Ocean Water Desalination Treatment

## By MIRA (Mixed Ions Reactive Approach) engine and Redox Master dryer.

Water molecules, heat of vaporisation, clusters and hydrogen bonds.

First, let me explain the physical and chemical features of the MIRA engine and Redox Master.
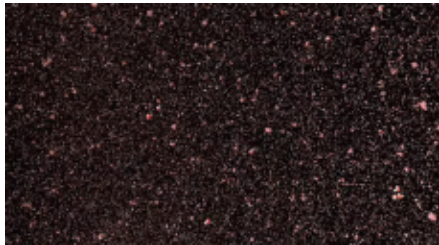The main feature of the Redox Master dryer with MIRA engine is its ability to utilise the unique properties of water as a substance to dry water or water content in the object to be dried quickly and at low temperatures, i.e. with low energy and low cost.
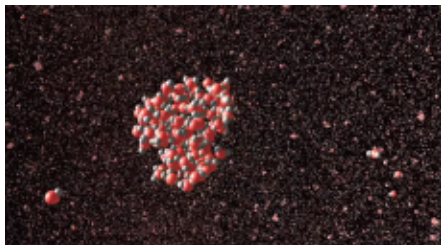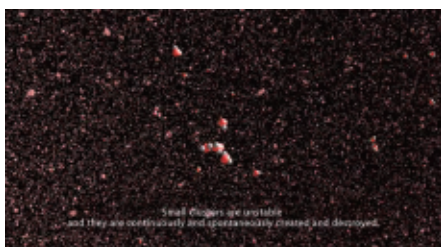
①3.4 cubic micrometres of air
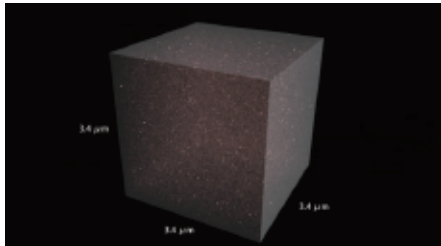
②Atmospheric moisture

③Water droplets (clusters of tens to hundreds of millions of water molecules aggregated (liquid) by hydrogen bonding)

④Clusters of small size with hydrogen bonds broken electromagnetically by the RM dryer/MIRA plasma engine.

Water has many strange properties, some of which are particularly relevant to the MIRA engine.
Water (H2O; molecular weight 18) is a compound almost the same size as methane (CH4; molecular weight 16). However, whereas methane has an ultra-low vaporisation temperature of -162°C, the vaporisation temperature of water reaches 100°C. The vaporisation temperature of water is no different from the boiling point of toluene (C6H5-CH3; molecular weight 92), which has a much larger molecular weight than water - 111°C. One of the reasons for this is that when water changes into water vapour, water molecules evaporate in clusters of about five (pseudo-large molecules or aggregates, held together by weak electromagnetic forces called hydrogen bonds). (Our research team believes that hydrogen bonds are so weak that even if there are actually more than five water molecules, they gradually start to evaporate as they get smaller and smaller).

When the relationship between the boiling point of water and the heat of vaporisation is compared with other liquids, water (boiling point 100°C, heat of vaporisation 2,250 kJ/kg), ethanol (boiling point 80.3°C, heat of vaporisation 393 kJ/kg) and ether (boiling point 34.5°C, heat of vaporisation 327 kJ/kg). Compared to substances with boiling points relatively close to water (physically and chemically, a difference of a few tens of degrees Celsius is perceived as very close), these substances have extremely high heat of vaporisation. This is also thought to be due to the fact that water molecules are polarised and polarised, causing hydrogen bonds to act and form clusters, known as clusters. *1

Glencal Technology's MIRA engine and Redox Master dryer utilise unique ionising technology to break up clusters of water molecules, which are said to number from a dozen to several hundred million under normal conditions, using weak electromagnetic force energy (the water molecules themselves are not broken up. The decomposition of water molecules, which are covalent bonds with strong binding forces, requires much stronger energy than the miniaturisation of cluster size). By making the clusters as small as a few pieces, the evaporation of water is carried out with low air heating and small energy.

As you may have already noticed, in the past, water and minerals were separated from seawater using high heat (e.g. flash and MSF methods) and membranes (e.g. RO membranes) in order to convert seawater into fresh water. technology with MIRA engines and Redox Master dryers may be considered a type of flash method, but it is a low energy desalination technology that can be used at 30 °C to 70 °C and can be considered a low-energy desalination technology with low CAPX/OPEX, with sufficient distillation capacity.

