TEACHING ANALYTICAL CHEMISTRY AT THE MOLECULAR LEVEL

Carlos A. Rius-Alonso, Alain Quere Thorent, Yolanda González-Quezada

Universidad Nacional Autónoma de México (MEXICO)

Abstract

Analytical chemistry of solution deals with reactions and equilibrium state of solutes in order to find appropriate conditions to characterize or quantify analytes. Chemical kinetics, study how fast reactants and product concentration are changing, whereas chemical equilibrium tells us, what those concentrations are once they have stopped changing.

Keywords: Chemical reactions, analytical chemistry, molecular modeling, kinetics, equilibrium state.

1 INTRODUCTION

Chemical kinetics, study how fast reactants and product concentration are changing, whereas chemical equilibrium tells us, what those concentrations are once they have stopped changing. Analytical chemistry of solution deals with reactions and equilibrium state of solutes in order to find appropriate conditions to characterize or quantify analytes.

The studies of equilibrium provide the information needed to affect the final concentrations of products by altering conditions. Le Chatelier´s principle is very important to explain the equilibrium; it states that the direction in which the system proceeds back to equilibrium is such that the change is partially offset until the equilibrium is reached. This principle has a significant implication in Analytical Chemistry.

During this part of the course, the relation between the structure and chemical equilibrium is discussed using Molecular Modeling programs. As reaction's changes greatly in their speed, they also varied in their extent. Fast reactions can give products in high yield or in a very low yield. The kinetic of a reaction is related to the speed, the concentration of product that is appearing per unit time. The equilibrium of a reaction applies to the extent of it, the concentration of product when no further change is observed.

One of the main objective of the course is to teach students the equilibrium state at the macroscopically and molecular levels, and then focus on the equilibrium constant and its relation to the balanced equation. At the Faculty of Chemistry (UNAM) we are using several Molecular Modeling programs as Spartan, Odyssey, AtomsInMotion and Mol Lab MS to teach students the molecular and macroscopic behavior of reaction.

The importance of chemistry is that everything is made of atoms, all the different sate of the matter; solids, liquids and gases are all made of atoms. There are a lot of different types of atoms called elements. Each element has specific properties due to it's mass and atomic number. [1-14]

1.1 Reactions

At room temperature, the molecules of gases and liquids are moving very fast. They are continuously bouncing of each other; the speed at which they move can be very fast up to 1,700 km per hour that means, they have a very large kinetic energy. If the collision is between reacting molecules, at the proper orientation, a reaction can take place. Some reactions can take place in fractions of seconds and other reaction take longer period of times. It depends of several factor; reactivity, internal energy, reaction barrier, orientation, pressure, temperature etc.

Kinetic energy is proportional to the mass of the atom multiplied by the square of the molecule's speed. The form of measuring the energy of matter is by temperature, this gives the average kinetic energy of the system. In this way if the temperature increase, the kinetic energy of the system increase and also the velocity of the reacting molecules. Each atom has a different kinetically energy some move very fast and other slow. As the atoms bounce off of each other they transfer energy back and forth, and the average energy in the system at a set temperature, remains constant. The larger the mass of the molecules the slower speed they move.

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In order to have chemical reactions the molecules has to collide each other. Although molecules are attracted to one another, these attraction forces, only act over relatively short distance. Most of the molecules in gas phase move about in straight lines unaware of the other molecules. Decreasing the temperature, the kinetic energy of the molecules decreases and begins to move more slowly. As the temperature lowers the molecules don't have enough kinetic energy to escape each other interactions. The molecules start to clump together into small groups and move about in these groups. These groups are liquid droplets of the molecules, and when this begins to happen in the gases, are said to be condensing.

The difference between gases and liquids or solids is a matter of spacing, only when the atoms are far apart from each other and acting independently they are gases. When they are close together they condense in liquid or solids. Reactions in solid state are very slow due to the low mobility of the molecules, y liquid phase they tend to collide and in gas phase are very fast.

