Proton Transfer in Ice:

Evaluation of Proton Diffusion Rates in Ice, Based on the Density of D_2O and H_2O

Research Experience for Teachers

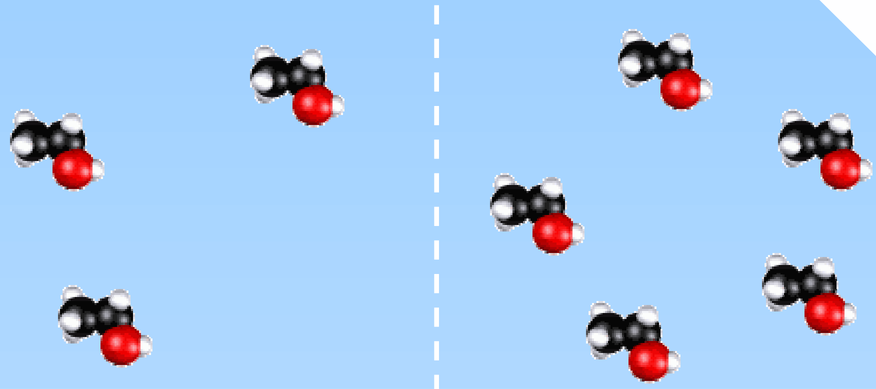
Mentor: Rafael Tadmor

Chae Meadows
Teacher grades 5-8, Casmalia School District

Funded by

Introduction

Physical Chemistry Department



Diffusion occurs as a consequence of the spontaneous and random thermal motion of atoms, molecules, and particles. This results in matter moving from areas of higher concentration to areas of lower concentration. While molecules are constantly moving into and out of each area, the net flow is from areas of higher concentration to areas of lower concentration, and, generally, the greater the difference in concentration, the faster the rate of diffusion will be. The end result would be an equilibrium, a constant concentration of each of the components throughout the volume available to diffusion.

The Experiment

The diffusion studied in this experiment was on the atomic level, that of protons hopping of hydrogen atoms from one H_2O molecule to another in ice. Proton transfer is a random process which leads to diffusion of the protons. It is commonly believed that proton transfer takes place in ice without the introduction of a stimulus into the environment. If this is true, then proton transfer should occur in samples of ice made from heavy or deuterated water (D_2O) fused with ice made from pure H_2O and stored at –20° C during the length of an experimental run.

Don’t Drink the Water!

Milli-Q water has been filtered and treated.

Preparing the Samples

Two 5cm trays are prepared. One with D_2O and one with H_2O.

The Deep Freeze

4° C

–20° C

The Experimental Run Begins

Once they are frozen, they are fused together with a drop of H_2O and then placed in the –20° C cold room.

Experimental

The idea behind the experiment was to have the ice cell that was formed divided into one centimeter sections and the density of each section calculated. If proton diffusion had occurred, there would be changes in density of the former place of D_2O and the former place of H_2O, the region where the heavy water used to have been decreasing in density as the region where the pure water used to have been increased in density, beginning at the interface of fusion of the two ice cells and diffusing over time throughout the sample.

Divide and . . .

The ice was removed from the tray, broken into 1cm sections, and then placed in labeled vials.

