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Carbon dioxide adsorption through carbon adsorbent structures: Effect of the porosity size, chemical potential and temperature

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ABSTRACT

In the present paper, the carbon dioxide molecule adsorption through nanoporous carbons has been studied at 248 [K], 298 [K] and 323 [K]. The 3-stage graphite, turbostratic carbon and activated carbon have been taken into account as nanoporous carbon structures with nearly the same simulation box size, i.e. 30 × 30 × 30 [Å]. The numerical experiments of the adsorption phenomenon of CO_2 molecule have been successfully achieved by user-written massively parallel codes via MPI paradigm which has been carefully examined and evaluated including electrostatic charges, 3-site CO_2 molecule and linear scalability issues for the parallel programming purposes. By taking advantage of the parallel programming and efficient algorithm paradigm, very accurate outcomes and highly portable implementations for High Performance Computing (HPC) have been obtained. The effect of nanoscale pore size and its distribution for the above-mentioned nanoporous carbons which are generated via user-written C++ codes, have been studied by means of scalable parallel code. In the first stage, the carbon dioxide at bulk state has been investigated. Afterwards, the adsorption simulations have been achieved on regular and nearly regular nanoporous structures, i.e. 3-stage graphite including 6 [Å] and 12 [Å] interlayer distances (pore width), receptively. The activated carbon structure which is generated via Reverse Monte Carlo in Pikunic et al. (2003), has been considered for numerical experiments of adsorption as well. The comparison among these nanoporous carbons reveals a cross-over trend beyond a specific Adams constant value and this issue can be found out for the above-mentioned carbons as well as bulk case.

1. Introduction

1.1. General introduction

The consumption of fossil fuels as well as other human activities have led to a huge amount of carbon dioxide in the atmosphere. This issue makes one of the primary environmental issues facing the humanity. Basically, a great amount of carbon dioxide sustains greenhouse gas effect as discovered in the early 20th century [2,3]. Additionally, it is not suitable for durability of most of human-made infrastructures, e.g. cement carbonation [4] conducting reinforced concrete bars corrosion issue. The protection issue and adsorption of carbon dioxide gas may be one choice among the available way-outs. The adsorption in nanoporous materials is widely applied for separation purposes in several industrial and geological applications. Furthermore, it is also applied in pollution control, mixture separation, environmental protection, water purification and gas storage purposes [5,6]. Moreover, the gas adsorption experiments are extensively applied as very useful way in characterization of porous materials in materials science community [7,8].

1.2. Problem statement

Nowadays, the computational materials science takes advantage of High Performance Computing and there are a bunch of algorithms dealing with thermodynamic, structural and dynamic bulk fluid properties. The Monte Carlo simulations are substantially applied in discovery process at micro and meso scales. The main advantage of the above-mentioned simulations is that they link macroscopic and microscopic behaviors involving the statistical mechanics as a scientific

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Nomenclature

ε/B_k	first parameter of Lennard-Jones over Boltzmann's constant in [K]
ε_0	$8.854187817620 \times 10^{-12}$ ideal gas constant in $[C^2.N^{-1}\,m^{-2}]$
$\varepsilon_{ij}^{A,B}$	first Lennard-Jones parameter in [J]
$\mathfrak{R}$	$N_A \times B_k = 8.314462145 \times 10^{-03}$ ideal gas constant in $[KJ.mol^{-1}\,K]$
σ	second parameter of Lennard-Jones in [Å]
$\sigma_{ij}^{A,B}$	second Lennard-Jones parameter in [Å]
dr_{max}	maximum translation for stochastic displacement in [Å]
dt_{max}	maximum rotation angle for stochastic rotation in [°]
θ	angle between O=C=O in CO_2 molecule in [°]
a	empirical constant 24.7233×10^{-3} $[Pa.m^6.mol^{-2}]$
b	empirical constant 0.0266×10^{-3} $[m^3.mol^{-1}]$
B_k	Boltzmann's constant $1.3806488 \times 10^{-23}$ $[J\,K^{-1}]$
e	elementary charge $1.6021766208 \times 10^{-19}$ [C]
h	Plank's constant, $6.626070040 \times 10^{-34}$ [J.s]
l	distance between C and O in CO_2 molecule in [Å]
N_A	Avogadro's constant $6.022140857 \times 10^{23}$ $[mol^{-1}]$
q	point charge in [e]

