Characterization of $CO_2$ Flow Through Charged Carbon Nanotubes

Dimitrios Mantzalis, Nikolaos Asproulis, Dimitris Drikakis

Fluid Mechanics and Computational Science Department, Cranfield University, UK
E-mail: n.asproulis@cranfield.ac.uk

Abstract. The equilibrium transport of $CO_2$ through infinitely long charged and uncharged single-walled carbon nanotubes has been examined by employing molecular dynamics simulations. It has been shown that the molecular transport concludes into a Fickian diffusion for all the examined cases. Ballistic and single-file diffusion mechanisms have been met especially in cases where the degree of loading is low since at higher pressures the electrostatic interactions derived by the charge of the nanotubes is canceled by the stronger SWNT-$CO_2$ interactions.

1. Introduction
In 1991, Iijima [1] enriched the family of carbon based materials with a forth member known as Carbon Nanotubes (CNT). Numerous studies have been carried out since then, both numerical and experimental, aiming to shed lights in nanofluidics topics. The investigation of confined fluids to nanopores encompasses various aspects with the diffusive and adsorptive behavior of gas molecules in nanosized porous materials is considered of vital importance for a series of applications spanning from materials science and gas separation [2, 3, 4, 5] to nanoelectronics and biology [6, 7]. Liquids in confined nanoflows exhibit considerable differences in the diffusion mechanisms compared with flows in bulk. The differences can become more eloquent when the molecular diameter of the confined fluid obtains a size comparable to the characteristic length of the confining environment [8, 9, 10]. Over the past years, a great number of studies have been focused in studying the potential capabilities of CNTs in the fields of gas filtering, separation and storage. Both computational and experimental works have attempted to show that fluids can experience a transport inside single walled carbon nanotubes (SWNTs) characterized by orders of magnitude faster compared to traditional microporous materials [11] such as the zeolites, which are considered among the conventional means of filtering and storage. Their small pore size along with the nearly frictionless curved graphitic surfaces provide a rare combination of high selectivity and transport efficiency [12] making them ideal gas adsorbents [13].

