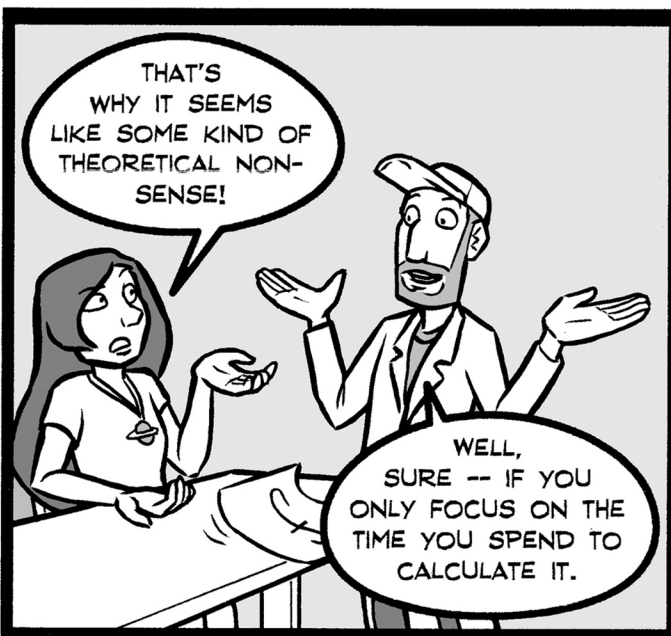
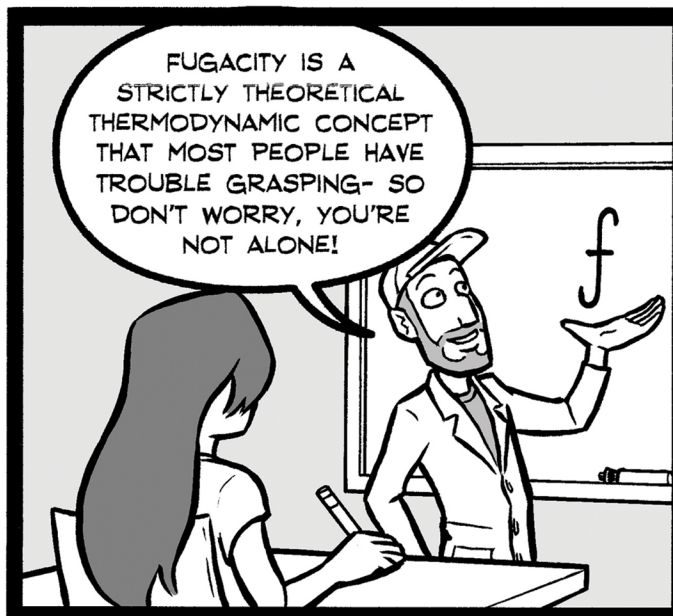


# FUGACITY

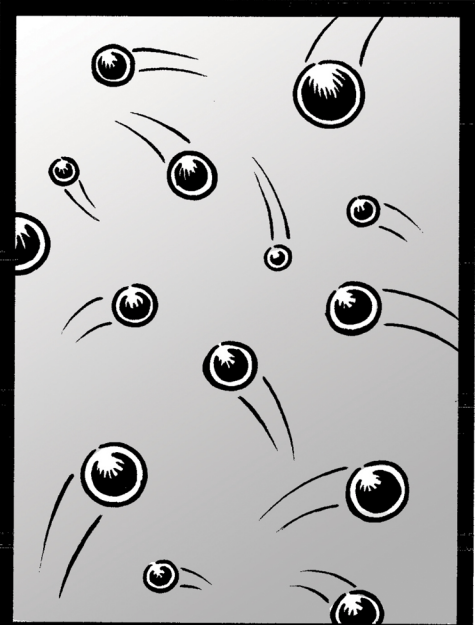
WRITTEN BY: DANTE SHEPHERD  
DRAWN BY: JOAN COOKE



SO WHAT IS FUGACITY? WELL, LET'S CONSIDER A CLOSED SYSTEM CONTAINING SEVERAL DIFFERENT SPECIES.

