

TORQUE BOUNDS OF DUMBBELL-LIKE MOLECULAR MOTORS AT THE INTERFACE OF 2 FLUIDS – BEYOND THE KRAMERS REGIME

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ABSTRACT

We study a dumbbell-like biological rotatory molecular motor whose two ends are separated by a membrane, where each end is in contact with fluids of different viscosity[1]. The motor operates cyclically in the over-damped regime[2]. We compute bounds for τ the torque (maximum and minimum) when the motor operates in the regime of maximum diffusion, beyond the Kramers regime[3]. These bounds are calculated solely on long-time observables and our findings complement the entropy generation bounds offered by the well-known TUR[4]. The cyclic operation of the motor in the overdamped regime is well described by $V_{eq}(\phi) - \tau\phi$ a tilted periodic potential[2] and solutions for the long-time drift velocity and diffusion are known[5]. The entropy generation rate of such a model can be computed as the product of generalized thermodynamic forces and associated current. In the case of a rotatory motor with only one degree of freedom, τ is the thermodynamic force and ω the angular velocity of its associated current. Thus, the rate of entropy production is: $T\sigma = \omega\tau$. When the motor operates either very-close-to or very-far-from equilibrium the TUR provides a tight bound for the rate of entropy generation. However, the TUR bound is very loose close to the regime of maximum diffusion[6]. For the particular system studied here, the TUR bound becomes $T\sigma \geq \omega^2/D_\phi$, where D_ϕ is the rotational diffusion.

The challenges present in most in-vivo experiments with molecular motors: i) direct measurement of the thermodynamic torque (force) applied(generated) is not possible, ii) precise determination of the viscous drag is challenging. Thus, when the TUR is a tight bound, the estimation of this torque(force) based on diffusion and drift values solely is straightforward[6]. However, if the motor operates close to the regime of maximum diffusion, the TUR is a loose bound, and estimating the torque is no longer trivial. Additionally, motors like the bacteria flagellar motor (BFM) operate in a fashion such that the motor's outer and inner parts are of very different sizes and subject to different sources of friction. In the present work, for the vicinity of maximum diffusion, one viscous drag-independent equation between torque(force), ω , D_ϕ , and E_a (the energy barrier at equilibrium corresponding to the underlying $V_{eq}(\phi)$) is found:

$$k_B T \frac{\omega}{D_\phi} \left[1 + \frac{a_1}{E_a^2} \tau^2 + a_2 \tau^4 \right] - \tau - \frac{a_3}{E_a^2} \tau^5 = 0. \quad (1)$$

Depending on the E_a value the torque is bound. With the torque estimated, we compute the effective viscous drag using the general relation for current and thermodynamic force[5]. The effective drag computed this way includes the motor's outer and inner parts contribution. In experiments, only the outer part of motors like the BFM is in contact with probes, resulting in several previous studies not accounting for any inner part contribution. The results of our study emphasize that this contribution is not negligible, and that in many circumstances dominates the dynamics of the system.

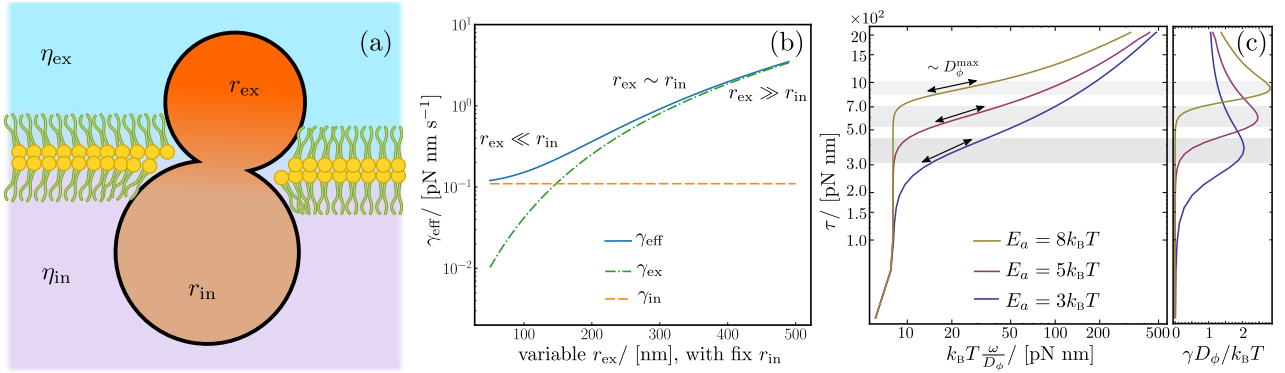


Figure 1: (a) Dumbbell motor scheme. (b) Effective viscous drag as function of motor's external radius. (c) Torque bound according to Eq.(1).

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