However, the amount of studies relating with gasses’ nanofluidics is much smaller compared with water which is the greatest ”rival” [14, 15, 9, 8]; hydrogen keeps the greatest portion within the gas studies for energy reasons [16, 3] with carbon dioxide [5, 17, 18] to possess an even lower position in the ”preferences”. This tendency altered partially its direction since the green house effect exerted extra pressure in the already large volume of environmental problems that modern world faces. Carbon dioxide is known as the main gas responsible for the increase of temperature with the green house effect to be the most obvious result. The atmospheric concentration is continuously rising [19] with billions of tones of $CO_2$ to be produced each year...
basically originated from the fossil fuel plants and the vehicles. The increasing quantities of \( CO_2 \) dispersed in the atmosphere have emerged the scientific community in developing new CNT-based technologies aiming to reduce its concentration through sequestration and storage techniques [11, 20, 5, 18]. Recent numerical studies, have investigated how \( CO_2 \) is formulated in regions close to the CNTs [17, 5]. Both groups showed that carbon dioxide accumulated in the proximity of the carbon walls forming concentric layers with the tubes. This behavior has been considered as a \( CO_2 \)-philic feature accompanying the hydrophobic properties of the curved graphitic walls comprising into repelling for example water molecules from the carbon surface while they tend to stay together because of the stronger hydrogen bonding network that has been developed. The former property is explainable by the stronger attachment in case of \( CO_2 \)-CNT compared to \( CO_2 \) – \( CO_2 \) molecules. In one of our previous studies [5] we have shown that well defined patterns of \( CO_2 \) layers formations have been predicted, with the parameters that affect the adsorbate's behavior to be concluded in the pore diameter and the gas-structure interactions. Molecular simulations have been carried out indicating that besides the primary layers formed around the carbon surface, secondary and some times tertiary layers have been observed in the internal regions of the tubes depending on the pore’s width. Further focusing in the permeability and the selectivity of several porous membranes dedicated in gas separation both the adsorption and the diffusion processes have to be explored for the captured gas species. In this context, Skoulidas et al. [21] investigated the adsorption and the diffusion mechanisms of \( CO_2 \) and \( N_2 \) within SWNTs at room temperature for different pore widths. The employed techniques allowed them to study how two different gas species behave confined into the interior of rigid tubes. In case of carbon dioxide, both spherical and linear models have been studied predicting qualitatively equivalent performances for the adsorption isotherms, especially in cases where the loadings correspond to low pressures indicating that the most favorable adsorption area for the \( CO_2 \) molecules, at room temperature locates near the tube walls. These differences in the diffusivities tend to dissolve both for the transport and the self-diffusion showing that the computed diffusion mechanism is not of Knudsen-type but configurational. In this framework, Arora et al. [2] place in the adsorbate’s role nitrogen to investigate the adsorption and the diffusion within SWNTs using molecular simulations means for a wide range of tube diameters at 100 K and 298 K . They proposed a steric resistance that may lead in a core structure of nitrogen molecules characterized by a higher mobility compared with the molecules located in the annular layer enhancing molecular diffusion. Detailed visualizations revealed a worm-like topology when pressure approaches the saturation point. The narrowest tubes demonstrated the highest diffusivities in case of loadings corresponding to saturation pressure. Confined flows of \( H_2 \) and \( CH_4 \) within carbon nanotubes and zeolites with comparable pore sizes have been reported using molecular dynamics simulations [11]. Skoulidas et al. focused into the adsorption by the interior of the tubes and not by the interstices nor the external surfaces. Equilibrium adsorption isotherms have been calculated for pure hydrogen and methane in (10,10) SWNTs, namely, silicalite and ZSM-12 through molecular simulations with the three materials to present similar adsorption performances in a volumetric basis. Skoulidas et al. [11] have calculated self (\( D_s \)) and transport diffusion (\( D_t \)) by performing a series of simulations both canonical Molecular Dynamics (MD) and Monte Carlo (MC). Alike isotherms, self diffusion presented a difference of 3-4 orders of magnitude higher than in the zeolites, with the aforementioned deviations to presumably attributed in the innate frictionless carbon surfaces while transport diffusion to comply with the same strikingly difference among the three adsorbents. Higher pressures lead in a decrease of self diffusivities, with this drop to be more pinpointed in case of the SWNTs, as the fluid-fluid collisions include a dominated mechanism of momentum decorrelation over the fluid-tube collisions. Finally, unlike the calculated adsorption performance, the gas transport of the adsorbed gases is not significantly affected by the fluid-adsorbate interaction potentials since the rapid transport is induced by the no-correlation in the potential energy surface (PES).
The same group [22], performed a work for $D_s$ and $D_t$ of argon and neon in (8,8),(10,10) and (12,12) SWNTs for a wide range of loadings related to bulk phase pressures between 0 and 100 bar. To perform comparable results with the diffusivities of Ar and Ne in silicalite they used the same pressure range. Once more, Ackerman et al. [22] spotted the better performance of SWNTs over any known microporous adsorbent considering diffusion within them.

Although the great amount of studied that have been devoted in confined liquids within CNTs, pure or functionalized, little attention has been attracted for the charged CNTs. An electric field may generate important effects in nanofluid properties such as the transport behavior, the filling rate, the topology of the developed layers, while some claim that it may affect the fluid velocity [23]. Huang et al. [24] studied the developing water structures inside a charged (10,10) SWNT both negatively and positively. In case negative charges have been applied, they showed that water molecules favor the regular structures compared with uncharged SWNTs [25], while for positively charged tubes different orientations have been predicted. Benerjee et al. [26] have also studied how the charge influence apart of the structure of the water molecules the dynamics, proposing that the hydrophobic properties that characterize uncharged CNTs alter to hydrophilic. A change like this, leads to higher rates of filling but at the same time hobbles the flow through them.

In the present article, we focus in the diffusion mechanism of carbon dioxide in charged and uncharged (8,8) SWNTs, close to the room temperature. We investigate how the different degrees of filling within infinitely long SWNTs affects the diffusion mechanism in charged and uncharged narrow cylindrical pores. Furthermore, an extensive investigation has been made how the presence of different charges, both in sign and in absolute values, may affect the transport properties of the confined liquid. The results are presented with respect to the MSD as a function of time validating the existence of transition periods from ballistic to Fickian diffusion through a single file mechanism. In section 2 we present the simulation methodology along with the models that have been used while in section 3 a thorough discussion is offered. In section 4 we outline the main conclusions of the study.

