

# FOOD SCIENCE AND TECHNOLOGY

## Lecture21

### Lecture 21: Water and Ice

Hello everyone, Namaskar.



So, today we are starting Module 5. So, in these 5 lectures of Module 5, we will talk about food macronutrients, particularly their structure and functions. So, the first lecture of this module—and overall Lecture 21 of the course—today we will talk about water.



We will discuss how water is important in food systems, the structure and properties of water and ice, the effect of solutes on water structure, and the concept of free and bound water. Also, we will talk about water activity, absorption isotherms, and molecular mobility versus food stability.

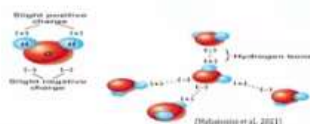
## Importance of water in foods

- Water is the most abundant constituent in most foods.
- Apart from quantitative presence, water offer functional importance in foods.
- Water is essential for the good texture and appearance

Food	Water (%)
Cucumbers	95-96
Tomatoes	93-95
Cabbage	90-92
Orange juice	86-88
Apples	83-87
Cow milk	86-89
Eggs, whole	74
Chicken, broiled	68-72
Hard cheese	30-33

## Structure and properties of water and ice

- Water is the major constituent of almost all life forms, with most animals and plants containing >60% water by volume.
- The two slightly negatively charged hydrogen atoms and a positively charged oxygen atom create a polar molecule.
- Attraction and repulsion between the positive and negative charges produce angular or V-shaped molecule.

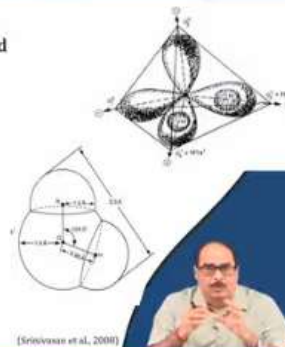


- Ice forms when water vapor or liquid water freezes below 0°C (32°F).

So, let us see how water is important in the food system. You know, different foods contain varying amounts of water. In earlier modules, we have already studied that food is essentially a mixture of various chemicals and biochemicals in water. So, you can say water is one of the most abundant constituents in most foods, apart from— quantitatively, water also offers functional importance in food. It is very essential for giving properties to food, particularly its texture and appearance—for fruits, vegetables, cereal grains, etc. All those things. In fact, water is the medium through which most cellular components, whether in plant or animal systems, operate. Water is a universal solvent, and this characteristic property of water as a solvent is very important in the case of tea, coffee, beverages, etc. When you are making any tea brew or coffee brew, it is basically the flavoring and coloring compounds present in the tea or coffee. They get extracted, and we sip it and enjoy the color and flavor of the coffee and other things. Water is a very essential and important component in food. It is related to various chemical reactions, microbiological reactions, enzymatic reactions, and all those things. Accordingly, water is also one of the major culprits. As far as the spoilage of food is concerned, alright. In fact, it encourages the growth of spoilage microorganisms and other factors responsible for the spoilage of food, like enzymatic reactions. In fact, one of the major aims of modern food technology is to reduce the water content to increase the shelf life of food. So now, it is well established that the effect of water on the stability of food cannot be ignored. It depends not only on the quantity of water present but also on the form and manner in which the water is present. How the water is structured, how it interacts with various components, etc., and that we will talk about later in this lecture.

### Structure of water

- A water molecule consists of two hydrogen atoms bonded to the  $sp^3$  orbitals of an oxygen atom.
- They form two covalent sigma ( $\sigma$ ) bonds of 40% ionic character, each of which has a dissociation energy of  $4.6 \times 10^2$  kJ/mol.
- The localized molecular orbitals are assumed to remain symmetrically oriented about the original orbital axes, hence retaining an approximate tetrahedral structure.
- In addition to the common isotopes of oxygen and hydrogen,  $^{16}\text{O}$  and  $^1\text{H}$ , also present are  $^{17}\text{O}$ ,  $^{18}\text{O}$ ,  $^2\text{H}$  (D), and  $^3\text{H}$  (T) with a resultant 18 isotopic variants of molecular H-OH.



So, let us see the structure and properties of water as well as ice. You know, water is the major constituent of all life forms, animals, and plants. They contain more than 60 percent water by volume in their body weight—animal body weight, cell body weight—60 percent or so. And the two slightly negatively charged hydrogen atoms and one positively charged oxygen atom create a polar water molecule, and there are attractions and repulsions between the positive and negative charges that produce an angular or V-shaped structure of the water molecule and ice forms when water vapor or liquid water freezes below 32 degrees Fahrenheit or below 0 degrees Celsius. So, if you look at the structure of water, a water molecule consists of two hydrogen atoms bonded to the  $sp^3$  orbital of an oxygen atom. And they form two covalent, that is, sigma bonds of 40 percent ionic character. Each of which has a dissociation energy of about  $4.6 \times 10^2$  kilojoules per mole. The localized molecular orbitals are assumed to remain symmetrically oriented about the original orbital axis, hence retaining an appropriate or approximate tetrahedral structure. In addition to the common isotopes of oxygen and hydrogen like  $^{16}\text{O}$  and  $^1\text{H}$ , there are also present  $^{17}\text{O}$ ,  $^{18}\text{O}$ ,  $^2\text{H}$ , and  $^3\text{H}$  with a resultant. There are about 18 isotopic variants of molecular OH and OH.

### ❖ Though water is an electrically neutral molecule, there is an imbalance of charge because of the arrangements of atoms.

- The oxygen atom of the water molecule on one side is slightly more electronegative and the sides where the hydrogen atoms are located are slightly more positive.
- This polar nature of the water molecule results in each hydrogen atom being attracted to the oxygen atom of another molecule and the oxygen atom to the hydrogen atom.
- This type of attraction leads to multiple hydrogen bonding on a three dimensional basis.
- Each water molecule is able to hydrogen bond with a maximum of 4 other molecules.
- Extra energy required to break these hydrogen bonds provide logical explanation for the unusual properties of water.