1.1.1 Atomistic Simulation

The Molecular Modeling programs compute the motions of atoms by integrating all the forces that the atoms exert on each other. These forces arise from changes in potential energy that depends on the separation distances between the atoms. All the atoms are simulated as if they were classical particles that move according to Newton's laws of motions (F=ma). Molecules consist of several atoms interacting by bonds. The bonds have to be accounted in the model. There are two type of bonds ionic (the bond is electrostatic and strong) and covalent bonds (the electrons are shared between the atoms)

1.1.2 Salts

All the minerals classified as salts are held together through ionic bond. One atom gains an electron and other loses it, the net change of the compound is zero. A positively charged ion is called a cation and the negative charged ion is called an anion. The amount of net charge depends on how many electrons have been removed or gained. If an atom loses or gains an electron the net charge of the atoms will be negative or positive. This charge is the difference between the number of electrons and protons. When the atom has a positive charge it called a cation and when the net charge is negative in known an anion. The net charge depend of how many electron have been removed (+) or accepted (-).

In Analytical Chemistry the solutions plays a very important role and students have some difficulties to conceptualize the phenomenon. The use of the program AtomsInMotion (salts) can be used to teach the concept, first a simulation can have only Sodium cations and because all of them have positive charge the ions distribute throughout the simulation and attempt to maximize the spacing between each other (Fig 1).

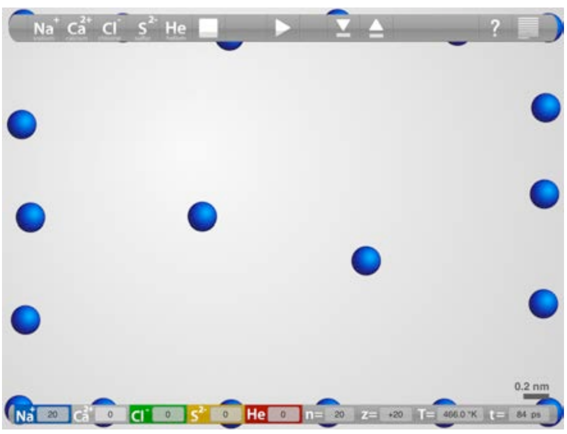


Fig 1 20 Sodium cations

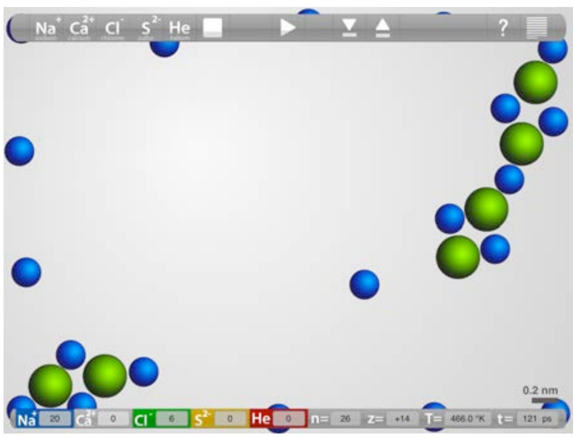


Fig 2 20 Sodium Cations and 6 Chloride anions

When Chloride anions are added the cations tend to neutralize the negative charge. Fig 2.

If the same number of cations and anions are present the salt tend to form a stable crystal structure. Fig 3.

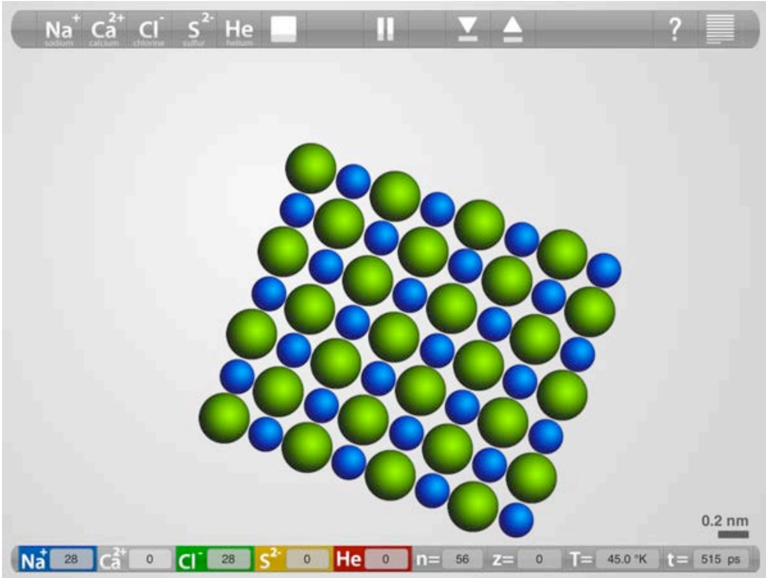
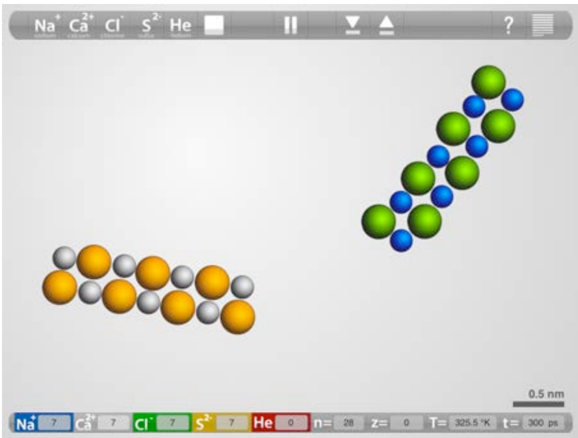