*1 Technical and professional commentary:

1. the water molecule consists of one oxygen atom and two hydrogen atoms covalently bonded together. The distance between the hydrogen and oxygen atoms is 0.0956 nm and the bond angle between oxygen and hydrogen is 104.5°. The oxygen atom has a greater electronegativity than the hydrogen atom and attracts electrons more strongly, so the oxygen atom is slightly negatively charged and the hydrogen atom is slightly positively charged and electrically polarised. The polarity of the water molecules allows **hydrogen bonds to act, forming clusters, known as clusters.** Hydrogen bonds are much weaker than covalent bonds, but they are also responsible for the higher melting and boiling points of water compared to other small molecules.
Hydrogen atoms tend to polarise to a positive charge and interact strongly with electrically negative atoms. Hydrogen atoms are so small that they can easily approach and interact more strongly with the atoms with which they interact. **The substance of hydrogen bonding is electrostatic interaction**, and the largest contribution to the binding energy is the electrostatic potential energy due to polarisation, the dipole-dipole interaction. In addition to this, there is stabilisation through charge transfer interactions. Dipole-dipole interactions and charge-transfer interactions are directional, with hydrogen-bonding interactions being responsible for the directional nature. There are also contributions from induced dipole-dipole interactions, dispersive forces, etc.).
References [1] Introduction to Molecular Interactions, H. Sugimura, Department of Materials Science and Engineering, Graduate School of Engineering, Kyoto University.

2.Evaporation rate of water
The evaporation rate of water, v, and the heat of vaporisation, Lv , are linked by the **Clapeyron - Clausius** relationship.
$v = v_0 \exp (- m L_v / k_B T)$
(1)
Determine the ratio of the evaporation rate to the evaporation rate when the heat of vaporisation is 2250 kJ / kg.
(2) expressed in Eq.
$v / v (2250 \text{ kJ} / \text{kg}) = \exp [m (2250 - L_v)/ k_B T]$

Figure 1 shows the results of equation (2) when T = 300 K. As the heat of vaporisation decreases, the evaporation rate increases and more water can be expected to evaporate with the same energy. In the Redox Master, experimental values of heat of vaporisation = 1150 kJ / kg have been obtained. Compared to a heat of vaporisation = 2250 kJ/kg, a theoretical **evaporation rate of about 2500 times higher** can be expected.

Figure 1 Results of equation (2) with T = 300 K
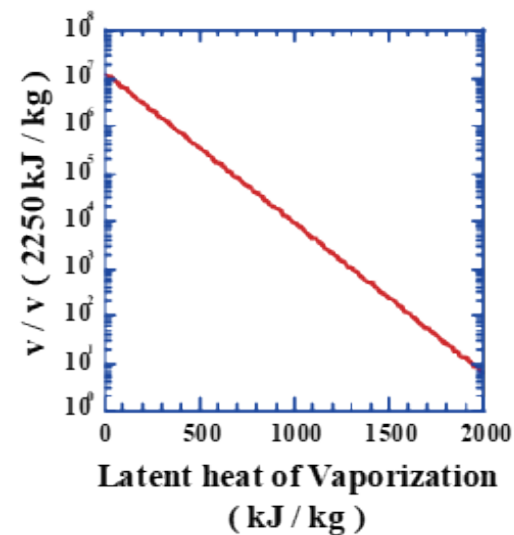
3.Quantitative evaluation of the relationship between water molecule cluster size and heat of vaporisation by non-empirical molecular orbital calculations. Molecular orbital calculations are calculations that solve the Schrödinger equation to determine the most stable structure of a molecule, molecular orbitals and their energy levels, ionisation potential, electron affinity, heat of vaporisation (evaporation enthalpy), heat of formation, charge distribution, spin distribution, dipole moment, transition state structure, activation energy, etc. The calculations are used to determine. It is also possible to predict UV-visible absorption spectra, emission spectra, IR spectra, Raman spectra and NMR spectra. The Schrödinger equation contains many complicated calculations, such as integrals, and is classified into semi-empirical molecular orbital methods and non-empirical molecular orbital methods, depending on the method used to solve the part. The non-empirical molecular orbital method does not use empirical parameters in integral calculations and calculates accurately within an approximation.

Non-empirical molecular orbital calculations for the H_2O molecule were performed using the non-empirical molecular orbital calculation programme GAMESS. Figure 2 shows the HOMO (highest occupied orbital) of the H_2O molecule, which is the orbital with the highest energy among the orbitals in which electrons are present, and therefore is an indicator of "where reactions are likely to occur" in orbital-dominated reactions.