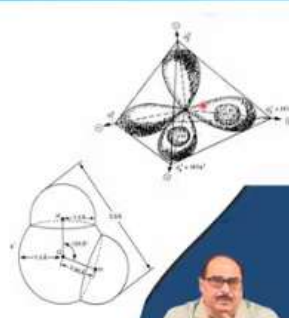
Structure of water (Contd...)



As you can see here in this structure, though water is considered to be an electrically neutral molecule, there is an imbalance of the charges between the arrangement of the atoms. That is, you see that is the 2H here in this structure. They are slightly on one side of the oxygen molecule. So, the side where the hydrogens are attached to the oxygen molecule is slightly more electropositive. Whereas, this area where it is open is slightly more electronegative. So, this polar nature of water results because it has both positive and negative charges, and the polar nature results in each hydrogen atom being attracted to the oxygen atom of another water molecule, and then it bonds with another molecule, and the oxygen atom bonds to the hydrogen atom. So, this interaction occurs in such a way that there are multiple hydrogen bonds—hydrogen attracts water, water attracts hydrogen, and thus, hydrogen bonding occurs. So, in this water structure, multiple hydrogen bonds are formed on a three-dimensional basis, and you can say each water molecule is able to hydrogen bond with a maximum of four other molecules, and it is the extra energy required to break these hydrogen bonds that provides a logical explanation for the unusual properties of water if you compare it with molecules of similar atomic weight or similar atomic structure, etcetera.

**Theories of water structure**

- **Homogeneous model**  
Intermolecular hydrogen bonds are distributed uniformly throughout water, so that each water molecule has essentially the same environment.
- **Mixture model**  
The intermolecular hydrogen bonds are concentrated, at any given moment, in localized multi-molecular clumps or clusters of water molecules.
- ❖ **The most widely accepted model is the mixture model.**

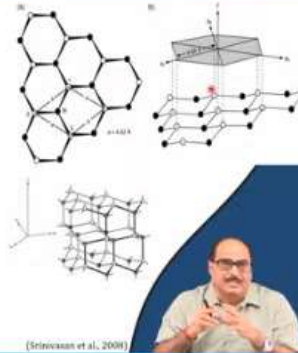


[Srinivasan et al., 2006]

So, there are two theories that explain the structure of water: one is the homogeneous model, and the other is the mixture model. So, in the homogeneous model, it is said that intermolecular hydrogen bonds—suppose there are many water molecules—are distributed uniformly throughout the water. So, each water molecule has essentially the same environment throughout the system. Whereas the mixture model says no. In contrast to the homogeneous model, the mixture model says that the Intermolecular hydrogen bonds are concentrated at a given moment in localized multi-molecular clumps or clusters of water molecules. The most widely accepted model is the mixture model.

### Structure of ice

- Ordinary ice belongs to the dihexagonal bipyramidal class of the hexagonal system of crystal symmetry.
- It can exist in 9 other crystalline polymorphic structures and also in an amorphous or vitreous state of uncertain, but largely non-crystalline structure.
- Real ice crystals are never perfect, and the structural defects encountered are usually of the orientational type or ionic type.
- Structural defects in ice explain the high mobility of protons and the small decrease in electrical conductivity when water freezes.



Now, let us talk about the structure of ice. So, you have seen that water is an open hydrogen-bonded structure of the water molecule. Now, when water is frozen into ice, the ice has a closed structure. That is, the open hydrogen-bonded structure of water is converted into a closed hydrogen-bonded structure. And almost a regular hexagonal pattern of molecules appears, in which there are a lot of void spaces inside. So, ice can exist in nine other crystalline polymorphic forms and also in an amorphous or vitreous state of uncertain, but largely non-crystalline structure. And there are, as I told you, hexagonal bipyramidal classes of crystal symmetry systems. So, real ice crystals are never perfect, and the structural defects encountered are usually the orientational or ionic types. So, structural defects in ice explain the high mobility of protons and the small decrease in electrical conductivity when water freezes.

The physical states of water

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### Structure of ice (Contd...)

- The hydrogen bonding in water also determines the structure of ice.
- When water freezes into ice a regular hexagonal pattern of the molecules results.
- This structure of ice accounts for its properties.
- Ice at 0 °C is actually less dense than water due to more empty space in ice.
- It is difficult to visualize what our world would be like if ice did not float on warmer water beneath it.
- The fish population that presently thrives under the insulating blanket of ice in the winter time would clearly be the first victim if water's unusual properties were not the rule.

So, as I told you, these are the closed hydrogen-bonded structures of ice; that is, when ice freezes, a regular hexagonal pattern of molecules results in the structure of ice. This basically accounts for its properties, and you know that it is well-known that ice at 0 degrees Celsius is usually less dense than water at that temperature. And that is mainly



because ice has a lot of empty void spaces in it, okay, and it is difficult. Because of this, there are a lot of oil spaces, it has a volume, and it has a light weight, and this ice floats on the water. It would be visualised what our world would be like if the ice did not have this unusual property of floating on the water. That is warmer water beneath it, and the fish population, particularly during the winter season, when this surface water freezes to ice, then the fish population, or other aquatic animals, etc. they survive inside the insulating blanket of the ice. Below the ice layer, the water is a little warmer, and the aquatic population survives in it.

**Unique physical properties of water**

- Water is a tasteless, odourless, and colourless liquid over the temperature range of 0-100°C at ambient pressure.
- It is transparent and only strong UV light is slightly absorbed.
- Water has a high specific heat capacity and a high latent heat of vaporization due to extensive hydrogen bonding.
- This allows water to absorb and release heat slowly, making it ideal for heating and cooling processes. It also conducts heat better than any liquid except mercury.
- Pure water has low electrical conductivity, but it increases significantly with the addition of ionic material. The conductivity rises as ion concentration increases since electrical current is carried by ions in solution.