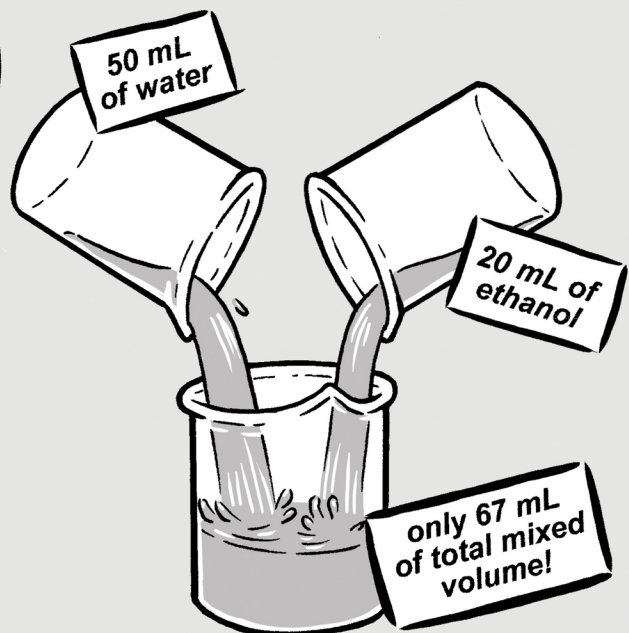


INSIDE, EACH SPECIES TAKES UP ITS OWN VOLUME AND EXERTS ITS OWN PRESSURE, BOTH OF WHICH ARE FRACTIONS OF THE WHOLE, RIGHT?



WELL, IF WE TREAT EACH CHEMICAL SPECIES AS IDEAL, WE WOULD ASSUME THAT EACH SET OF MOLECULES TAKE UP SPACE WITHOUT INTERACTING WITH EACH OTHER--SOMETHING WE KNOW IS NOT REALISTICALLY TRUE!

IN REALITY, THE PRESENCE, MOVEMENT, AND ACTIVITY OF EACH MOLECULE--AS WELL AS THE ATTRACTIONS BETWEEN DIFFERENT MOLECULES - WILL AFFECT ALL THE OTHER MOLECULES PRESENT! THIS INTERACTION AFFECTS THE PRESSURE AND VOLUME AND CHANGES THE OVERALL CONDITIONS WITHIN THE SYSTEM.





THIS BRINGS US TO CHEMICAL EQUILIBRIUM--HOW EACH CHEMICAL SPECIES WILL BALANCE IN DIFFERENT PHASES PRESENT WITHIN A SYSTEM, LIKE WATER AND OXYGEN PRESENT AS BOTH A GAS AND A VAPOR. THIS CHEMICAL EQUILIBRIUM IS BASED ON GIBBS FREE ENERGY--THE MAXIMUM AMOUNT OF USEFUL WORK THAT CAN BE PULLED FROM A CLOSED SYSTEM.

EACH SPECIES PRESENT HAS WHAT ITS OWN PURE FREE GIBBS ENERGY WOULD BE--THE TOTAL ENERGY IT WOULD CONTRIBUTE TO THE MIXTURE AS AN INDIVIDUAL SPECIES.

BUT BECAUSE WE DO HAVE DIFFERENT SPECIES PRESENT, THERE IS AN OVERALL GIBBS FREE ENERGY OF THE SYSTEM.

WE DEFINE THE CONTRIBUTION OF EACH SPECIES TO THE OVERALL GIBBS FREE ENERGY AS THE CHEMICAL POTENTIAL,  $\mu$ .

IT'S THIS CHEMICAL POTENTIAL--WHICH, YES, IS AN ABSTRACT CONCEPT--THAT IS THE DRIVING FORCE FOR MASS TRANSFER, FOR SPECIES TO MOVE TO DIFFERENT PHASES OR DIFFERENT SPACES!

THIS IS WHERE FUGACITY COMES IN.

FINALLY!

