WATER STRUCTURES AND THE SEPARATION EFFECT ON WATER–ALCOHOL SOLUTIONS IN CARBON NANOTUBES UNDER THE INFLUENCE OF ELECTRIC FIELDS

March 2016

WINARTO

別表６
（３）

Keio University

Thesis Abstract

No._____

Registration Number	□ “KOU” □ “OTSU” No. *Office use only	Name	WINARTO

Thesis Title:

WATER STRUCTURES AND THE SEPARATION EFFECT ON WATER–ALCOHOL SOLUTIONS IN CARBON NANOTUBES UNDER THE INFLUENCE OF ELECTRIC FIELDS

Thesis Summary:

Carbon nanotubes (CNTs) are promising for nanofluidic-based applications such as separation membranes and nanopumps. However, a better understanding of the properties of water molecules in CNTs is required to develop such kinds of CNT-based nanofluidic devices, since they can be very different from those in the bulk. Using molecular dynamics simulations, we investigate the effects of axial electric fields on the water molecules in CNTs. Moreover, this work investigates the effect of electric fields for separation of water–methanol solutions and water–ethanol solutions by CNTs. An alternative method for alcohol separation from aqueous solution is urgently needed for production of biofuel because the separation with distillation consumes a large amount of energy.

An electric field aligns the dipole moment of water molecules parallel to the direction of the electric field. Water molecules thus have the same orientation in the CNTs. The uniformity of the orientation then facilitates the water molecules to build hydrogen bond network for formation of ordered structures. The structures are solid-like structures or ice nanotubes structures. The electric field induces phase transition from liquid to solid in the CNTs. Although the water structures are like solid but they can flow through CNTs. Formation of the ordered structures strengthens the hydrogen bond (or electrostatic interaction) between the water molecules. This promotes the water structures in the CNTs to be more stable and water molecules prefer to fill CNTs. The preference of water to fill CNTs under the influence of an electric field is an important property to produce a separation effect.

Without an electric field, methanol molecules or ethanol molecules fill the CNTs in preference to water molecules. The preference of methanol or ethanol to occupy the CNTs over water results in a separation effect. The van der Waals interaction of CNT–methanol or CNT–ethanol is the main factor for inducing the separation effect without the electric field. However, the van der Waals interaction significantly decreases with the increase of CNT diameter. Consequently, the separation effect without an electric field is strong for small CNT diameters and significantly decreases with the increase of diameter. In contrast, under an electric field, water molecules strongly prefer to occupy the CNTs over methanol molecules or ethanol molecules, resulting in a separation effect for water. The electrostatic interaction within the water molecules structures is the main factor for inducing the separation effect with an electric field. Thus, the formation of water structures in CNTs induced by an electric field has an important role in the separation of water from methanol or ethanol. The electrostatic interaction depends more on the molecules structures rather than the CNT diameter. As the result, the separation effect with an electric field is stronger and does not decrease with the increase of CNT diameter.