The slide includes a small video inset of a man with glasses and a mustache, wearing a light blue shirt, gesturing with his hands while speaking. At the bottom left, there are logos for 'APJKTU' and 'NPTEL'. The name 'Dr. Manoj Kumar' is written in the bottom right corner of the slide area.

Now, let us talk about physical properties of water and this is because of this structure hydrogen bonded water is a closed dense hydrogen bonded structure and ice is the closed water is a open handed bonded structure or ice is a closed hydrogen bonded structure and because of this structural differences in the ice and water there is also the differences in the properties of ice and water. First, we take the property that water is A tasteless, odourless and colourless liquid over the temperature range of 0 to 100 degrees Celsius at ambient pressure. It is transparent, and only strong UV light is slightly absorbed in water. Water has a high specific heat capacity and high latent heat of vaporisation, and that is mainly because of the Extensive hydrogen bonding. There is more heat required to break these hydrogen bonds, and this allows water to absorb and release heat slowly, making it ideal for heating and cooling processes. Water also conducts heat better than any liquid except mercury. Pure water has low electrical conductivity, but it increases significantly with the addition of ionic material. The conductivity rises as ion concentration increases since electrical current is carried by ions in the solution.

Physical properties of water	
Property	Value
Molecular weight	18.0153
Melting point (at 101.3 kPa)	0 °C
Boiling point (at 101.3 kPa)	100 °C
Critical temperature	373.99 °C
Critical pressure	22.064 Mpa
Triple point temperature	0.01 °C
Triple point pressure	611.73 Pa
$\Delta H_{\text{vap}}$ at 100°C	40.647 kJ/mol
$\Delta H_{\text{sub}}$ at 0°C	50.91 kJ/mol
$\Delta H_{\text{fus}}$ at 0°C	6.002 kJ/mol

In this table, I have tried to give you the important physical properties of water, like its molecular weight, melting point 0 degree Celsius, boiling point 100 degree Celsius, its critical temperature, critical pressure, triple point, even latent heat of fusion at 100 degree Celsius, latent heat of sublimation, latent heat of evaporation, all these things are given. These values are well known in any book; you can get them.

Temperature dependent properties				
Properties	Temperature (°C)			
	Ice		Water	
	-20	0	0	20
Density (g/cm <sup>3</sup> )	0.9193	0.9168	0.99984	0.99821
Vapor pressure (kPa)	0.103	0.6113	0.6113	2.3388
Heat capacity (J/g/K)	1.9544	2.1009	4.2176	4.1818
Thermal conductivity (W/m/K)	2.433	2.240	0.561	0.5984
Thermal diffusivity (m <sup>2</sup> /s)	$11.8 \times 10^{-7}$	$11.7 \times 10^{-7}$	$1.3 \times 10^{-7}$	$1.4 \times 10^{-7}$
Compressibility (Pa <sup>-1</sup> )	-	2	4.9	-
Permittivity	98	90	87.9	80.2

Similarly, the temperature-dependent properties and a comparison with these properties of ice and water, like density—that is, you see at 0 degree Celsius, the density of ice is 0.9168 gram per cubic centimeter, whereas the water is 0.99984. So, water is more dense than ice at 0 degree Celsius. Similarly, if you compare vapor pressure, heat capacity, normal heat capacity of ice, water is more than that of ice. Thermal conductivity, however, of ice is more than that of water. Similarly, thermal diffusivity of ice is also more than that of water. Then, permittivity is normally almost the same, but if you look at 0 degrees Celsius, the water has a little less—it is 87.9, and the ice has 90.

### ❑ Effect of solutes on water structure

In all food systems, both water and solutes are present. Therefore, it's essential to discuss how solutes affect the nature and behavior of water molecules, including their solvent properties.

#### ❖ Water-solute interactions in aqueous solutions

- The mixing of solutes and water alters their properties due to molecular interactions, which depend on the solute's molecular nature.
- Ions interact with water mainly through electrostatic forces, which can either enhance or disrupt the typical orientations of water molecules.
- Hydrophilic solutes strongly interact with water, altering its structure and mobility, while water modifies the solute's reactivity and sometimes their structure.
- The hydrophobic groups of added solutes interact only weakly with adjacent water, seeming to prefer a nonaqueous environment.

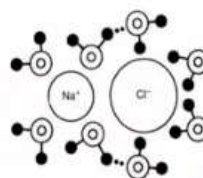


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So, the effect of solutes on water structure is that when any chemical, a soluble chemical like, for example, sugar, is added into the water, it dissolves, or any other salt added into water. So, let us see what happens when any salt is dissolved and put into it, then there is an effect on the regular hydrogen-bonded structure of water. And then, let us see what happens. Now, in a food system, both water and solute are present. Therefore, it is essential to discuss how these solutes affect the nature and behaviour of water molecules. Particularly, the hydrogen-bonded structure of water molecules, including their solvent properties. So, if you see water-solute interactions in liquid solutions, the mixing of solute and water alters their properties due to molecular interactions, which depend on the solute's molecular nature. Ions interact with water mainly through electrostatic forces, which can either enhance or disrupt the typical orientations of water molecules in the pure hydrogen-bonded structure of water. So, hydrophobic solutes strongly interact with water. They alter the structure and mobility of water molecules, while the water modifies the solute's reactivity and sometimes its structure as well. The hydrophobic groups of added solutes interact only weakly with adjacent water molecules, seeming to prefer a non-aqueous environment.