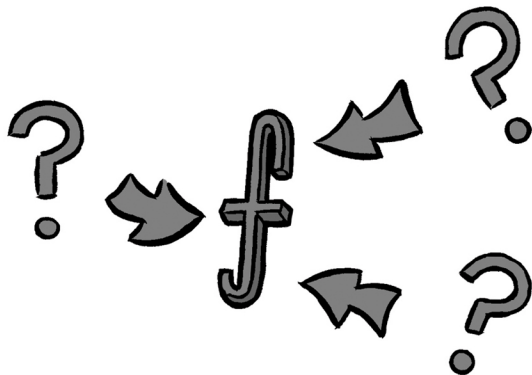
CHEMICAL POTENTIAL IS A PAIN TO WORK WITH MATHEMATICALLY. BASED ON ITS DEFINITION, FOR CERTAIN CASES LIKE INCREDIBLY SMALL CONCENTRATIONS IN A MIXTURE, CHEMICAL POTENTIAL BECOMES USELESS.



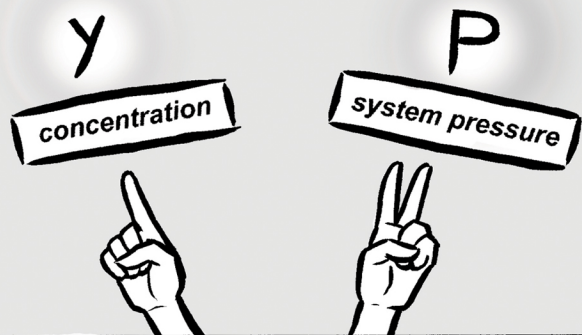
WHICH BRINGS US TO FUGACITY. IT'S RELATED TO CHEMICAL POTENTIAL, BUT CAN BE USED WITH GASES, LIQUIDS, OR SOLIDS TO HELP CHARACTERIZE CHEMICAL EQUILIBRIUM!



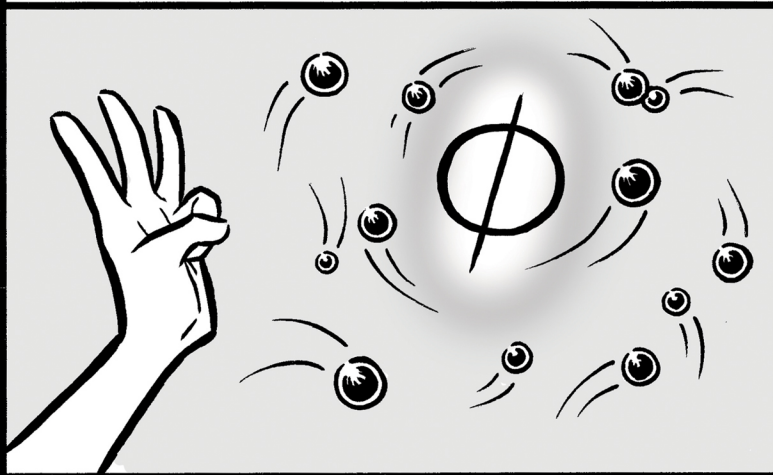
THINK OF FUGACITY AS "CORRECTED PRESSURE." EACH CHEMICAL SPECIES CAN BE DETERMINED FROM THE PRODUCT OF THREE COMPONENTS.



FOR A GAS, WE TAKE THE SPECIES' CONCENTRATION AND THE SYSTEM PRESSURE--THAT COMBINATION ALONE DESCRIBES THE PARTIAL PRESSURE THAT EACH SPECIES NORMALLY TAKES UP WITHIN THE ENTIRE SYSTEM'S PRESSURE.



BUT THERE'S A THIRD COMPONENT: A COEFFICIENT TO DESCRIBE HOW IDEAL THE SPECIES IS BEHAVING! HERE IS WHERE THOSE INTERSPECIES INTERACTIONS MATTER SO MUCH! FOR A GAS, THIS COEFFICIENT IS APTLY NAMED THE FUGACITY COEFFICIENT.

