

October 28, 2016

Physics 131

Prof. E. F. Redish

■ **Theme Music:**

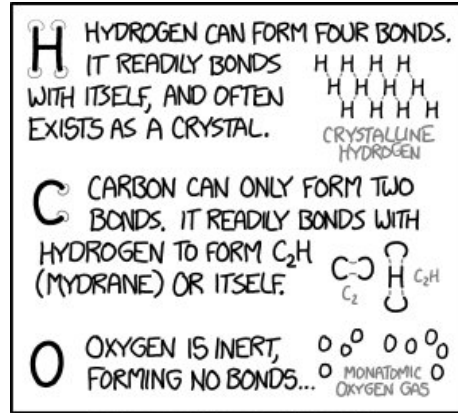
**Willie Nelson**

*The Gambler*

■ **Cartoon:**

**Randall Munroe**

*xkcd*



TYPOGRAPHIC CHEMISTRY

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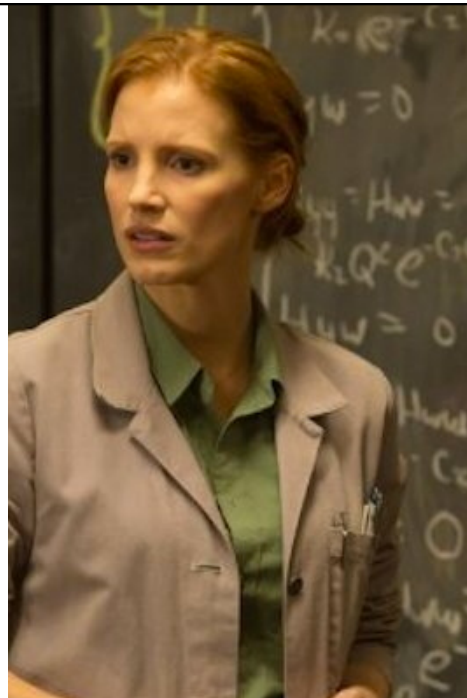
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**The Equation of the Day**

Fick's Laws

$$\langle (\Delta x)^2 \rangle = 2D(\Delta t)$$

$$J = -D \frac{dn}{dx}$$



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## Foothold principles: Fick's first Law



- If a set of molecules is not distributed uniformly in 1D (there is a concentration gradient) there will be an effective flow of those molecules according to

$$J = -D \frac{dn}{dx}$$

(or in 3D)  $\vec{J} = -D \vec{\nabla} n$

- In a gas, the diffusion constant  $D$  is given by  $\frac{1}{2\sqrt{3}} \lambda \bar{v}$
- In a liquid, the diffusion constant is given by  $D = \frac{k_B T}{6\pi\mu R}$

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## Foothold principles: Fick's second Law



- The average square displacement of a random walking molecule in a thermal bath after a time  $t$  is given in 3D by Fick's second law:

$$\langle \Delta r^2 \rangle = \langle \Delta x^2 \rangle + \langle \Delta y^2 \rangle + \langle \Delta z^2 \rangle = 6D\Delta t$$

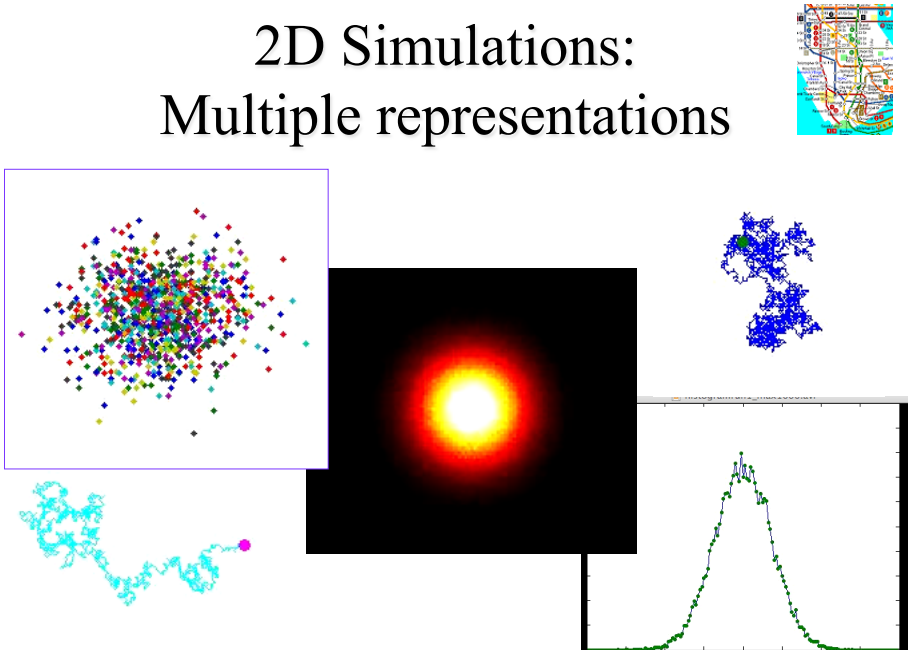
- The radius of a small blob of chemical in a liquid will grow at this rate.
- The displacement,  $\Delta r = \sqrt{\langle \Delta r^2 \rangle}$ , only grows like  $\sqrt{\Delta t}$ . For larger organisms, this is too slow and is the reason transport systems for air and blood have evolved.