2. Simulation methods and model
The governing system of equations for molecular dynamics is a system of Newton’s equation of motion

$$m_i \ddot{r}_i = -\frac{\partial V_i}{\partial r_i}$$

for each atom $i$. These are modelled as mass points with position $r_i$ and mass $m_i$. Each atoms potential energy $V_i$ is the sum of semi-empirical analytical functions that model the real interatomic forces. The atomic trajectories are calculated by time integration of Equation 1 for all atoms. The time integration is performed by a finite difference method such as the predictor-corrector method or the Verlet algorithm [27, 28]. Despite the apparent simplicity, the simulations are extremely demanding computationally due to huge number of atoms involved, even in the smallest systems. The nanotubes considered in the present work are of type armchair while their carbon atoms, $C^*$, are modeled as Lennard-Jones spheres, holding them in their equilibrium crystallographic positions during the simulations. In practice, carbon nanotubes are flexible materials mainly those with large pores; the choice of frozen curvature reduces the computational cost compared with a flexible model. Several studies have shown that the deviations observed into these two approaches can be initially ignored; self-diffusion computed for simple fluids in rigid tubes has been found to predict higher values compared with cases that flexibility is involved in the computations. This effect is negligible in narrower pores in cases where the confined liquid reaches high densities. The choice of frozen curvature in combination with the fixed relevant motion between $C^*$ atoms, reduces the computational cost compared with
a flexible model. However several studies have shown that the disagreements between the two techniques can be ignored in first place. In the present work, the nanotubes have been assumed to be rigid as in case of the narrow (8,8) SWNT, the $C^\ast$ vibrations are not expected to affect the diffusion mechanism of carbon dioxide molecules bearing in mind the small overestimation of self-diffusion as stated by Skoulidas et al. [11].

The present study is primary focusing in exploring the transport properties of carbon dioxide confined in uncharged and charged (8,8) SWNTs studying how the presence of a charge may affect the type of diffusion. Basing our work in previous studies that had investigated the above in confined water molecules, here we will adopt uniformly charged CNTs namely as $\pm0.01e, \pm0.1e and \pm0.5e$. The microcanonical ensemble (NVE) [28] has been used for the integration of the equations of motion, where the number of molecules in the system (N), the volume of the simulations box (V) and the system’s total energy (E) are kept constant. The calculations have been performed with LAMMPS [29] while the integration timestep is $\delta t = 0.5$ fs for the uncharged SWNT while for the charged the time step chose to be $\delta t = 0.25$ fs to avoid large fluctuations of the total energy and the temperature of the system arising from the presence of more electrostatic interactions. The system has been equilibrated for 200 $- 600$ ps, period that has been disregarded for the further calculations according to the charge of the CNTs.

To ensure that the temperature fluctuations will not will not considerably deviate from the set value of 300 $K$, a temperature rescaling has been employed during the equilibration period every 1000 timesteps achieving the temperature fluctuations to never exceed 34 $K$ in case of the charged SWNTs and 36 $K$ for the charged cases. After equilibrating the system, the temperature is allowed to fluctuate while $CO_2$ positions were stored every 5.0 $ps$ a value that has been found to minimize the correlation effects of the mean square displacements (MSD). For studying the diffusion mechanism only the MSD in the axial direction has been taken into consideration.

The modeling of carbon dioxide has been implemented through the 3-site model proposed by Murthy et al. [30]. A previous computational study [31] focusing in the transport properties of $CO_2$ in bulk has investigated that deviations among the linear models [30, 32, 33, 34] used in conjunction with MD simulations lead to small discrepancies in these properties; for example, the diffusion coefficient differs less than 5%. The SHAKE algorithm [35] has been applied so both bonds and angles in carbon dioxide are being reset to their equilibrium length and angular values, retaining the geometry of each adsorbate molecule rigid in practice, allowing longer time steps to be employed. $CO_2-CO_2$ interactions have been described through a 12–6 LJ potential, to calculate the dispersive terms, augmented by the electrostatic interactions. The employed parameters are $\varepsilon_{CC}/k_B = 29.0$ $K$, $\varepsilon_{OO}/k_B = 83.1$ $K$, $\sigma_{CC} = 2.785$ $\AA$ and $\sigma_{OO} = 3.014$ $\AA$ with the $CO_2$ mass being (44.010 g/mol). Partial charges have been assumed at carbon and oxygen sites with ($q_C = 0.5957e$) and ($q_O = -q_C/2$), respectively.

