CHAPTER 1

INTRODUCTION

1.1 Problem Identification

1.1.1 Computational Science

Computer technology has now been integrated into every field in science. In chemistry, the accessibility to high performance computer in the last decade has opened computational chemistry research to the real world applications of chemistry, once restricted to model chemical systems. The widely used computational chemistry techniques are quantum chemical calculations and statistical mechanics simulations. The aim of this research is to investigate microstructures dynamic and thermodynamics properties of chemical systems.

Computational Science is interdisciplinary area, which uses numerical computations and graphic visualization to find out interested information for scientific investigations. While *Computer science* concentrate on the study of computer, algorithm and computer systems, including hardware and software, Computational Science uses computer technology to study and solve problems in the fields of mathematics, physics, chemistry, biology, other applied sciences and engineering. So that computational science should be separated from computer science. Computational scientists must be familiar with both fundamentals of computer science and in the scientific field whose problems need to be solved.

One of the computational science techniques is the use of a simulation that simulate physical events from large amount of generated or collected data. Thus

computer simulation is now established as a third basic methodology of doing scientific research, in addition to theory and experiment. The importance of computer simulation is illustrated by the *grand challenge, drug design* and *product design* problems, whose solution is beneficial to society but will require vastly powerful computers and more efficient technique to solve them.

Models of chemical systems are mainly constructed in the form of quantum chemical calculations and statistical mechanics simulation. These tools are widely applicable for many systems, especially for investigation of microscopic properties of the system. The result of computer simulation can be directly compared with those of experiment.

Computational simulations can fill the gap between theory and experiment because its results can be compatible with experimental results and it gives an insight, which could not be obtained by experiments. More over, simulation results can also used to test theoretical models.

Computer simulation methods, such as Monte Carlo (MC) practically introduced by Metropolis [1], and Molecular Dynamics (MD), introduced by Alder and Wainwright [2-4], are tools which widely used for studying statistical and dynamical properties of liquid and solutions. Both simulation methods can be employed to evaluate structural properties of systems, included some information unacquirable by experimental techniques. However, Molecular Dynamics methods show not only the structural properties but it can also predict dynamical properties of the system.

1.1.2 Pair Potential Function

The studies of the computer simulation run for chemistry system can be set up in the same way as experiments. The condition, for example, temperature, pressure and density of the system can be adjusted. And it can be applied to any condition, also for the systems, which are not stable. However, it is practically impossible to calculate energy of all simulation steps based on quantum chemical method, even using the fastest computer which available up to now. Because the mathematical concept behind the system is totally complicate. The alternative choice is to use the hypothesis of pair interaction. That is, complexation energy of the system (ΔE) can be estimated from sum of the complexation of each pair of molecule or ion (ΔE_{ij}),

$$\Delta E = \sum_{i}^{N-1} \sum_{j>i}^{N} \Delta E_{ij} \qquad (1.1)$$

where N is total numbers of molecules and/or ions in the system and

$$\Delta E_{ij} = E_{ij} - E_i - E_j \qquad (1.2)$$

here, E_{ij}, E_i and E_j are total energies, calculated using quantum chemical calculations, of the complex ij and monomer i and j, respectively.

The calculation of ΔE using equations (1.1) and (1.2), is still unpractical. This is because particles in the system have to be moved million times for each simulation run and ΔE has to be calculated for each step. Therefore, ΔE is normally calculate from the *Pair Potential Function*.

The Pair Potential Function is a mathematical equation that constructed to explain interaction between two particles, molecule or ion. The quality of the simulation depends strongly on the quality of the function used. It is generally agreed that the progress in the field of computer simulation is obstructed by the reliability of the function and the difficulty in developing it. The main goal of this study is to simplify the process for developing the Intermolecular Pair Potential Function and make it easy and convenient for scientists, especially for those are not familiar in this field.

1.1.3 Programming languages

FORTRAN (FORmula TRANslation) has been the most common programming language for scientific research, in view of its suitability for scientific applications, with a variety of mathematical functions, and the availability of FORTRAN compilers producing efficient code. The importance of extracting the most from the computer in the early days of simulation is emphasized by the use of assembler coding, instead of FORTRAN, for the most time-consuming program sections (the 'inner loop'). With some exceptions, the situation has changed somewhat since the early days. Now, computer time is more plentiful, and the gaps in speed between assembler and compiled FORTRAN, and between FORTRAN compilers and other languages, have narrowed. Rather more significant now is the programmer effort required to translate an idea into a working program. A scientist's time is valuable, and more structured programming languages (C, PASCAL) may be preferable to FORTRAN (at least to the older FORTRAN-66 or FORTRAN-IV dialects) in this respect. Having said this, the FORTRAN-77 standard incorporates many of the elements of these languages, notably the IF THEN...ELSE...ENDIF construct, which greatly simplify the writing, and final appearance, of programs. There are still some drawbacks to FORTRAN-77 (restriction to six-character variable names, absence of DO WHILE...ENDDO and CASE statement, and

recursion, although these may appear in extended versions of the language on many machines) but the widespread implementation of FORTRAN-77, the features built into it, and its historical position, still make it the natural choice for any users. In this work, FORTRAN-77 has been use to develop the program.

1.2 Objectives and Scope of the Research

The aim of this work is to develop program which creates the Intermolecular Pair Potential Function in the semi-automatic manner. This function is then used in further simulation calculation. The program language chosen is FORTRAN-77 for the solve of compatibility to the simulation program. To perform this configurations of the complex are generated and the corresponding interaction energies are calculated. The selected systems to test the performance of the program (also to test the quality of the function, which will be given elsewhere [5]) are the NH_3-Li^+ and NH_3-NH_3.

1.3 Expected output

An expected output from this study is part of the semi-automatic Fortran program for generating the Intermolecular Pair Potential Function which is possible to be used even for the novice users (scientists).