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## 2D Simulations: Multiple representations




10/28/16 *Simulations by Alex Morozov & Kerstin Nordstrom* **10**

## 2D Simulations: Multiple representations



1. Watch all the particles.
2. Look at the density of the particles
  - What do the colors represent?
3. Look at a plot of the density along a slice through the middle.
  - What it will look like and what it will do.
4. Look at the motion of individual particles.



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## Foothold ideas: Pressure 1



- In a gas the molecules are moving very fast in all directions. On the average their momentum cancels out.
- If you put in a wall keeping the gas on only one side, only the momentum in one direction acts on the wall ( $N_1$ ,  $N_2$ ,  $N_3$ ), resulting in a force.
- In a non-flowing gas, the force/area is a constant, the pressure. It is proportional to the number of molecules and their  $mv^2$ .

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## Foothold ideas: Gases – Kinetic Theory II



- Newton's laws tell us that motion continues forever unless something unbalanced tries to stop it, yet we observe motion always dies away.
- Our model of matter as lots of little particles in continual motion lets us “hide” the energy of motion that has “died away” at the macro level in the internal incoherent motion.
- The model unifies the idea of heat and temperature with our ideas of motion of macroscopic objects.

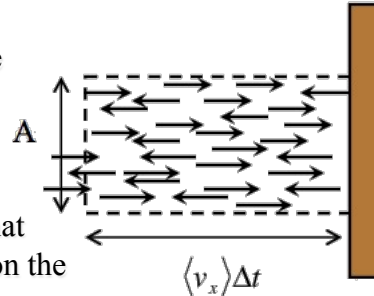
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## Summarizing the model

- In between collisions each molecule moves in a straight line – ignoring gravity. (We've used  $N!$ )
- Ignore up and down motions.
- Momentum change of a molecule that bounces off the wall exerts a force on the wall.
- The force on the wall will be the change in momentum of all the molecules that bounce off the wall in a time  $\Delta t$  divided by  $\Delta t$ .
- Calculate this using density.



$$F = \left( \frac{2mv_x}{\Delta t} \right) \left( \frac{1}{2} n A v_x \Delta t \right) = nmv_x^2 A$$

$$p = \frac{F}{A} = nmv_x^2 = \frac{N}{V} mv_x^2 = \frac{N}{V} \frac{1}{3} m \langle v^2 \rangle$$

$$F = \frac{dp}{dt}$$

**Average force is an emergent property!**

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## The Ideal Gas Law

Chemist's form

$$pV = n_{\text{moles}} RT$$

$$n_{\text{moles}} = \frac{N}{N_A}$$

$$R = k_B N_A$$

Physicist's form

$$pV = Nk_B T$$

$$p = nmv_x^2$$

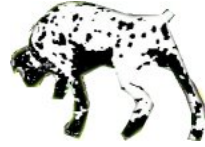
$$\frac{3}{2} k_B T = \frac{1}{2} mv^2$$

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## Interpreting



- The “physicist’s form” of the ideal gas law lets us interpret where the  $p$  comes from and what  $T$  means.
- $p$  arises from molecules hitting a wall and transferring momentum to it;
- $T$  corresponds to the energy of motion of one molecule (up to a constant factor).

$$p = nmv_x^2 \qquad k_B T = \frac{2}{3} \left( \frac{1}{2} mv^2 \right)$$

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