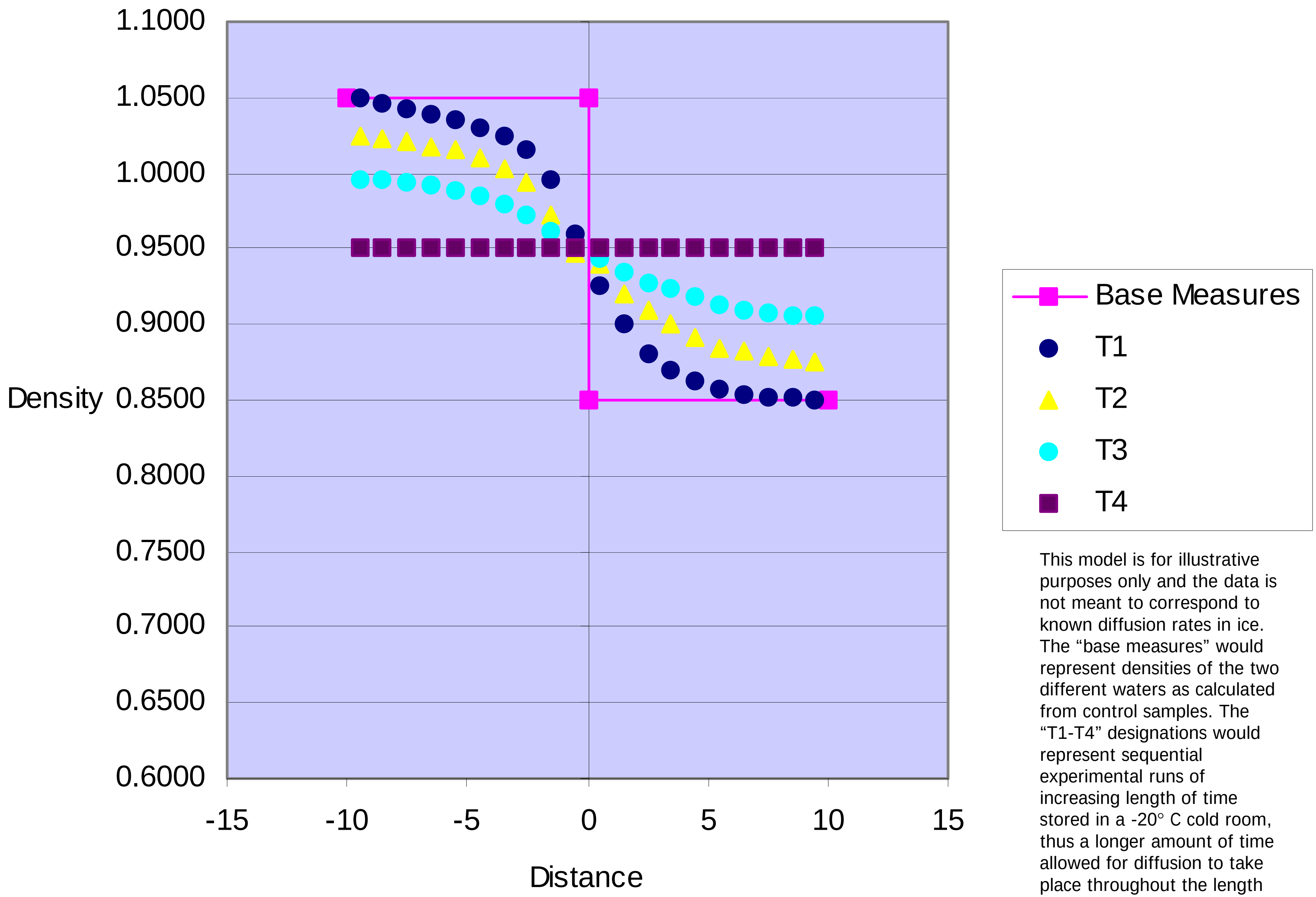
Measure

This scale measures to the 100,000th place. The samples in the vials were weighed and their density calculated.