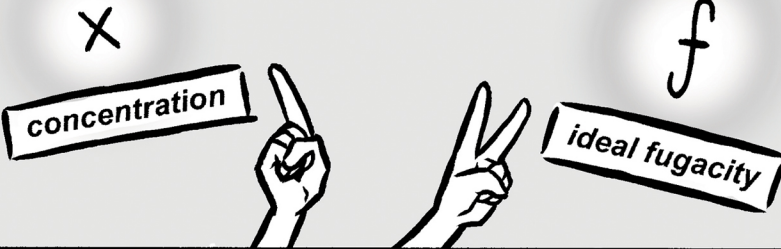


$$\hat{f}_i^v = y_i \phi_i^v P$$





FOR A LIQUID OR A SOLID, IT'S A LITTLE DIFFERENT. WHILE FUGACITY IS STILL A COMBINATION OF CONCENTRATION, AN IDEALITY COEFFICIENT, AND PRESSURE, YOU NEED TO REMEMBER THAT PRESSURE IS EXERTED A LITTLE DIFFERENT ON LIQUIDS AND SOLIDS THAN ON GASES.



SO WHILE CONCENTRATION IS STILL A FACTOR, INSTEAD OF PRESSURE, THE CONTRIBUTING COMPONENT IS THE "IDEAL FUGACITY," WHICH CAN BE DETERMINED AS THE FUGACITY OF THE SPECIES WHEN IT IS A PURE SPECIES.

FOR LIQUIDS AND SOLIDS, THAT COEFFICIENT SPECIFICALLY DESCRIBING IDEALITY IS THE ACTIVITY COEFFICIENT - AGAIN, DESCRIBING THE ACTIVITY OF THE CHEMICAL RELATIVE TO AN IDEAL STATE.



SO WE HAVE FOR A LIQUID:

$$\hat{f}_i^l = x_i \delta_i f_i^l$$

AND FOR A SOLID:

$$\hat{f}_i^s = X_i \Pi_i f_i^s$$

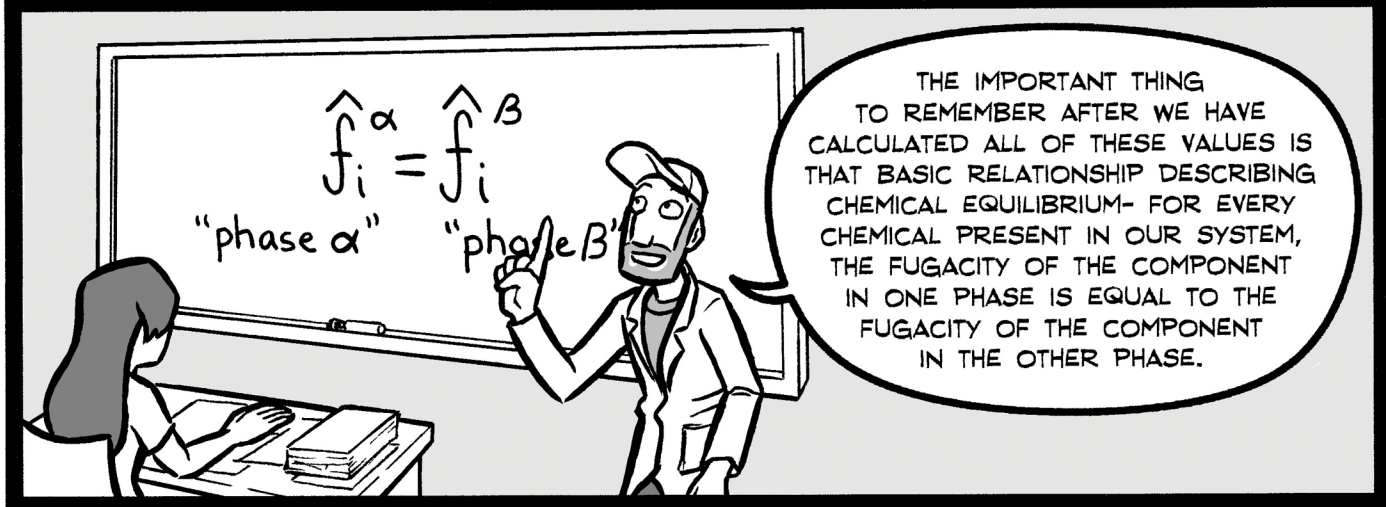
BUT WHAT DOES IT ALL MEAN?