#### ❖ Interactions of water with ions and ionic groups

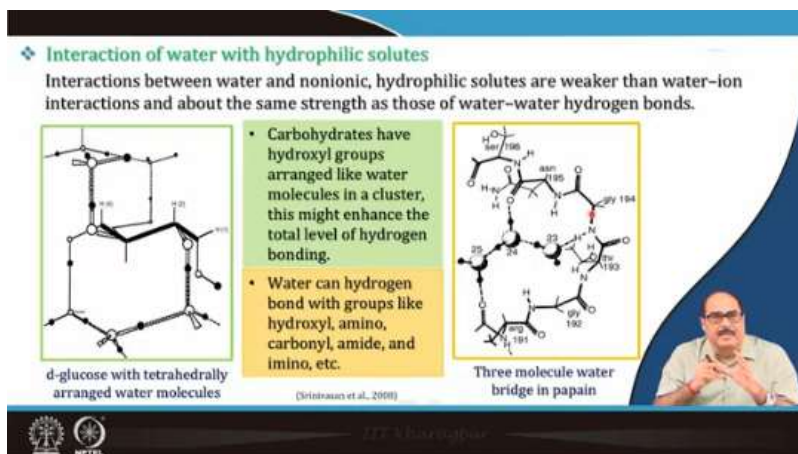
- Ions and ionic groups of organic molecules significantly hinder or influence the mobility of water molecules more than other solutes.
- The strength of electrostatic water-ion bonds is greater than that of water-water hydrogen bonds, but still much less than that of covalent bonds.
- Water and simple inorganic ions undergo dipole-ion interactions, for e.g. hydration of the NaCl ion pair.



Dr. Manoj Kumar



As far as the interaction of water with ions and ionic groups is concerned, like sodium ion, when it is dissolved, it dissociates into sodium positive and chloride negative ions. So, these ions and ionic groups of organic molecules significantly hinder or influence the mobility of water molecules more than other solutes. So, you can see here how water molecules are moving. So, the strength of electrostatic water-ion bonds is greater than that of the water-water hydrogen bonds, but is still much less than that of the covalent bonds. So, water and simple inorganic ions undergo dipole-ion interactions, for example, hydration of the sodium chloride and ion pair, and so on.



So, regarding the interaction of water with hydrophobic, like interactions between water and nonionic hydrophilic solutes are weaker than water-ion interactions and about the same strength as those of the water-water hydrogen bonds. And you can see here in the picture, it has been shown: glucose with tetrahedrally arranged water molecules. Whereas here, three water molecules bridge in a papaya. So, carbohydrates have hydroxyl groups arranged like water molecules in a cluster, and this might enhance the total level of hydrogen-ion bonding. Also, water can hydrogen bond with groups like hydroxyl, amino, carbonyl, amide, and amino, etc and these interactions between the ions, etc., may sometimes enhance the hydrogen bond structure or sometimes destroy it. depending upon the ions.

❖ Interaction of water with nonpolar substances

❖ Water and apolar groups exist in an antagonistic relationship, water structure adjusts to minimize contact with apolar groups.

(a) hydrophobic hydration, and (b) hydrophobic association

[Schirmer et al., 2000]

Also, regarding the interaction of water with non-polar substances, as you can see here, there is hydrophobic interaction in picture A as well as hydrophobic hydration, and then hydrophobic association in pictures B and C is shown. So, water and a polar group exist in an antagonistic relationship; water structure adjusts. To minimise contact with apolar groups.

❑ Ice in the presence of solutes

- The presence of solutes influences both the amount (through thermodynamic effects) and the propagation patterns (through kinetic effects) of ice in an aqueous system.
- As the concentration of a particular solute increases, the amount of ice formed at any temperature decreases. This is a manifestation of freezing point depression and colligative effects.
- The amount and kind of solutes present influence not only the quantity, but also the size, structure, location, and orientation of ice crystals resulting from any particular cooling protocol.
- The hexagonal form of ice, which is highly ordered, is found in foods unless extremely rapid freezing occurs or solutes significantly restrict water molecule mobility.

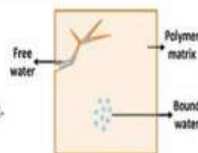
So, regarding ice, ice in the presence of solutes, the presence of solute influences both the amount, that is, through the thermodynamic effect, and the propagation pattern. The propagation pattern is influenced by the kinetic effects of ions in an ecosystem. As the concentration of a particular solute increases, the amount of ice formed at any temperature decreases. This is a main manifestation of freezing point depression and colligative effects. The amount and kind of solutes present influence not only the quantity, but also the size, structure, location, and orientation of ice crystals resulting from any particular cooling protocol. And the hexagonal pattern of ice, which we discussed earlier—which is highly ordered—is found in food unless extremely rapid freezing occurs or solutes significantly restrict water molecular mobility.

## Free and bound water

Natural foods typically contain up to 70% water, with fruits and vegetables holding up to 95%. Easily extractable water is called **free water**, while water that's not easily extracted is termed **bound water**.

### Free water

- Water that is not chemically bound to other materials and can move or be extracted easily.
- Easily obtained by pressing, squeezing, or cutting.
- Acts as a solvent and participates in biochemical reactions.
- Has a higher vapor pressure and can freeze at moderate temperatures.



Almouyri et al. 2014


Now, let us talk about the free and bound water concept, which is again very, very important as far as food science is concerned—food stability is concerned, here, water activity comes into play. So, as I told you earlier, natural food typically contains up to 70 per cent or, in some fruits and vegetables, up to even 95, 98 per cent. Easily extractable water is called free water—that is, the water which is physically entrapped among the cellular matrix, like in any fruit or any juice, let us say tomato or such others. If you squeeze with your hand, you get the juice, but if you squeeze grain, wheat grain, paddy grain, etc., rice grain, you will not get free water, you will not get juice in the form of juice. So, that is the tomato in such other material, the water is physically entrapped inside the cellular matrix, as you can see here in this picture. So, that is called free water and the water that cannot be easily extracted which cannot come out by just simply squeezing or pressing is the bound water means it is present in the form of bound in the bound form it is in the form of with the other polymer matrix other components of present in the food it is bound with them. So, free water is that water that is not chemically bound to any other material and can move or be extracted easily. It is easily obtained by pressing, squeezing or cutting and acts as a solvent and participates in biochemical reactions. Many of the water-soluble components are present in these physically entrapped waters, and when you get the juices, then the water-soluble components also. They come in along with it. This free water has a higher vapor pressure and can freeze at moderate temperatures.