To represent the interactions between the CNTs and carbon dioxide, the AMBER force field [36] has been employed as described in our earlier publications [5] with the parameters to be ($\varepsilon_{CC}/k_B = 28.0068$ $K$) and ($\sigma_{C^\ast} = 3.4$ $\AA$). Additionally, cross interactions have been calculated through the Lorentz-Berthelot mixing rules. The long range electrostatic interactions are treated according to the particle-particle particle-mesh solver (PPPM) [37]. The length of both nanotubes is 150 $\AA$ however to ensure that the finite size effects this choice do not affect our calculations, as proposed by Striolo [9], the MD configurations have been replicated four times towards the axial direction. The diameter of the (8,8) SWNTs have been defined as the distance between the centers of two carbon atoms laying opposite in the tube. To implement the PPPM solver, the nanotubes have been placed along the Y axis in a rectangular parallelepiped computational boxes with the X- and Z- directions with size of 50 $\AA$. The size in the Y-direction equals with the length of the nanotubes, while periodic boundary conditions have been assigned to all three directions.
3. Results and Discussion
The transport mechanism within a CNT is mainly affected by the interactions between the surface and the confined molecules along with the pore width of the membrane [38] while the ratio of the fluid’s molecular size to the pore’s diameter [39] is a factor with equivalent influence. To explore the diffusion mechanism of fluid molecules through a CNT the scaling behavior between the MSD and the time can be employed. The diffusion transport in narrow pores is broadly classified in the following mechanisms; The normal-mode or Fickian diffusion where the molecules are able to surpass each other in the flow direction with the MSD to scale linearly with time noting that this type of diffusion is an innate fluid property in bulk systems. The single-file diffusion (SFD) where the MSD scales with the square root of time being met in cases where the degree of confinement is higher and the molecules are not allowed in passing each other. The last type of diffusion is the ballistic mechanism where it scales proportional to the square of time and the flow can be characterized by a higher degree of coordination. The three previously described diffusion mechanisms can be expressed through the following equations as [9, 8]

\[
\lim_{t \to \infty} \langle (y(t) - y(0))^2 \rangle = 2Dt \tag{2}
\]

\[
\lim_{t \to \infty} \langle (y(t) - y(0))^2 \rangle = 2S\sqrt{t} \tag{3}
\]

\[
\lim_{t \to \infty} \langle (y(t) - y(0))^2 \rangle = 2Bt^2 \tag{4}
\]

where \( \langle (y(t) - y(0))^2 \rangle \) is the axial MSD of the adsorbed molecules [40], \( \langle \rangle \) refers to the average over the molecules into the interior of the SWNT and \( y(t) \) is the position of a molecule within the nanotube in its axial direction as a function of time \( t \). In Eqs. 2-4 the coefficients \( D, S \) and \( B \) denote the Fickian, single-file and ballistic diffusion mobilities respectively [41, 42]. It has been shown that the constrained molecular diffusion is the main transport mechanism of gases in micro- and nanopores, channels with pore widths up to 2 \( \text{nm} \) [43], expecting to obey the Fickian dependence in general. However several studies have shown that the diffusion mechanisms presents a more than one stage mechanisms with the final observation to be in most of the cases the Fickian one. The type of diffusion is more complicated in narrow nanotubes whereas in wider tubes things are more lucid. Aiming to enhance our understanding in diffusion mechanism within the uncharged and charged (8,8) SWNTs, the double logarithmic plots of the axial MSD against time along embraced with the typical plots for the three diffusion mechanisms are illustrated in Figs. 1-4 for different \( \text{CO}_2 \) loadings.