THAT'S NOT WHAT YOU'RE REALLY ASKING. YOU'RE ASKING, WHY DOES THIS EVEN MATTER, RIGHT?

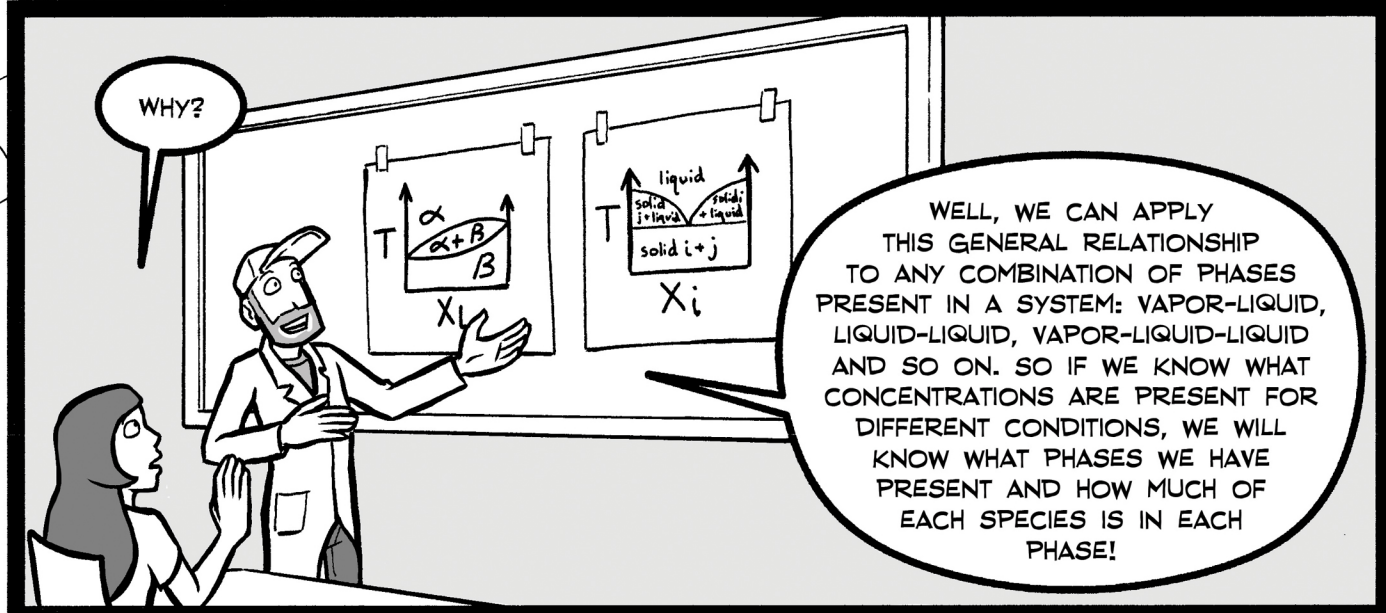
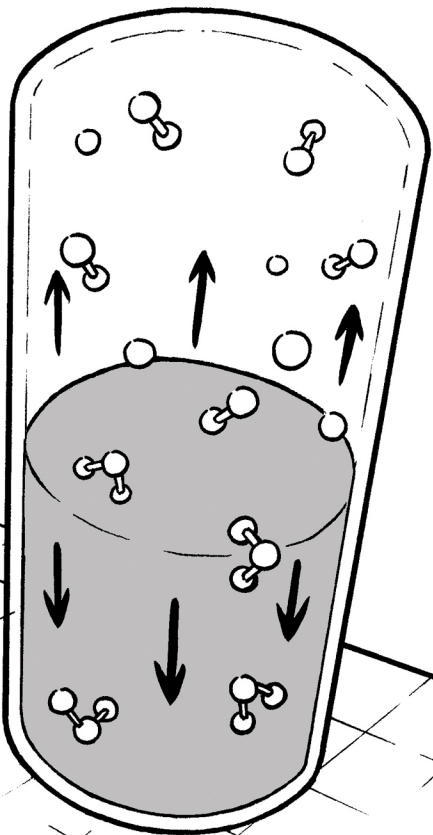
WELL, YES.





