Poster presented at the 65th international astronautical congress (IAC 2014): our world needs space, 29th September - 3rd October 2014, Toronto, Canada.
Proceedings published by the International Astronautical Federation are available (ISBN: 9781634399869)

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Equilibrium Molecular Dynamics Modelling of Diffusion and Adsorption of Fluids in Armchair Single Walled Carbon-nanotube

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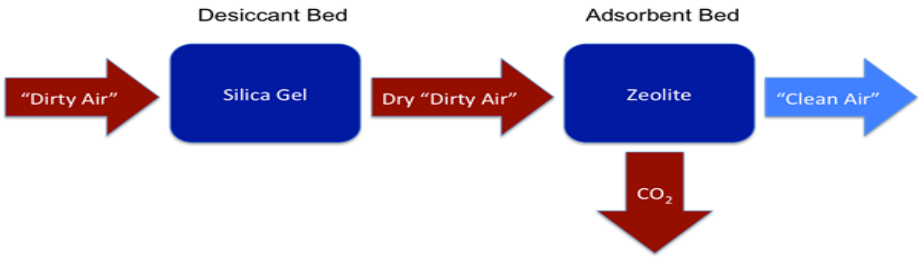
Introduction

Frequently flying modules and nodes on-board the international space station (ISS) to meet carbon-dioxide/oxygen removal requirement will be too expensive making their application impractical. Currently, the (ISS) have the carbon-dioxide removal system (CDRA), multifilters for advanced water recovery and the new Sabatier assembly. These systems and process ensure the safe removal of Co_2 from the ISS with the use of zeolite membranes and filters. This work models adsorption of Co_2 in single-walled carbon nanotubes (SWCNT) with possible application as a filter membrane.

Fig. 1 Co_2 Removal Process in ISS



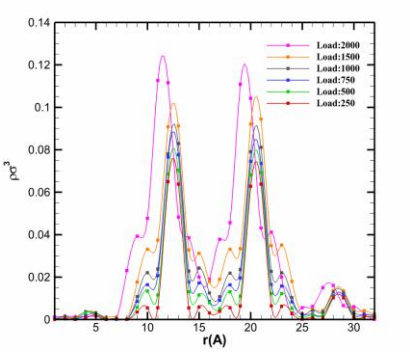
Computational Process

A simulation of CNT configuration of (10x10) and (16x16) with a length of 60 Armstrong is chosen, with periodic boundary conditions. The Lennard jones model describes the non-bonded interaction of Co_2 and Argon with $\varepsilon_{Co2\text{-}Ar}/k_B$ =235.9K. 50ps equilibration time and 1fs simulation time was chosen with a time step of 0.005τ.

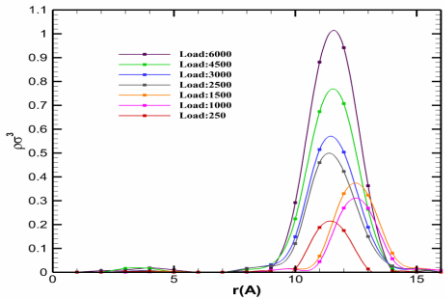
Fig. 2 Sabatier assembly module (Node 3) ISS.

Results

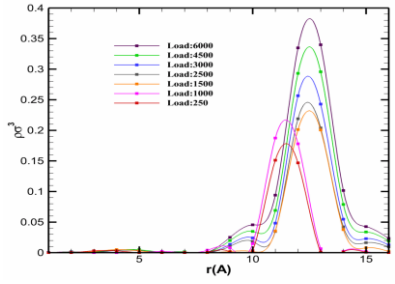
Adsorption of Argon for (10x10) SWCNT



Adsorption of Ar-Co_2 for (10x10) SWCNT



Adsorption of Ar-Co_2 for (16x16) SWCNT



Conclusion

The study shows that Co_2 sticks and forms adsorption sites and layers around the walls of carbon- nanotube.10x10 CNT is found to trap and remove more Co_2 with the aid of argon atoms and can be used as a filter membrane in the international space station.

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2014-12-31
International Astronautical Federation (IAF)
https://dspace.lib.cranfield.ac.uk/handle/1826/11499
Michael Kio, Nickolaos Asproulis Laszlo Konozsy and Dimitris Drikakis. Equilibrium molecular dynamics modeling of diffussion and adsorption of fluids in armchair single walled carbon-nanotube. Proceedings of the 65th international astronautical congress (IAC 2014): our world needs space, 29th September - 3rd October 2014, Toronto, Canada.

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