Free and bound water (Contd...)

❑ **Bound water**

Water that exists in the vicinity of solutes and other nonaqueous constituents, and that as a result of its location exhibits apparent properties that are significantly altered from those of 'bulk water' in the same system.

- ✓ It is the stable water content of a sample at a specific temperature and low humidity.
- ✓ Remains unfrozen at temperatures as low as  $-40^{\circ}\text{C}$  or below.
- ✓ Unavailable as a solvent for additional solutes.
- ✓ Bound water is the water that moves with macromolecules during sedimentation, viscosity, or diffusion experiments.

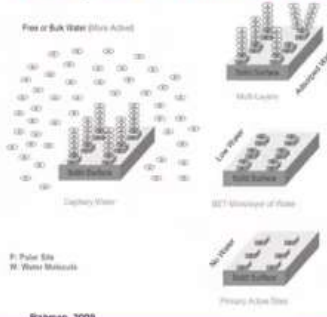


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On the other hand, the bound water is the water that exists in vicinity of solutes and other non-aqueous constituents. And that as a result of its location, it exhibits apparent properties that are significantly altered from those of the bulk water or free water in the same system. This bound water is the stable water content of a sample at a specific temperature and low humidity. It remains unfrozen at temperature as low as at minus 40 degree Celsius or below. It is unavailable as a solvent for additional solutes. Bound water is the water that moves with macromolecules during sedimentation, viscosity or diffusion experiments. Means it is rightly adhered to these macromolecules, etc. So, it moves along with the macromolecules.

❑ **Concepts of BET mono and multi layers water**



Free or Bulk Water (Highly Active)

Adsorbed Water

Capillary Water


BET Monolayer of Water

Primary Active Sites

P: Polar Sites  
H: Water Molecules

Rahman, 2009

- BET (Brunauer-Emmett-Teller) theory explains water adsorption on solid surfaces in food systems at varying moisture levels.
- **BET monolayer water**  
A single, tightly bound layer of water molecules adsorbed onto a food surface, critical for stability and not supporting microbial growth.
- **BET multilayer water**  
Additional, loosely bound water layers that form after the monolayer, affecting texture, reactions, and microbial growth.



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Now, this at least free water and bound water, various water types, how these are present in the biological system, or how they influence the various characteristics of the food, etc., can be understood with the BET, monolayer or multilayer water concepts. So, BET means Brunauer-Emmett-Teller, which is the BET theory that explains water absorption on solid surfaces in food systems at varying moisture levels. Like you can see, that is bulk or free water, how it is produced in the capillary water or even BET. Multi-layer, monolayer water is primarily active. sites etcetera. So, the BET monolayer of moist water is a single tightly bound layer of water molecules which is adsorbed onto a food surface, and it is critical for


the stability of the food material and does not support microbial growth, etc. This is the monolayer moisture content that is  $m_0$  value in the BET equation, which is multilayer water, meaning additional loosely bound water layers that form after the monolayer and this is the water multilayer water you can see which is present here all these things ok, which is basically that is the it affects the it is above the monolayer and it affects the texture even reactions it encourages it allows support the various chemical reactions, microbial reactions and all those reactions, etcetera.

Water activity (Contd..)

- Water activity is defined as 'the ratio of the vapour pressure of water in a food to the saturated vapour pressure of water at the same temperature.'

$$a_w = P/P_0$$

Where,  $a_w$  = Water activity;  $P$  (Pa) = Vapour pressure of the food;  
 $P_0$  (Pa) = Vapour pressure of pure water at the same temperature

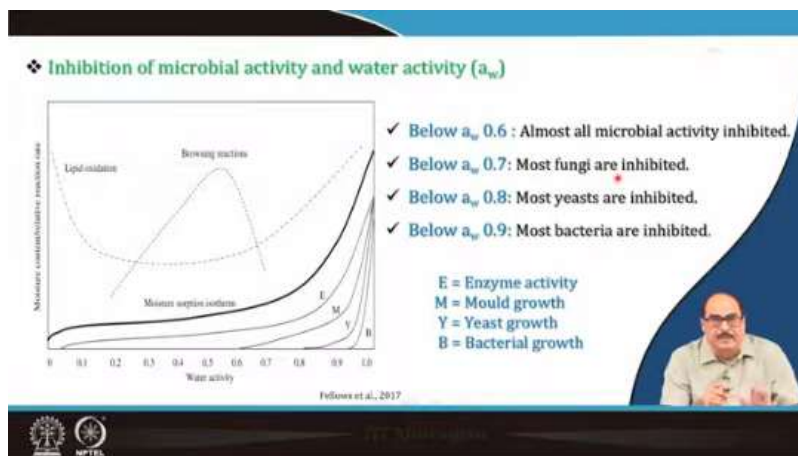


- Water in food exerts a vapour pressure, and the size of the vapour pressure depends on
  - ✓ the amount of water present
  - ✓ the temperature, and
  - ✓ the concentration of dissolved solutes (particularly salts and sugars) in the water.