THE IMPORTANT THING TO REMEMBER AFTER WE HAVE CALCULATED ALL OF THESE VALUES IS THAT BASIC RELATIONSHIP DESCRIBING CHEMICAL EQUILIBRIUM- FOR EVERY CHEMICAL PRESENT IN OUR SYSTEM, THE FUGACITY OF THE COMPONENT IN ONE PHASE IS EQUAL TO THE FUGACITY OF THE COMPONENT IN THE OTHER PHASE.

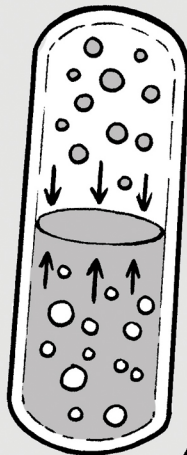
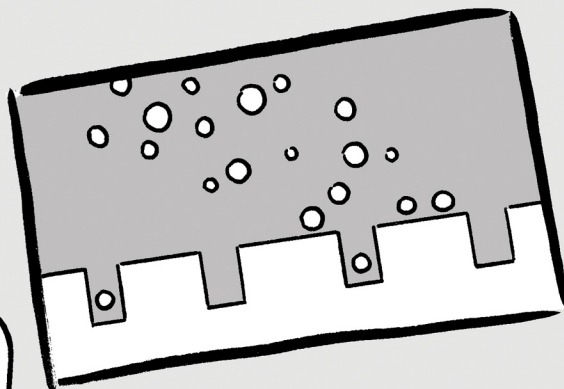
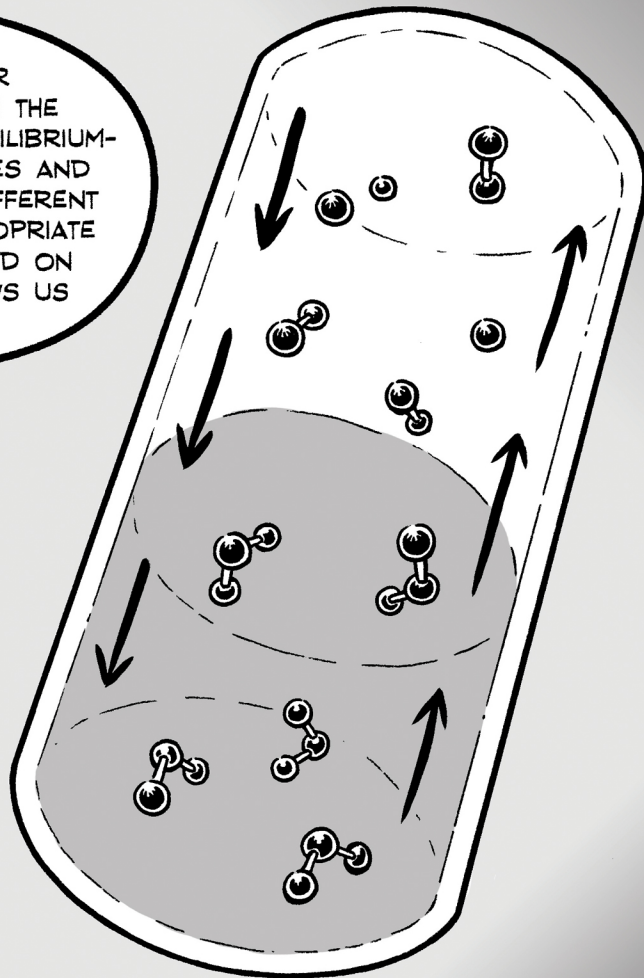
SO IF WE HAVE TWO CHEMICALS PRESENT IN A GAS-LIQUID SYSTEM - IF WE CAN DETERMINE THE IDEALITY AND PRESSURE OF THE SYSTEM, ONCE WE KNOW THE CONCENTRATION OF A SPECIES IN ONE PHASE, WE CAN DETERMINE WHAT THE CONCENTRATION IS IN THE OTHER! AND THAT HAS HUGE IMPLICATIONS!



