ABSTRACT

ATP synthase (F$_1$F$_0$-ATPase) is an essential enzyme for life. Powered by an electrochemical proton gradient, it catalyzes ADP and phosphate into ATP. The F$_1$-subunit of ATP synthase is called F$_1$-ATPase as it also independently catalyzes the reverse reaction in absence of F$_0$-part. The nearly 100% energy conversion efficiency of the molecular motor has attracted the attention of many physicists and biologists to explore the underlying thermodynamics. Recently, a new nonequilibrium equality derived by Harada and Sasa (Harada & Sasa, 2005) was applied to the experimental time series data on F$_1$-ATPase to extract heat flow to the environment. A phenomenological model for rotary motion was proposed and shown to reproduce key experimental features. Interested in the high efficiency of F$_1$-ATPase and the good performance of the corresponding model, we carried out a detailed computational study of the model to understand its behavior in a broader range of parameter values. We solved the model using a modified Gillespie algorithm for stochastic simulation and by integrating the Fokker-Planck equation. Various physical properties of the model, such as the relation between rotational velocity and parameters characterizing angular dependence ($q$) and ATP switching rates ($W$), the relation between two kinds of dissipation and rotational velocity, the negative heat flow from environment to system through ATP binding etc. are analyzed in detail. Importantly, we modified the driving potential to investigate the factors affecting the efficiency. Additionally, we found some inconsistences between properties of this model and previous studies and we could unify them by some adjustments, which may be useful for constructing more precise models in the future.
TABLE OF CONTENTS

ABSTRACT .................................................................................................................. ii

ACKNOWLEDGMENTS ......................................................................................... iii

TABLE OF CONTENTS ......................................................................................... iv

LIST OF FIGURES ................................................................................................. vi

LIST OF ABBREVIATIONS ...................................................................................... viii

1. Introduction and thesis Outline ................................................................. 1
   1.1 The F₁F₀-ATPase ........................................................................ 1
   1.2 The mechanochemical coupling of F₁F₀-ATPase .................... 2
   1.3 High frequency measurement of rotary motion .................. 3
   1.4 Theoretical studies of the energy conversion efficiency ....... 4
   1.5 Organization of the thesis ......................................................... 5

2. Review of Experiments ................................................................................. 6
   2.1 The energy transduction ............................................................... 6
   2.2 Four experiments and previous data analysis ......................... 7
      2.2.1 The direct analysis from trajectories ............................. 8
      2.2.2 Calculating the rotary dissipation by HSE .................... 9
      2.2.3 Calculating the torque by Fluctuation Theorem .......... 11
      2.2.4 Stall torque method ....................................................... 12
   2.3 Summary ..................................................................................... 13

3. Stochastic Model and Simulation ............................................................. 14
   3.1 The totally asymmetric allosteric model ................................. 14
   3.2 Langevin simulation ................................................................. 17
   3.3 Fokker-Planck equation and simulation ................................. 20
      3.3.1 The Fokker-Planck equation for F₁-motor ................ 20
      3.3.2 Equation governing the steady-state distribution .......... 21
   3.4 Difference scheme .................................................................. 24
   3.5 The physical quantities ............................................................... 25
   3.6 Simulation performance ............................................................. 26

4. Numerical results and analysis ................................................................. 27
   4.1 The rotational velocity as a function of parameter q and W .... 30