Analyzing the Data

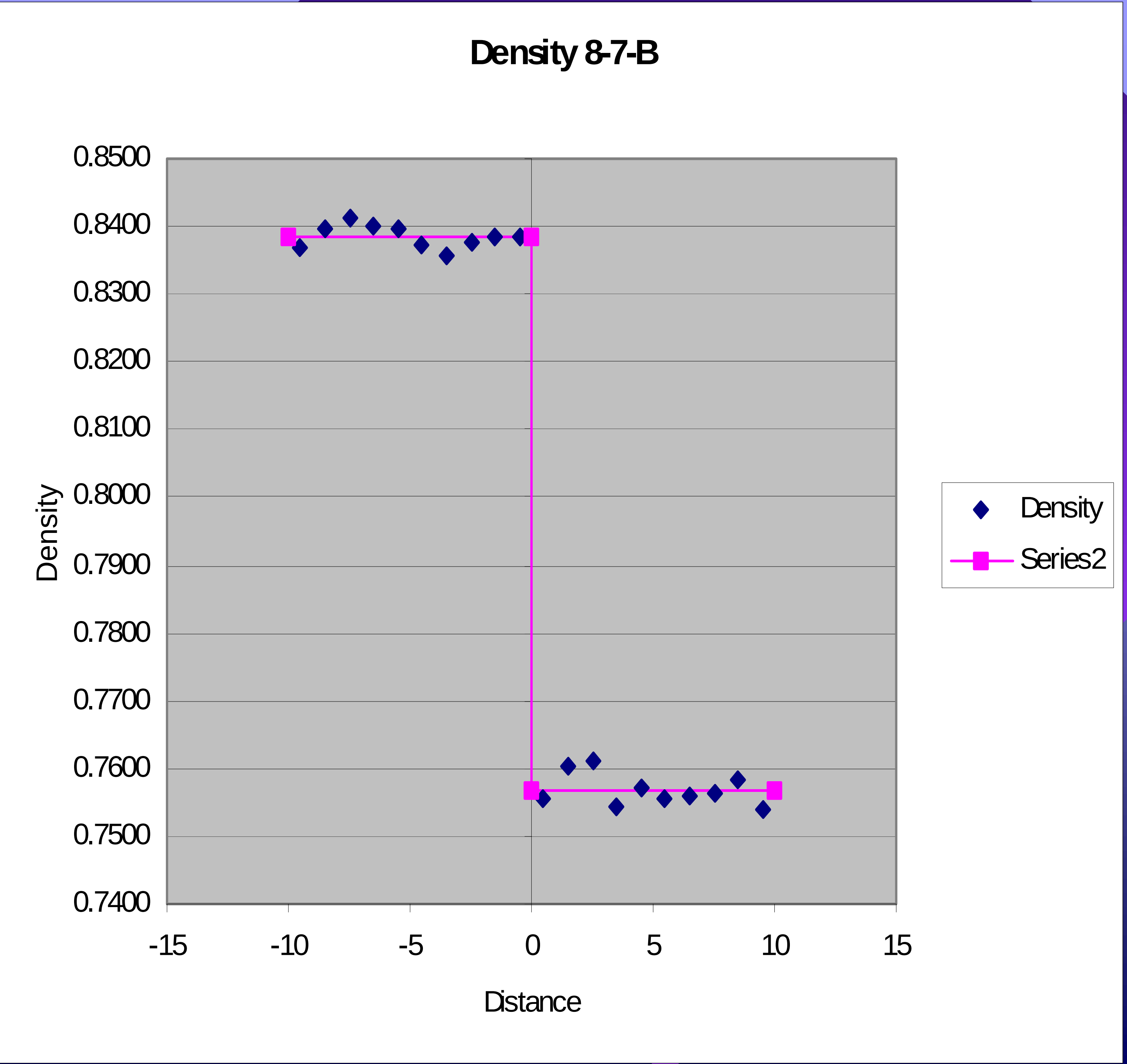
The data was organized in a spreadsheet and plotted. The graphs of the data should show a transition in densities from high to low, evening over time as in the following model:

Density Model



This model is for illustrative purposes only and the data is not meant to correspond to known diffusion rates in ice. The “base measures” would represent densities of the two different waters as calculated from control samples. The “T1-T4” designations would represent sequential experimental runs of increasing length of time stored in a -20° C cold room, thus a longer amount of time allowed for diffusion to take place throughout the length of the ice cell.

Typical graph showing data groupings with no density measure-ments between the high and low values that would indicate that diffusion has taken place.