WELL, WE CAN APPLY THIS GENERAL RELATIONSHIP TO ANY COMBINATION OF PHASES PRESENT IN A SYSTEM: VAPOR-LIQUID, LIQUID-LIQUID, VAPOR-LIQUID-LIQUID AND SO ON. SO IF WE KNOW WHAT CONCENTRATIONS ARE PRESENT FOR DIFFERENT CONDITIONS, WE WILL KNOW WHAT PHASES WE HAVE PRESENT AND HOW MUCH OF EACH SPECIES IS IN EACH PHASE!



WHICH IS USEFUL IN REAL-WORLD APPLICATIONS! FOR EXAMPLE, DISTILLATION IS BASED ON THE ENTIRE CONCEPT OF VAPOR-LIQUID EQUILIBRIUM--WE APPLY A RANGE OF TEMPERATURES AND PRESSURES TO BE ABLE TO DRIVE DIFFERENT SPECIES APART--AND KNOWING APPROPRIATE RANGES OF CONCENTRATIONS, BASED ON OUR FUGACITY RELATIONSHIP, ALLOWS US TO OPTIMIZE OUR SYSTEM.



WE HAVE SIMILAR RELATIONSHIPS FOR ABSORPTION OF GAS PARTICLES ON A SOLID FILTER SURFACE, OR THE SEPARATION OF CHEMICALS IN IMMISCIBLE LIQUID PHASES--WORKING WITH THE CHEMICAL EQUILIBRIUM EQUATION PRODUCED BY FUGACITY, WE CAN DETERMINE THE OPTIMAL OPERATING CONDITIONS.



LET'S LOOK AT SOME EXAMPLES. FIRST, CONSIDER A CASE WHERE WE'VE GOT MIXTURES IN TWO DIFFERENT BEAKERS SEPARATED BY A VALVE. ONE SIDE HAS JUST A LITTLE BIT OF A PURE SUBSTANCE (WE'LL CALL IT A,) WHILE THE OTHER SIDE IS A LOT OF A 95% A/5% B MIXTURE.



WHEN I OPEN THE VALVE, WHICH DIRECTION WILL A AND B PARTICLES TRAVEL?

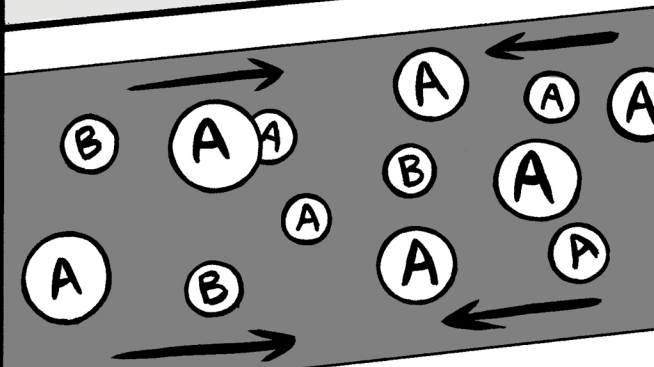


WOULDN'T THEY BOTH GO FROM THE SIDE WITH THE LARGER VOLUME TO THE SIDE WITH LESS?

YOU WOULD THINK THAT--BUT MASS TRANSFER IS DRIVEN BY FUGACITY--AND FUGACITY IS PARTLY DEPENDENT ON CONCENTRATION, NOT VOLUME!



SO EVEN THOUGH THE SIDE WITH THE MIXTURE HAS FAR MORE A IN TERMS OF VOLUME THAN THE PURE SIDE, WHILE PARTICLES OF B TRAVEL FROM THE MIXED SIDE TO THE PURE SIDE, PARTICLES OF A WILL TRAVEL FROM THE PURE SIDE TO THE MIXTURE!