Fig 3. NaCl crystal structure.

Crystals are formed by the Coulombic forces between the anion and cations. In NaCl both have +1 and -1 charge. If a crystal if formed with CaS they have +2 and -2 charge, the forces between ions are 4x stronger en CaS than NaCl this can be correlated with their melting points, (NaCl mp=801°C, CaS mp=2,525°C). Fig 4 are both crystals at low temperature, Fig 5 is when the sample is heated above NaCl mp a rupture of the crystal is observed.



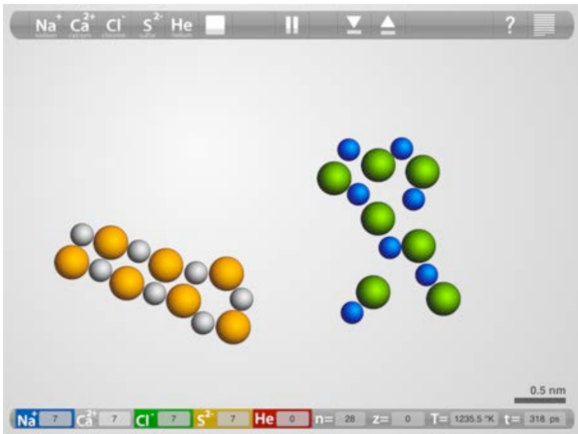


Fig 4 325 °K CaS and NaCl

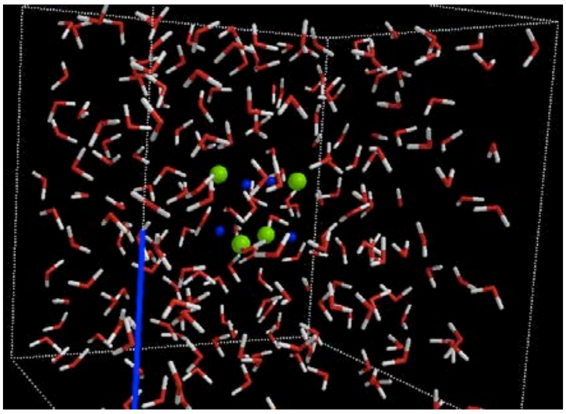
Fig 5 1235°K CaS and NaCl

1.1.3 Standard Solutions

The standard solution is used very often in Analytical Chemistry consist in dissolving 1mol of the compound in 1 liter of solvent. 1 mol of a compound is the molecular weight of the compound in grams. In order to find how many molecules are present in one mole the Avogadro number is used

$$N_a = 6.0221415 \times 10^{23} \text{ mol}^{-1}$$

this is a very large number to perform simulations if we are using water as solvent the MW=18 and 1l is 1000g that means 55.55 moles or 333.333 x 10^{23} water molecules we can make a simple approximation and for a AB type electrolytes we will consider 55 water molecules per 1 cation and 1 anion. In Fig 6 we simulate 4 molecules of NaCl in 220 molecules of water to have a 1 molar solution. After some 15 *p*s (Fig 7) the NaCl start dissolving and after 100 ps (Fig 8) is dissolved.



