Introduction

Water substance attracts the attention of scientific community at all the times. It is the most abundant material and the source of life on earth. It is content almost in every field from atmospheric sciences to planetary research, agriculture to cryobiology, combustion chemistry to reactor engineering. Its unique properties inspire scientists and engineers, whether it is a gas at high temperature and pressure or it is a liquid deeply supercooled into the metastable region.

Circulation of water is a key factor in the climatic changes. The characteristics of air such as salinity and humidity are altered while passing across the oceans, and transmitted to the continents. Another process that commonly occurs in the atmosphere is the nucleation of ice. As an example, supercooled microdroplets in clouds initiate the precipitation of hail through ice nucleation.

Besides atmospheric events, water has a large impact on the continuity of our ecosystem. One of the unique properties maintained by liquid water is its expansion on freezing. This property makes it possible for ice to float on liquid water, which protects the living organisms from cold weather in lakes. On the other hand, freeze and antifreeze processes occur through controlled ice-nucleation within plants and animals living in cold climates(Franks 2003).

Water also plays a central role in numerous industrial processes. Liquid water is a good solvent and maintains optimum conditions for a myriad of chemical reactions. Several engineering applications get use of the properties of steam and liquid water. Besides, ice has tetrahedral packing in all known phases of it. Liquid water is also known to be a tetrahedrally coordinated liquid. SiO_2 and GeO_2 which are known for their geological and technological importance display similar features to those of water, which might be originating from their common tetrahedral configurations(Stanley, Buldyrev et al. 1998).

The behaviour of water, i.e. its thermodynamic and transport properties under various conditions, continuously challenge the researchers in finding reliable explanations. With all its benefits in evaluation of life, industrial processes and technological advancements, it is worth spending time and efforts to study the challenging properties of water.

The intention of the following work is to find a model of liquid water which allows the calculation of homogenous nucleation rates of ice in supercooled liquid water. The proposed model of water should be checked by related experiments. The outline of this study is given below:

1. The first chapter is devoted to review the structure and key properties of liquid water, and the historical development of water models.
2. In the second chapter, a modified model of liquid water based on statistical thermodynamics will be developed.
3. In the third chapter, a review of classical nucleation theory will be given. Its strength and weakness in describing the nucleation phenomena, and in estimating the homogeneous nucleation rates of liquid water will be discussed. Finally a new kinetic approach will be developed, which allows the calculation of homogenous nucleation rates of ice in supercooled liquid water and binary liquid mixtures of water with non-electrolytes.
4. In the fourth chapter, the experimental results for water + ethanol, water + isopropanol, water + glycol, water + 1,4-dioxane liquid mixtures, and aqueous urea solutions will be presented.
5. In the fifth chapter, the experimental determination of nucleation rates by the levitated-single-droplet experiments will be described.
6. The sixth chapter will contain the summary of the results.
7. The appendices contain the Fortran code for the statistical thermodynamic calculations. In addition, all the measurements of nucleation times and the corresponding ln (N_u/N_0) vs. $V_d \cdot t$ graphs are documented.