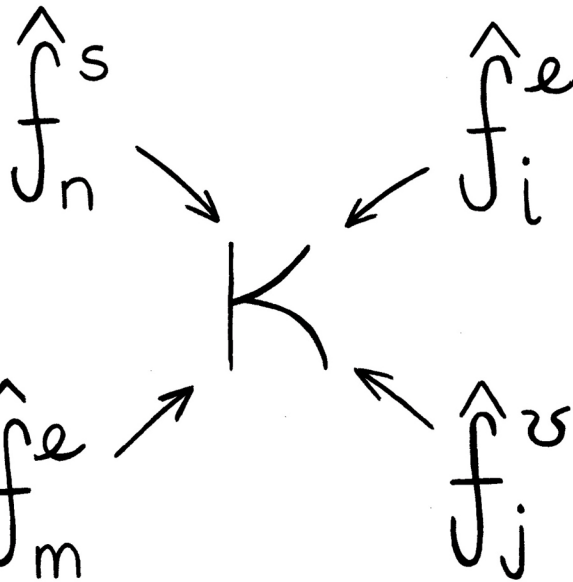


SIMILARLY, BY CALCULATING THE FUGACITY FOR DIFFERENT TEMPERATURES AND PRESSURES, WE CAN DETERMINE WHAT CONCENTRATIONS WE WILL HAVE AND HOW WELL OUR SYSTEMS ARE MIXING OR SEPARATING!





BUT IT GOES FURTHER- THE TERM FOR CHEMICAL EQUILIBRIUM,  $K$ , IS DEPENDENT ON THE PRODUCT OF ALL FUGACITIES OF ALL SPECIES PRESENT IN A SYSTEM.



SO?

SO, THIS MEANS THAT IF WE CAN CALCULATE THE FUGACITY FOR EACH COMPONENT IN A REACTIVE SYSTEM, THEN WE CAN DETERMINE WHAT THE OUTPUT CONCENTRATION WILL BE FROM A REACTOR! SO THROUGH FUGACITY, WE CAN ACTUALLY DETERMINE HOW EFFECTIVELY A REACTOR IS WORKING AND HOW MUCH OF OUR DESIRED PRODUCT IS BEING PRODUCED!



SO YES, FUGACITY IS COMPLICATED. BUT IT'S INCREDIBLY USEFUL WHEN WE REALIZE WHAT IT MEANS AND HOW IT IS APPLIED!



I THINK I GET IT. THERE ARE SO MANY EQUATIONS AND DERIVATIONS FOR CALCULATING FUGACITY COEFFICIENTS AND THE OTHER COMPONENTS OF FUGACITY...

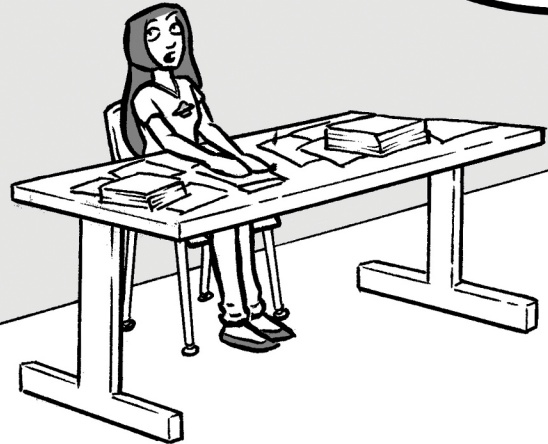


BUT WHEN WE PIECE IT ALL TOGETHER, FUGACITY TELLS US WHAT CHEMICALS AND PHASES WE HAVE, AND HOW OUR REACTORS AND SEPARATOR SYSTEMS ARE PROCEEDING!



RIGHT!

HANG IN THERE! FUGACITY IS LATIN FOR "TENDENCY TO ESCAPE"- BUT KEEP AT IT AND IT WON'T ESCAPE YOUR GRASP!



AND WHAT A TERRIBLE JOKE TO END ON.