Can nanoscale pores be used to separate H_2 and D_2 ?
An Executive Summary

Gas separation techniques are used worldwide and is a big part of industrialisation. For example, separating nitrogen in air can help us produce fertilisers for agriculture. Using such techniques, we hope to get the most amount of desired products, and at a higher rate and lower price. Understanding these flowing behaviours at the molecular level, we can apply it to water filtration and desalination in water treatment plants[1]. Therefore, we are proposing the question whether nanoscale pores can be used to separate hydrogen (H_2) and deuterium (D_2), which can be done if the nanoscale pores satisfy certain requirements, namely its width, length, interior design, and stability.

The nanoscale pores can be visualised as tiny tunnels with some length L, some width w. w should be wide enough for desired molecules to pass through. Given a pressure difference, nanoscale channels (w=10nm-100nm) have been shown[2] to let helium (He) gas through. Both H_2 and D_2 can pass through similar channels with similar values of w, if they are both gases in some set conditions.

We would not need to consider L, as the flow rate Q is independent of it[2]. Q is the number of particles passing through the nanoscale pore per second. As L increases, more time is needed to cross it, therefore a slower rate. Q increases as L decreases[2]. However, this classical proportionality, as described by **Knudsen diffusion**, is invalid for He flowing through graphene nano-channels[2]. We must visualise He particles bouncing off the walls of the channel, as if light is shone on mirrors. Light can pass to the other side with no obstacles[1]. Similarly, He, D_2, and H_2 can pass through the nanoscale pores without hindrance, with the particles bouncing off the walls of the pores. This is called **specular surface scattering**[2]. Thus, L does not affect Q of H_2 and D_2, and does not need to be considered while constructing our nanoscale pores.

The main obstacle for separating D_2 and H_2 is to find their critical difference. D_2 is an isotope of H_2. The former is heavier, as it has one more neutron in the nucleus than the latter. Both have the same number of electrons, thus having the same chemical properties, and both have the same molecular diameter. Using the classical theory of **Knudsen diffusion** as discussed, we would expect Q of the heavier D_2 to be greater[2]. However, the contrary has been observed[2]. This phenomenon, named the **reversed isotope effect**[2], is true only if we treat particles as waves.

Matter has both wave and particle properties. The relation can be expressed in the following equation: $\lambda_b = \frac{h}{mv}$. For a particle having mass m and velocity $\mathbf{v}$, it has a wavelength of λ_b. (h is the Planck's constant.) We can see that as m increases, λ_b decreases. The wavelength of a D_2 molecule is thus shorter than that of a H_2 molecule, which helps us in distinguishing between the two. Within the graphene nanotubes, specular reflection[2] differs for the molecules. H_2 bounces off the walls of the nanoscale pores less than D_2[1], therefore H_2 gas flows much faster than D_2.

To achieve separation, we would want H_2 transport to be highly promoted, and D_2 transport to be highly inhibited. Similar materials has been synthesised and tested[2]. Nanoscale channels made of roughened graphite and molybdenum sulphide (MoS_2) inhibits the flow of He[2], since it takes more bounces off rougher surfaces for the He particles[1]. Oppositely, channels made of graphite and hexagonal boron nitride (hBN) promotes He flow[2], since it takes less bounces off smoother surface for the He particles[1]. Hence, the interior walls has designed have to be smoother for H_2 and rougher for D_2, in order to separate them.

The nanoscale pore synthesised has to be stable in some set conditions[2]. The nanomaterials are shredded down to only a few atoms thick to make the atomically flat walls for the nano-channels, provided they do not collapse under some optimal conditions. The material used has to possess similar properties.

More research and experiments can be done to synthesise and examine the optimal nanoscale pore. The exact techniques, conditions, and mechanisms for separating H_2 and D_2 should be studied in detail. Furthermore, the proposed material does not guarantee full purity of the desired product. The product (H_2) after separation may have some D_2 impurities, as some D_2 gas may get through the channel the same rate as the majority of the H_2 gas. Future research and evaluation should be done to decrease this probability significantly.

In conclusion, given the correct materials and conditions, nanoscale pores can be used to separate H_2 and D_2. By exploiting the fact that the two molecules have different wavelengths, thus different flow rates through nanoscale channels[2], the material used should promote H_2 transport and inhibit D_2 transport. It should be stable in some set conditions, possessing a width w to permit molecules to pass through, and independent of length L[2]. Further research and detailed experiments should be conducted to evaluate and improve the proposed method. We can have studies on increasingly complicated systems in the future. For example, separating different isotopes of carbon, or some mixture of gases. The end goal will be to further expand its use, utilize it effectively, and ultimately industrialise it, so we can improve and provide to our society in its development.

Total word count: 897

3.1 3.2 3.3 3.5 3.4 3.6

References

[1] Atomic-scale ping-pong, Phys.org, 20 June 2018
https://phys.org/news/2018-06-atomic-scale-ping-pong.html

[2] Keerthi, A., Geim, A.K., Janardanan, A. et al. Ballistic molecular transport through two-dimensional channels. Nature 558, 420–424 (2018).
https://doi.org/10.1038/s41586-018-0203-2

Index of comments

1.1 General comments

1.2 Technical criteria

1.3 Technical argument comments

1.4 Rubric comments

1.5 7(a) The introduction attempts relate the importance of work to a more general example but the context (status quo) is not discussed

1.6 1(a) VISION

1.7 7(b) the introduction does not prepare the reader for what comes next.

1.8 10(a) the topic sentence does not reference what the rest of the paragraph will be about

1.9 2(a) this is really hard to follow and too technical.

1.10 2(b) concepts in this paragraph are not explained clearly and hard to follow - why is Knudsen diffusion invalid for He?

1.11 2(c) Knudsen diffusion is jargon

2.1 1(c) TECHNICAL PROBLEM

2.2 12(e), (h)

2.3 10(b) TS test fail

2.4 1(e) NEW SOLUTION

3.1 1(f) OBSTACLES

3.2 1(g) DISCUSSION/ FUTURE/ PROGNOSIS

3.3 8(a) The conclusion does not address what impact the research has - this links to not having defined a technical problem in the introduction. If the problem being solved was known, it would have been easy to answer how the work changes the world in a narrow way

3.4 4. There is some attempt to apply critical thinking and logic when discussing future research. The summary does not probe the usefulness of the techniques presented at all, nor does it present why the advances in the field are needed.

3.5 3. The summary misses the mains points presented in the abstract of the paper completely. There is no reference to some crucial discoveries made in the paper.

3.6 5. The summary attempts to answer the questions but it goes off track. The writing gets caught up in defining the equations at times