Summary of Experi-mental Runs

#	Run	Length	Solution	Duration	Conclusion/Comment
1	17-6-A	20cm	D_2O and H_2O	19h 3m	First run, trial run for procedure, data unreliable.
2	17-6-B	10cm	D_2O and H_2O	21h 26m	Data grouped at D_2O density and H_2O respectively. No indication of diffusion/transfer.
3	18-6-A	20cm	D_2O and H_2O	1d 0h 19m	Data groups discrete. No evidence of proton transfer.
4	18-6-B	20cm	D_2O and H_2O	12d 23h 25m	Samples reduced by evaporation. Low D_2O measurements. Data groups discrete. No transfer noticed.
5	20-6-A	20cm	D_2O and H_2O	6d 21h 52m	Data groups discrete. No transfer noticed.
6	20-6-B	20cm	D_2O and H_2O	6d 21h 57m	Data groups discrete. No transfer noticed.
7	20-6-C	20cm	D_2O and H_2O	3d 21h 57m	Data groups discrete. No transfer noticed.
8	20-6-D	10cm	D_2O and H_2O	3d 21h 27m	Data groups discrete. No transfer noticed.
9	20-6-E	10cm	D_2O and H_2O	3d 21h 30m	Data groups discrete. No transfer noticed.
10	1-7-A	20cm	+ 2.5% glycerol	19h 37m	Data groups discrete. No transfer noticed.
11	1-7-B	20cm	+ 2.5% glycerol	23h 9m	Data groups discrete. No transfer noticed.
12	1-7-C	20cm	+ 2.5% glycerol	6d 20h 42m	Data groups discrete. No transfer noticed.
13	3-7-A	20cm	+ 2% acetic acid	3d 4h 40m	Data groups discrete. No transfer noticed.
14	3-7-B	20cm	+ 2% NaCl	3d 4h 4m	Data groups discrete. No transfer noticed.
15	8-7-A	20cm	+ HCl (1drop/50ml)	2d 23h 6m	Data groups discrete. No transfer noticed.
16	8-7-B	20cm	+ HCl (1drop/50ml)	6d 21h 51m	Data groups discrete. No transfer noticed.
17	10-7-A	10cm	+ HCl (1drop/50ml)	1d 0h 3m	Data groups discrete. No transfer noticed.
18	11-7-A	10cm	+ HCl (1drop/50ml)	4d 21h 31m	Data groups discrete. No transfer noticed.
19	15-7-A	10cm	+ HCl (1drop/50ml)	still running	
20	18-7-A	10cm	D_2O + acetic acid; H_2O + 2% NaOH		

Conclusion

There were no significant differences between data from D_2O and H_2O *without* dopants and D_2O and H_2O *with* dopants, nor did the type of dopant make a significant difference in the data obtained. Furthermore, other variables such as the duration frozen (within the range of this experiment), length of sample, or change in method of preparation of the sample, did not meaningfully affect the outcome. The grouping of data at each of the respective base measures of density and the lack of transitional densities between suggests that no measurable proton hopping or diffusion took place within the parameters of the experiment.

Some possible explanations for the difference in the findings of this experiment as compared to those found or suggested by others are as follows:

1. Diffusion rates are much slower than previously projected for non-excited ice.

2. A different chemical reaction than proton transfer is responsible for density changes.

3. Rates of previously measured proton transfer are higher because the local area that is being measured is heated with a laser, thereby inducing or enhancing the reaction and causing increased diffusion rates.

4. The system that we use consists of different molecules, which could form an interface between them (two phases). It could be that diffusion is not occurring across that interface.

What did I learn this summer?

- How scientific research is done.
- Diffusion and proton transfer.
- Be prepared for results that may be very different than expected.
- I enjoy teaching kids.

What will I take to my classroom?

- Develop a project-driven Science curriculum .
- Incorporate research and student developed experimentation.