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A Robust Mathematical Formulation for Studying Elastically Coupled Motor-Cargo Systems

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Molecular motors are small, and, as a result, motor operation is dominated by high viscous friction and large thermal fluctuations from the surrounding fluid environment. The small size has made it very difficult to study the physical mechanisms of molecular motors. It is already difficult enough to see the motor itself, let alone to control the motor directly by applying an external force. In many single molecule experiments and when carrying out its biological functions, a molecular motor may be coupled elastically to a cargo that is much bigger than the motor itself. Fortunately, current experimental technologies allow us to measure the external force acting on the cargo and the position of the cargo with the precision of piconewtons and nanometers. It is not clear, however, whether the measured force and position can be simply treated as the force acting on the motor and the position of the motor itself. Thus, to interpret correctly the experimental results, we need to study the behaviors of not just the motor itself but also the elastically coupled motor-cargo systems. To facilitate the modeling study of motor-cargo systems, we must develop the corresponding numerical capability for solving the modeling equations. In this study, we develop a robust mathematical/numerical formulation for simulating elastically coupled motor-cargo systems for the full range of elasticity.

Keywords: Molecular Motors, Motor-Cargo Systems, Langevin Equations, Fokker-Planck Equations, Stokes Efficiency, Binding Zipper Model.

1. INTRODUCTION

Molecular motors are very small and operate in a viscous fluid environment (water). Consequently, the motor motion is dominated by high viscous friction and large thermal fluctuations.[1] Because of the small size, molecular motors have several features that distinguish themselves from macroscopic motors. The most prominent feature of molecular motors is that the time scale of inertia (the time it takes for the motor to forget its current instantaneous velocity) is much smaller than the time scale of chemical reaction cycle in the motor. On the time scale of motor operation, the effect of inertia can be safely ignored. A related feature of molecular motors is that the instantaneous velocity, caused by the bombardments of surrounding fluid molecules, changes drastically over the time scale of chemical reaction cycle in the motor. The typical value of the stochastic instantaneous velocity is several orders of magnitude larger than the average velocity of the motor. In comparison, for macroscopic motors, the time scale of inertia is much larger than the time scale of reaction cycle, and the instantaneous velocity is almost constant over the time scale of reaction cycle. These peculiar features of molecular motors suggest that we have to model molecular motors as stochastic processes and take explicitly into consideration the large thermal fluctuations. In particular, results obtained for macroscopic motors should be examined carefully in the mathematical framework of stochastic processes before being applied to molecular motors. In both macroscopic motors and molecular motors, a unidirectional motion can be produced by generating an active force at the chemical reaction site and then using the active force to drive the motor forward. This mechanism of producing a unidirectional motion is called power stroke.[2,3] In molecular motors, a unidirectional motion can also be produced by a different mechanism: if thermal fluctuations in the backward direction are blocked by a free energy barrier, then the motor will be effectively carried forward by thermal fluctuations. This mechanism of producing a unidirectional motion is called Brownian ratchet[4–8] or information ratchet.[9] In a power stroke motor, the chemical reaction generates an active driving force, which corresponds to a gradually decreasing motor potential. In a Brownian ratchet, the chemical reaction establishes a free energy barrier, which corresponds to a vertical drop followed by a flat step in the motor

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