Then we talk about water activity versus water activity, as you saw that. Yes, that is the water activity. It is that if more free water has a water activity of 1. And when you lower the water content, the water activity reduces. So, it is not, as I earlier discussed, the total water content, but it is the water activity which becomes more important. That is, moisture content alone is not a reliable indicator of food stability. For example, you can say that peanut oil or any butter, oil, ghee, etc., fats can deteriorate if the moisture content is as low as 0.6 per cent. or even water activity less than 0.2 percent, 0.1 percent also. Whereas, potato starch and such other materials can remain stable at more than 20 percent moisture content. So, it basically is the water activity that defines the availability of the water for various chemical processes, etcetera. So, water activity. Actually,  $A_w$  determines the availability of water for microbiological, enzymatic, or chemical processes. It is directly linked to the shelf life of the food and is also known as relative vapor pressure (RVP). So, the water activity can be defined as  $a_w$  is equal to  $P$  by  $P_0$ , that is the ratio of the vapor pressure of water. of vapor pressure of water in a food to the saturated vapor pressure of water at the same temperature. Like that, these molecules you see exert pressure, all right? Various molecules. So, that is in the food along with the water; there are some other things, as we say, solutes, etcetera—all those things. So, that water vapor pressure—the vapor pressure of the water in the food system—what is present is the free water. Divided by—if that is  $P_0$ —it is only when there is pure water, how much

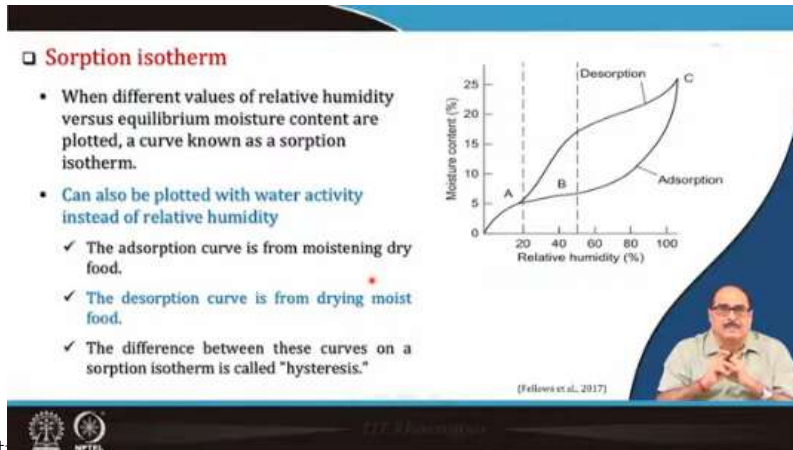


pressure it exerts is called the ratio of that, the water activity. In fact, you can say that if you say that the water activity of pure water, that is, water which is found in the seas, ponds, etc., free water, it has a water activity of 1. And when solutes dissolve into it, it causes the water—that is, some of the water is bound with the solutes, etcetera—and therefore, it results in the depression of the water activity. Water solute concentration increases; water activity decreases, OK? So, water—if the food exerts a vapor pressure—the size of the vapor pressure depends upon the amount of that, the water pressure  $P$ , which we are talking about—the amount it depends upon the amount of the water present. The temperature and the concentration of the dissolved solutes—particularly salts and sugars—which are there in the water, OK?



So, here you can see, as I was telling you, that once you go below that—the free water—that is, as a water activity ( $a_w$ )—and it will obviously support all the types of. So, when you go down, add solutes—particularly when what happens when we dry, we remove the moisture to water activity. So, water activity can be managed either by removing the moisture or by adding certain solutes to bind this water. So, when the solutes are there, the water activity will be less and by evaporation, the concentration of solutes increases in the water. So, water activity reduces. So, obviously, when the water activity reduces, the various enzymatic processes, chemical processes, microbial processes, etc., are required. That is, for example, if you bring about water activity below 0.9, most of the bacterial microorganisms, etc. they will not be able to grow in that food. Similarly, below 0.8 most of the yeasts are inhibited. if the water activity is brought below 0.7 even most of the fungi molds etcetera are also and if the water activity brought below 0.6 then most of the microbial almost all the microbial chemical and other processes are stopped only a few that is there is a lipid oxidation reaction as you can see in this figure it is there is some exception like they can they occur at a high rate at a lower water activity level. Otherwise most of the other reactions they are minimum at the boundary layer of isotherms of point zone 1 and

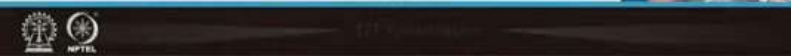
zone 2 and then they increase and there are maximum in the vicinity of around 0.8 or 0.9 in this all this process. So, water activity increases, the enzymatic activity, mold growth, yeast, bacterial all those things. So, this graph shows how the moisture content or relative humidity versus water activity and how it will influence the various reactions like moisture sorption isotherm with this, then browning reactions, lipid oxidation and other microbial growths and so on.



So, the Sorption isotherm you can see here. When different values of relative humidity versus equilibrium moisture content are plotted, a curve known as the sorption isotherm is obtained, and it can also be plotted with the water activity instead of relative humidity. So, you can see here that when there is an increase in water content, it is the adsorption, but when there is a decrease in water content. Again, the material is removed, dried, and then the water goes out, and it is called desorption. The desorption curve is from drying most of the foods. So, the difference between these groups that are present during adsorption and during desorption is that there is some change in the path, and that is called hysteresis, which is exactly what this is because of the many factors that are present in the food, such as the rate of adsorption. And the rate of desorption of water from the food system there is variable, and that hysteresis takes place.

#### ❖ Water activity short comings

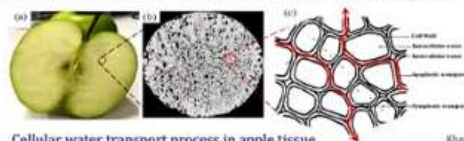
- Water activity has been a critical parameter in estimating food stability, particularly influencing microbial growth, enzymatic activity, lipid oxidation, and food texture during processing and storage.
- It measures the chemical potential of water, assuming food is in equilibrium with its environment, but most foods are not in equilibrium. This limits its accuracy in capturing the evolution of structural changes in food over its shelf-life.
- It also does not account for food microstructure or local variations in water content, which can affect microbial stability. Microorganisms are more sensitive to local properties than bulk water activity.
- Microbial response can depend more on the type of solute controlling water activity than on the water activity itself, underscoring the importance of solute-water interactions in food systems.
- Water activity reflects surface properties rather than internal molecular dynamics, and solutions with the same water activity can exhibit significant differences in kinetic properties like viscosity.