Scalar quantities

$\beta = \frac{1}{B_k T}$	in $[J^{-1}]$
ℓ_x	length of simulation box in [Å]
ℓ_y	width of simulation box in [Å]
ℓ_z	height of simulation box in [Å]
μ	chemical potential in [J]
μ_{ex}	excess chemical potential in [J]
$\sqrt{\alpha}$	width of the screening Gaussian $[Å^{-1}]$
E_P	efficiency in [–]
$P_{Creation}$	probability of creation in [–]
P_{Delete}	probability of deletion in [–]
S_P	speedup in [–]
T_P	runtime of the parallel algorithm with P processors in [sec]
T_S	runtime of sequential algorithm in [sec]
U	total energy of interactions in [J]
$U^{A,B}$	energy between two molecule in [J]
U_{EW}	electrostatic energy using Ewald summation in [J]
U_{Real}	short-term energy counterpart in real space in [J]
$U_{Reciprocal}$	long-range energy counterpart in Fourier space or so-called reciprocal space in [J]
U_{Self}	self-energy subtraction term in [J]
Λ	$\Lambda = \frac{h}{2\pi B_k T\,m}$, De Broglie wavelength in [m]
H_{iso}	isosteric heat of adsorption or so-called isosteric enthalpy in $[KJ.mol^{-1}]$
m	mass in [K g]
N	number of guest molecules or atoms in [–]
P_{vdW}	pressure in [Pa]
q_i^A, q_j^B	charge [e]
R_{cut}	cut-off radius in [Å]
$r_{ij}^{A,B}$	displacement between two molecules before the application of the periodic conditions in [Å]
r_j^A	atoms positions of molecule A in [Å]
r_j^B	atoms positions of molecule B, in [Å]
T	temperature in [K]
U_{new}	new energy of the molecule after the translation dr and rotation dt in [J]
U_{old}	energy of the molecule before the move action in [J]
V	volume of simulation box in $[Å^3]$
P	number of processors in [–]

Vector quantities

ρ	density in $[m^{-3}]$
P	pressure in [Pa]
U	potential energy in [K]
W	virial energy in [J]

backbone. The use of the computational aspects involving the appropriate algorithms gives rise to numerical solutions for basic and fundamental equations of the statistical mechanics. This is a great benefit for huge and very huge thermodynamic systems including a great amount of molecules and inter-molecule interactions. Basically, the computer methods are constantly growing in the past few decades and this matter makes too much easier to study the bulk fluid models from hard sphere assumptions or called 1-site models to the multi-site molecules. The very early computer methods for the liquids trace back to the early fifties [9]. The computer method known as Metropolis Monte Carlo has been mainly established to obtain the thermodynamic properties of bulk fluids. The main background of the above-indicated method is the use of probability rules [10,11]. The use of appropriate ensemble is crucially required to explore more complex gas and fluids and fluid mixtures. The numerical simulations are very useful to discover and understand the experimental results. Despite the fact that the computational aspects have extremely enhanced, there are also too many restrictions about number of molecules, simulation box size arising from disorder structures and non-periodical issues. Furthermore, it is necessary to take into account the electrostatic charges and other relevant issues in the computations to get more accurate numerical results. The multi-site molecular considerations increase number of iterations and interactions during calculations too. Traditionally, these computations have been handled via sequential codes. The main deficiency of these codes is that they are not able to take advantage of modern multi-core hardware architectures.[1] That is why the parallel programming is applied to handle this job and to reduce runtime using CPU or GPU computing [12]. This issue significantly speeds up the discovery process for large and very large molecular simulations involving an extremely great amount of iterations due to random translations and rotations for multi-site molecules and molecules mixture adsorption [13,14]. Consequently, very accurate and fast parallel computer method for adsorption is crucially needed. The outstanding issue in the computer methods in adsorption simulation is to provide accurate and highly scalable computer methods in which portability issue is fully satisfied.

As mentioned earlier, the adsorption simulations of carbon dioxide are carried out on nanoporous carbon materials (slit-shaped carbons and activated carbon). Clearly, the adsorption process is essentially controlled by several parameters such as: interactions between fluid-fluid, fluid-solid, pore size and thermodynamic conditions. The main

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[1] We note that there are several publicly available GCMC codes (e.g., https://www3.nd.edu/ed/research/cassandra.html, https://pypi.python.org/pypi/RASPA2.). Some of these packages take advantage of OpenMP parallelization. OpenMP parallel programming is only suitable for shared-memory computations, i.e. workstation computing. As a result, OpenMP parallel programming cannot be used in supercomputing and large clusters. Additionally, the use of the high level programming, e.g. Python may provide reduced performance due to technical issues on modern computational hardware. MPI parallel programming using low level programming (MPI C/C+ +) overcomes these issues for supercomputing.

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