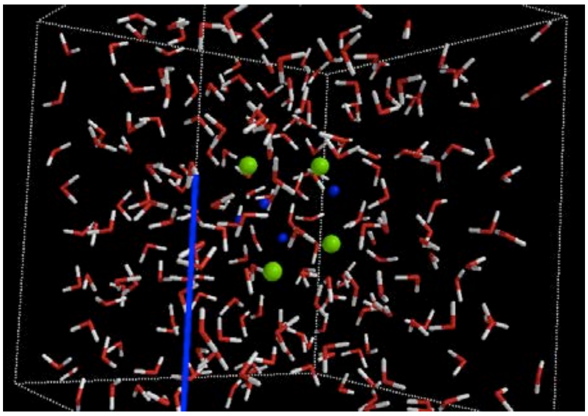


Fig 6 NaCl in water initial time   Fig 7 NaCl in water 20 ps

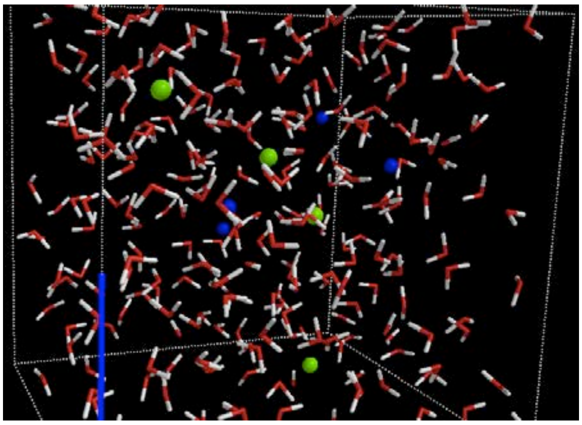
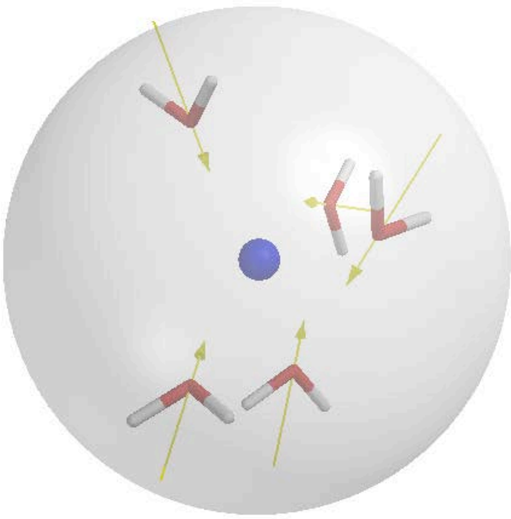


Fig 8 NaCl in water 100 ps

The ions can be view in detail surrounded by water molecules, the cation is neutralized by the more electronegative Oxygen of water (Fig 9) and the anions are neutralized by the more positive Hydrogen's of water (Fig 10).



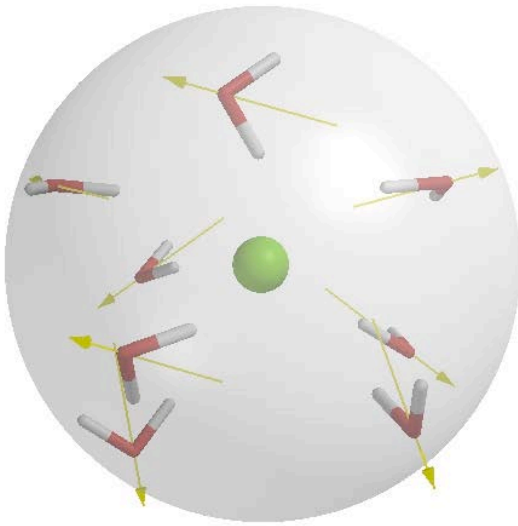


Fig 9 Na+ interacting with O   Fig 10 Cl- interacting with H

1.1.4 Equilibrium and Molecular Dynamics

Equilibrium is essential to Analytical Chemistry it depends on several factors as the dielectric constant of the solvent, the nature of the solute etc. When a substance is dissolved in a solvent and it´s ionized this substance is known and electrolyte. The individual components of the substance are dissociated due to thermodynamic interactions between the solvent and solute molecules. This includes soluble salts, acids and bases. They are called electrolyte because they can conduct electricity. The nature of the substance and solvent is important to understand the extent of dissociation [17].

Molecular Dynamics computes the motions of atoms integrating all the forces that the atoms exert on each other. In order to calculate the forces all the atoms are treated as if they are classical particles moving according to the Newton's lay of motion. The size of the atoms is modeled by the van der Waals diameters. The position of each atoms is updated after each computation, and the experiments proceed interactively until the time required.

2 CONCLUSIONS

The use of Molecular Dynamics programs allows a better understanding of the Analytical Chemistry. When students visualize at molecular level the behavior of the atoms and molecules, they understand the dynamics of the events and the equilibrium between different analytes.

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Fig 1 to 5 were done using Atoms in motion [15]

Fig 6 to 10 were done using Odyssey [16]

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