So, there are water activity basically there are shortcomings that water activity has been a critical parameter in the food stability, particularly influencing the microbial growth, enzymatic activity and many other biochemical processes like lipid oxidation, etc. So, it measures the chemical potential of water, assuming food is in equilibrium with the environment. But most foods are not always in equilibrium. So, this limits the accuracy in capturing the evolution of structural changes in food over its shelf life. Also, water activity does not account for the food microstructure or local variations in the water content, which can affect microbial stability. So, microorganisms are more sensitive to local properties than bulk water activity. Microbial responses can depend more on the type of solute controlling water activity than on the water activity itself. So, this underscores the importance of solute water interactions in the food system. Water activity reflects a surface property rather than the internal molecular dynamics, and the solutions with the same water activity can exhibit significant differences in the kinetic properties, like viscosity, etc.

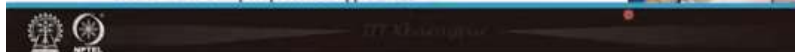
#### Molecular mobility and food stability

- Recent scientific research suggests that molecular mobility is a fundamental approach to fully attain food physical properties and stability
- Food systems are complex mixtures of water, biopolymers, ingredients, and colloids, where molecular mobility influences stability, physical state, microstructure, and food characteristics.
- Food water content, location, and interactions with other components are critical in microbial growth, degradation reactions, and sensorial aspects.

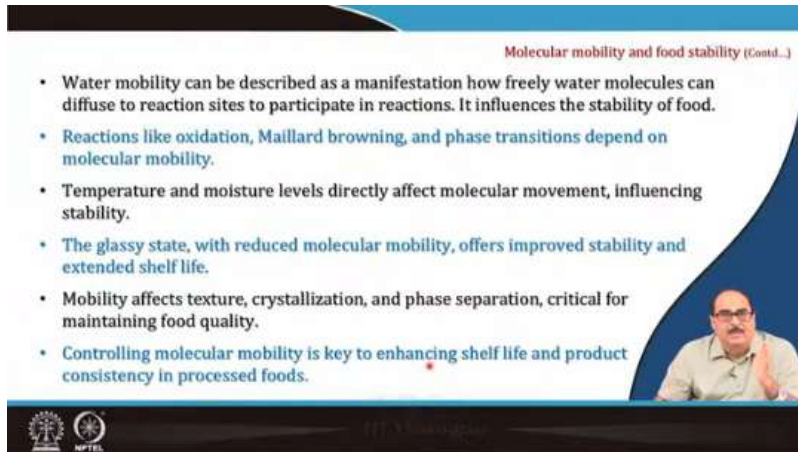


Cellular water transport process in apple tissue

Khan et al., 2018



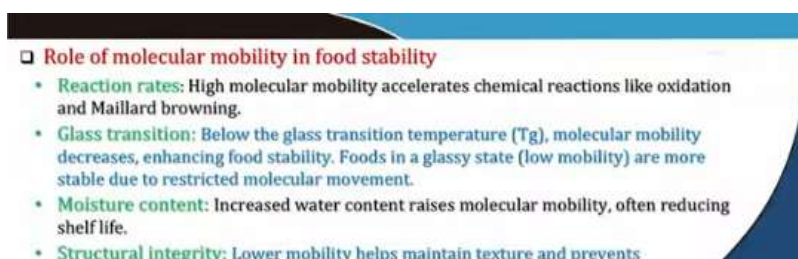
So, the molecular Mobility and the food stability we discussed recently, scientific research suggests that the molecular mobility is a fundamental approach to fully attain food physical properties and its stability. Food systems are complex mixtures of water, biopolymers, ingredients, colloids and how all these molecular mobility influences the stability, physical state, microstructure, food characteristics and so on. As you can see here, the cellular water transport process in an apple tissue is shown. This is a high, which is the larger size, right? So, inside the cell, how is this an intracellular water structure?.



**Molecular mobility and food stability (Contd...)**

- Water mobility can be described as a manifestation how freely water molecules can diffuse to reaction sites to participate in reactions. It influences the stability of food.
- Reactions like oxidation, Maillard browning, and phase transitions depend on molecular mobility.
- Temperature and moisture levels directly affect molecular movement, influencing stability.
- The glassy state, with reduced molecular mobility, offers improved stability and extended shelf life.
- Mobility affects texture, crystallization, and phase separation, critical for maintaining food quality.
- Controlling molecular mobility is key to enhancing shelf life and product consistency in processed foods.