Figure 1 illustrates the MSD obtained for 10 \( \text{CO}_2 \) confined molecules in differently charged (8,8) SWNTs corresponding to +0.01e,-0.01e, +0.1e,-0.1e and 0.0e; however more simulations have been carried out for additional charges. The conclusions generated here can be easily extended in all cases that have been simulated. The mechanism of diffusion is explained through a double logarithmic plot of the MSD as a function of time. For all the cases the results illustrate a complex diffusion mechanism when 10 molecules have been confined. For the uncharged SWNT, as it has been described earlier, a ballistic-type mechanism is illustrated persisting for \( \approx 100 \ \text{ps} \) followed by a short period of SFD while it concludes to the expected Fickian diffusion. Interestingly, compared to previous studies where the single-file mechanism is not observed, in the present work we find evidence of it as it has been proposed by others [44, 45] to explain the anomalous transport of nanoconfined carbon dioxide molecules mainly in short nanotubes. However it still persists for short periods indications that can be explained though the same reasons that the no evidence of SFD has been. The length of nanotubes can be recognized as a factor that may influence the computations. Charging the nanotube with −0.01e, we observe almost the same behavior with the uncharged case. The diffusion initiates
with a ballistic mechanism followed by a SFD and a Fickian type. The only difference that can be marked is located in the time interval where the Fickian diffusion is observed obtaining higher values of displacements. Increasing the charge to $-0.1e$ the electrostatic interactions affect the diffusion within the SWNT; the ballistic mechanism is restricted to $\approx 10$ ps while the SFD is visible for up to $90$ ps of simulation time with the Fickian mechanism at longer periods. Positively charging the SWNT, we observe once more some worth noting changes. In case a $+0.01e$ charged is obtained, the ballistic mechanism persists for $\approx 400$ ps accompanied by a SFD for an additional period of $\approx 700$ ps suggesting that the combination of the positively charged SWNT with the charged sites located in $CO_2$ produce a considerable force component in the already acting forces between the adsorbate and the adsorbent. Further increase in the charge does not produce a significant change in how the 10 molecules diffuse within the tube apart of adding a short period inside the ballistic mechanism where the diffusion acquires a SFD-like type which in practice is a deceleration which requires further studying.

Increasing $CO_2$ loading to 30 molecules (see Fig. 2) the type of diffusion alters with the impact of the charged CNTs to start reducing. In the uncharged case, the collective motion persists for a considerable shorter period ($\approx 20$ ps) while it is followed by a SFD and Fickian diffusion. Charging a SWNT with $-0.01e$, as in case of 10 molecules, does not have a practical impact in the diffusion mechanism compared with the uncharged SWNT. However, increasing the charge to $-0.1e$ significantly alters the diffusion of the 30 $CO_2$ molecules within the SWNT. The ballistic period is extended to $\approx 100$ ps with additional prolonged period with a single-file type. On the contrary, when the 30 molecules have been confined in a positively charged environment, we observe the greatest changes; the ballistic period is further suppressed compared not only to the rest cases in the 30 molecules framework but also with the 10 molecules case. The $400$ ps of ballistic diffusion in case of 10 molecules, with a $+0.01e$ applied, becomes $\approx 10$ ps
followed by a Fickian diffusion. Increasing to $+0.1e$ give birth to SFD even for a short period lasting $\approx 10 - 20 \text{ ps}$. When larger loadings (60 molecules see 3) are studied corresponding in higher pressure, the effect of the charge tends to diminish. The latter is mainly explicated by directly comparing the uncharged scenario with the charged cases. When $0.0e$ is employed there is a short ballistic period while in the charged cases this period is either vanished or remains unaffected ($-0.1e$). The aforementioned suggests that as the amount of the adsorbate increases the effect of the electrostatic interactions between the pore and the $CO_2$ molecules decreases; with the electrostatic effect to be canceled. The aforementioned is more lucid when the loading of the adsorbate approaches the number of adsorbed molecules near the saturation pressure where in practice there are no differences (see 4).

4. Conclusions
To summarize, we have investigated the axial diffusion of carbon dioxide within infinitely long narrow charged and uncharged SWNTs. It has been shown that in case of the uncharged (8,8) SWNT independently on the degree of filling a considerable long-time diffusion mechanism occurring for up to 400 ps. In first place the MSD follows a ballistic mechanism as a function of time except in the case where the adsorbate corresponds to close to saturation pressures. As the variable of charge is inserted into the simulation we observe that there is an influence in the diffusion mechanism within the tube. However the degree of influence is not of the same importance as the amount of loading especially in cases of higher amount of adsorbate. It seems that at higher pressures the CNT-$CO_2$ electrostatic interactions are canceled by the stronger van der Waals interactions between them. The results exhibited in the present study can be proved valuable in engineering CNT-based devices including carbon dioxide that require an in depth understanding of its flow in molecular level.
Figure 3. Mean square displacement along the pore axis for 60 carbon dioxide molecules confined within a (8,8) SWNT. The grey line represents the typical diffusion mechanisms of the Fickian type. The red, blue, green, black, purple lines are for +0.01e, -0.01e, +0.1e, -0.1e, Uncharged SWNTs respectively.

5. References

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Figure 4. Mean square displacement along the pore axis for 120 carbon dioxide molecules confined within a (8,8) SWNT. The grey line represents the typical diffusion mechanisms of the Fickian type. The red, blue, green, black, purple lines are for $+0.01e$, $-0.01e$, $+0.1e$, $-0.1e$, Uncharged SWNTs respectively.

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