *Heat conduction to the absorber material from the air.*
- *Consideration of thermal and viscous boundary layers and their interactions with the nanotubes.*
- *Flexibility of nanotubes and coupling with acoustic waves.*
- *Capability of simulating gaseous media.*

As indicated in Table 2, it was found that LBM shows improper results for the simulation of strong compressible me-

dia (i.e. gaseous media such as air) and is unable to simulate substantial heat transfer effects, which are the two important mechanisms that must be considered for the case of acoustic analysis of nanotubes. On the other hand, DSMC does not have any constraints for boundary conditions and is applicable for the whole Knudsen number range of flow regimes, thus being independent on continuum limitations. Moreover, Hanford (2008) indicated that sound propagation properties such as nonlinear phenomena and absorption are inherent in the algorithm, which makes DSMC more applicable for sound wave propagation. Considering those facts it can be concluded that DSMC shows the most potential as an appropriate method to simulate the acoustic flow propagation through the fibres at nano-scale. Based on this investigation of the applicability of molecular simulation between LBM and DSMC, it seems that DSMC would play a central role to analyse the acoustic flow behaviour of nano-scale fibres.

CONCLUSION

Investigating the absorption mechanisms of nanoscopic fibres is a potential research area and its significance is growing rapidly because of increased demand for thinner acoustic absorbers, combined with and recent trends of nanotechnology and nanomaterials. This study was intended to provide an overview on the potential simulation techniques to investigate the acoustic absorption of nanoscopic fibres. A rigorous review has been given on the applications, advantages and disadvantages of the two most popular particle simulation methods (LBM and DSMC) that could be implemented to solve the acoustic flow problem of nanoscale materials. This article has also discussed the phenomena most likely to be incorporated with the models for the simulation of nanoscopic fibres. Based on the previous research work on the transition flow regime for different Knudsen number and their application in sound wave propagation it can be concluded that DSMC is the most suitable model to be applied for this case as it has two major advantages such as the capability of simulating large Knudsen number flow and compressible media along with the effective simulation of heat conduction through the material. Future research will concentrate on using DSMC as a simulation tool to explore the absorption mechanisms of nanoscopic fibres. Results from these simulations will be employed to develop an optimum acoustic absorber and acoustic measurement will be conducted to verify the predicted performance.

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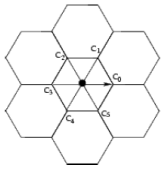
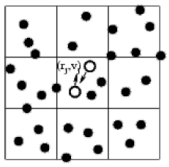
Table 2. Comparison on the advantages, disadvantages, limitations, applicability range of LBM and DSMC reported in the literature.

Simulation Method	LBM	DSMC
Approach	 The Collision grid for LBM (Czerwinska 2009) 1. Lattice gas based model. 2. Particles interact and move on the fixed lattice (Czerwinska 2009). 3. Kinetic Gas theory equations satisfied (Czerwinska 2009).	 The Collision space for DSMC (Czerwinska 2009) 1. Purely stochastic object oriented model. 2. Translation of particle position (Czerwinska 2009). 3. Calculation of collision rate; select collision pairs; adjust trajectories in the imposed mesh (Czerwinska 2009).
Advantages	• Simple collusion rules for the conservation of mass and momentum (Hanford 2008). • Simplification and discretisation of physical and velocity space (Hanford 2008). • Simple implementation of boundary condition and uniform grid (Aaltosalmi 2005). • Specific way of handling large computational meshes regardless of the complexity of the geometry of the structure (Bernsdorf 2008). • Computations can be performed on smaller grids with fewer iterations and the final values can be directly obtained without any time and space averaging process (Bernsdorf 2008). • Very high performance and nearly ideal scalability on high performance vector-parallel computers (Bernsdrof 2008). • Very efficient handling of equidistant Cartesian meshes generated by the semi-automatic discretisation of complex geometries (Bernsdrof 2008).	• Bypass continuum limitations (Hanford 2008). • Applicable for whole range of Knudsen numbers (Hanford 2008). • Minimised numerical complexity (Hanford 2008). • Computational flexibility for all Kn in a wide range of systems (Hanford 2008). • Not plagued by the boundary condition problems of kinetic theory predictions (Hanford 2008). • Sound propagation properties, such as nonlinear phenomena and absorption, are inherent in the algorithm, which make DSMC more applicable for sound wave propagation (Hanford 2008). • Unlike LBM, conservation laws are required to apply for individual molecules for molecule-surface interactions instead of using velocity distribution functions, which allows DSMC to be extended to include physical effects without major modifications in the basic procedure (Oran et al. 1998).

Disadvantages	• Solution of Boltzmann equation is improbable in the case of nontrivial gases or multidimensional flows, even using standard numerical methods (Hanford 2008). • Standard numerical method solutions only exist for simplified geometries or approximations to the Boltzmann collision integral (Hanford 2008). • Given information of boundary conditions has to be translated from macroscopic variable to distribution function (Aaltosalmi 2005).	• Time consuming computation. To minimise the computation costs, simulated domain length has to be negotiated to the range of a few wavelengths (Hanford 2008). • For much lower values of Knudsen number, DSMC extremely expensive to use (Oran et al. 1998). • A *priori* knowledge of the accommodation coefficients is required (Karniadakis 2005). • Produces unsteady flow simulation; hence, an ensemble of many computations is usually assembled and averaged to obtain acceptable statistical accuracy which results in large computational time marching process (Prasanth & Kakkassery 2006).
Limitations	• Inability to simulate heat transfer effect on transport properties (Hanford 2008). • Strong compressibility and substantial heat transfer cannot be simulated (Succi, 2001; Aaltosalmi, 2005; Bernsdorf, 2008). • Particle motion restricted to a lattice grid (Hanford 2008). • Difficulty in simulating flows at high Reynolds number (Aaltosalmi 2005). • Only applicable in the low Mach number limit to flows where there is a density variation which is much smaller compared to the mean density (Stansell & Greated, 1997; Buick et al., 1998).	• The cell size must be similar to the local mean free path (Prasanth & Kakkassery 2006) • The number of particles per cell must be roughly constant in order to preserve collision statistics (Prasanth & Kakkassery 2006). • Simulation time-step must be chosen so that particles only transverse a fraction of the average cell length per time-step (Prasanth & Kakkassery 2006). • Limited to binary collisions (Danforth & Long 2004a). • Extension of the model for multidimensional flows may create a memory intensive program, which could result in large computational time (Hanford 2008).
Potential Sources of Error	• Error mainly occurs due to the finite-size effects, compressibility effect and boundary effects (Aaltosalmi 2005). • Error due to finite-size effect caused by the limited number of grid points in the calculation lattice (Aaltosalmi 2005). • Compressibility errors can occur for the simulation in the case of both incompressible fluid and/or strongly compressible fluid. They are caused by the dependence of pressure on density and varying nature of the density in LBM assumptions (Aaltosalmi 2005).	• Statistical error corresponding to the stochastic nature of the method, which is induced by the use of a simulated molecule to represent a large number of actual molecules (Endo et al. 1998; Prasanth & Kakkassery 2006). • Deterministic error depends on the selection of numerical parameters such as the time-step, cell volume, and the total number of cell particles (Endo et al. 1998; Prasanth & Kakkassery 2006).

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