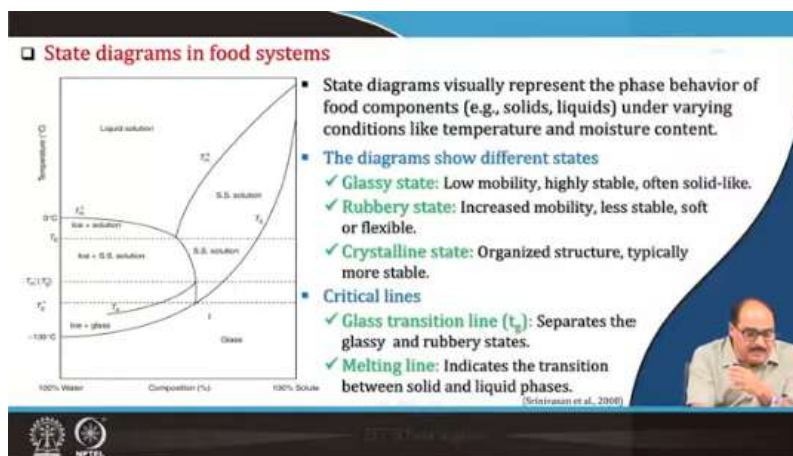
So, these food water content, its location, its interactions with other components, they are critical for all aspects, whether it is microbial growth, whether it is degradation reduction, sensorial aspects and so on. Water mobility can be described as a manifestation of how freely water molecules can diffuse to reaction sites to participate in various reactions, and therefore, it influences the stability of the food. Reactions like oxidation, Maillard browning, and phase transition reactions all depend upon the molecular mobility when the food is put under certain conditions, whether it is compressed, heated, or subjected to any process. So, how these molecules move, along with various micromolecules and how the water moves, etc., will depend. Temperature and moisture level directly affect molecular movement, influencing their stability. The glassy state with reduced molecular mobility offers improved stability and extended shelf life. Mobility affects texture, crystallisation, and phase separation, which are critical for maintaining food quality. So, controlling molecular mobility is key for enhancing shelf life and product consistency, particularly in processed foods. High molecular mobility accelerates chemical reactions like oxidation, Maillard browning, etc. Also, below the glass transition temperature ( $T_g$ ), molecular mobility decreases, enhancing food stability.



**Role of molecular mobility in food stability**

- **Reaction rates:** High molecular mobility accelerates chemical reactions like oxidation and Maillard browning.
- **Glass transition:** Below the glass transition temperature ( $T_g$ ), molecular mobility decreases, enhancing food stability. Foods in a glassy state (low mobility) are more stable due to restricted molecular movement.
- **Moisture content:** Increased water content raises molecular mobility, often reducing shelf life.
- **Structural integrity:** Lower mobility helps maintain texture and prevents

Foods in a glassy state, with low mobility, are more stable due to restrictions in molecular movement. Increased moisture content raises molecular mobility, often reducing shelf life. Structural integrity of the material: lower mobility helps maintain texture and prevents collapse in freeze-dried or dehydrated foods. Also, high molecular mobility enhances enzymatic reactions, leading to spoilage. Reduced molecular mobility delays unwanted crystallization or phase changes, preserving product quality. Also, this is the state diagram, you can see here that it visually represents the phase behaviour of food components like solid, liquid, etc., under varying conditions of temperature, moisture content, etc.



These diagrams show different statuses, as you can see here in the picture. There is a glossy state that has low mobility, highly stable, half solid, then there will be a rubbery state, and a crystalline state. So, all these rubbery states have increased mobility and a less stable and crystalline state that is an organised structure, typically more stable. So, the critical lines you can see here are that the glossy transition line  $T_g$  separates the glossy state from every state, and the melting line indicates the transition between the solid and liquid states. So, in this way, when you increase the composition and temperature that is a it gives various states that one side 100 percent water and this side is the 100 percent solute.

#### ❖ Limitations of the molecular mobility concept in food stability

- **Neglects chemical reactions:** Molecular mobility focuses more on physical changes and overlook chemical reactions that can occur independent of molecular movement.
- **Incomplete prediction:** Does not fully predict stability issues in multi-component systems, where different phases or regions may behave differently.
- **Temperature dependency:** The concept is heavily dependent on temperature, while other factors like pH, ionic strength, and mechanical stresses are often not considered.
- **Non-equilibrium states:** Fails to address non-equilibrium conditions that are common in real food systems, where molecular mobility does not behave as expected.



So, this molecular mobility concept in food stability has certain limitations as well, for example, it neglects the chemical reaction. Molecular mobility focuses more on physical changes and overlooks chemical reactions that can occur independently of the molecular movement. Similarly, the molecular mobility is almost completely predicted because it is such a complex system. So, it does not fully predict stability issues in a multi-component system where different phases or regions may behave differently. The concept of molecular mobility is heavily dependent on temperature, while other factors like pH, ionising strength and the mechanical stresses are often not considered. So, these are the limitations of this concept. Also, there is this mobility concept that fails to address non-equilibrium conditions, which are common in real food systems. where molecular stability and mobility do not behave as expected. In heterogeneous systems, it is difficult to apply the concept of molecular mobility in heterogeneous food materials with varying water activity and ingredient distribution. These molecular mobility concepts are limited in capturing dynamic changes over time, such as those occurring during long-term storage, where the food's physical structure evolves. So, these are some of the limitations of the molecular mobility concept in food stability, and this should be properly considered while designing all these processes.

## Summary

- Water is a polar molecule with a V-shaped structure due to its charged atoms; ice forms when it freezes below 0°C
- Water in food is vital for texture, taste, chemical reactions, preservation, and microbial control.
- Water activity ( $a_w$ ) measures the availability of free water in food, impacting microbial growth, chemical reactions, and food stability.
- Water mobility can be described as a manifestation how freely water molecules can diffuse to reaction sites to participate in reactions. It influences the stability of food.
- The glassy state, with reduced molecular mobility, offers improved stability and extended shelf life.



So, finally, I would like to summarize this lecture by saying that water is a very important component in food. It is an essential material for allowing various desirable reactions to take place, but it also enables undesirable reactions due to its presence. Water mobility can be described as a manifestation of how freely water molecules can diffuse to reaction sites to participate in reactions, etc. It influences the stability of the food. Water activity measures the availability of free water in the food, which impacts microbial growth, chemical reactions, food stability, and all those factors. In fact, water is what gives food its desirable characteristics, properties, texture, color, flavor, and even taste. Also, it is a very important component for providing useful properties, but at the same time, it is also one of the most addressed things from a spoilage point of view. The higher the moisture content, the higher the rate of microbial deterioration, etc. So, this is one of the reasons why, in drying or many other operations, water plays a very important role, and water activity is crucial in deciding the process conditions and giving stability to food. So, with this, these are the references.

Thank you very much for your patient hearing. Thank you.