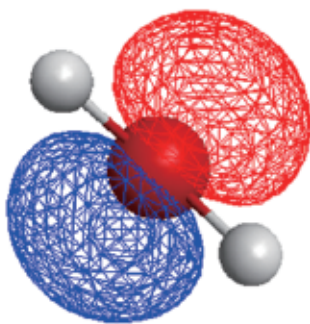Figure 2 H2 HOMO (highest occupied orbital) of an O molecule

Figure 3 shows the electrostatic potential map, on the isoelectronic density surface (= 0.02) of the H_2O molecule. In the electrostatic potential map, the areas marked in red attract the blue areas of other molecules, meaning that the red areas are repulsive to each other and the blue areas are repulsive to each other. In charge-dominated reactions, this is an indicator of "where reactions are likely to occur".

Figure 3 Electrostatic potential map of H2 O
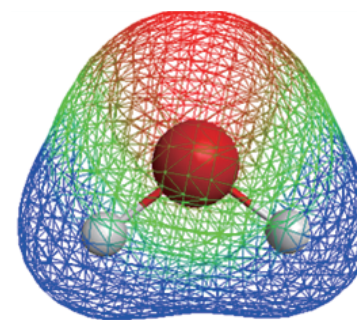
The total energy of the H_2O molecule was determined in GAMESS. - 76.0107465155 Hartree = - 2068.389751 eV = - 1.100716832 x 107 kJ / kg.

1 Hartree = 27.211806822906 eV for the H_2O molecule, 1 eV = 5321.612289 kJ / kg. $(H_2O)_2$ The total energy of the molecule was determined, the heat of vaporisation of dimeric water was determined and compared with the literature [3].

1 eV = 96.45178984 kJ / mol, obtained in GAMESS $(H_2O)_2$ The total energy of the molecule was - 152.0304564967 Hartree = - 4137.023413 eV, The heat of vaporisation of dimer water was 152.0304564967 Hartree - 2 x 76.0107465151 Hartree = 0.0089634665 Hartree = 0.2439121189 eV = 23.14842956 kJ / mol,. This value is not significantly different from the value of 21.9 kJ / mol given in Ref. Therefore, it was concluded that there were no **major errors in the calculations in this paper.**

References [3] A. J. Stone, Chem. Phys. Lett. 211 (1993) 101.

The total energies were also determined in GAMESS for the 3 - 5 water molecules, and **the heat of vaporisation for the 2 - 5 water molecules** was **determined** using the results of the total energy calculations for the 1 - 5 water molecules. The results are shown in Figure 4. From these results, it can be inferred that the **cluster size is about 3 in the redox master.**

The difficulty and rigour of non-empirical molecular orbital calculations should be noted: for n = 5, the total energy is - 380.110533 Hartree and the heat of vaporisation is 0.056800 Hartree = **1645.07 kJ/kg**, which means that a change in the fifth digit of the total energy will significantly change the value of the heat of vaporisation. The value of the heat of vaporisation changes significantly when the fifth digit of the total energy changes. For example, if the total energy is - 380.120533 Hartree, the heat of vaporisation is 0.06680 Hartree = 1.817767118 eV = **1934.69 kJ/kg**. Moreover, it is a large-scale calculation that requires more than five significant digits of energy. Therefore, no calculations have been carried out for hexahedra or larger in this paper.
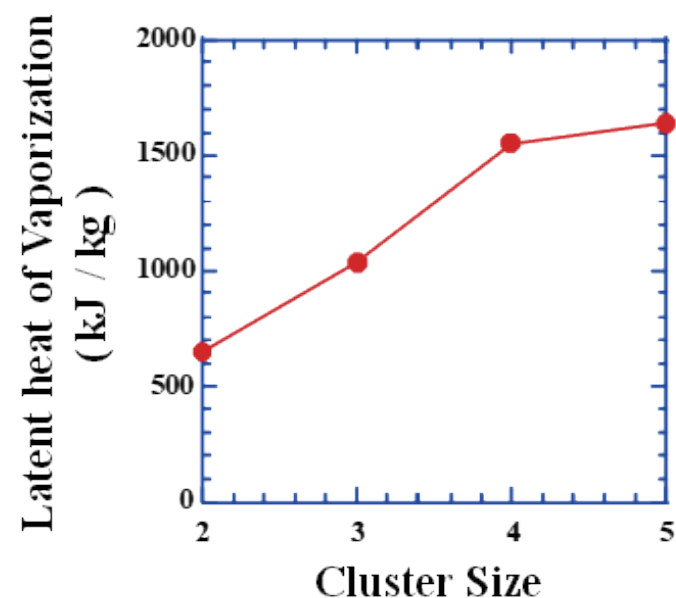
Figure 4 Heat of vaporisation of water molecules in 2 - 5 quantities

image RedoxMaster Desalination Treatment