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Entropy production for the terminal orientation of a half cylinder in a flow

Bong Jae Chung [1], **Blas Ortega** [2] **and Ashwin Vaidya** [2,*]

[1] Department of Bioengineering, George Mason University, Fairfax, VA, USA.
[2] Complex Fluids Lab, Department of Mathematical Sciences, Montclair State University, Montclair, NJ, USA.

* Author to whom correspondence should be addressed; E-Mail: vaidyaa@mail.montclair.edu, Tel.: +1-973-655-2139.

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Abstract: The terminal orientation of a rigid body is a classic example of a system out of thermodynamic equilibrium and a perfect testing ground for the validity of the maximum entropy production principle(MEPP). A freely falling body in a quiescent fluid generates fluid flow around the body resulting in dissipative losses. Thus far, dynamical equations have been employed in deriving the equilibrium states of such falling bodies, but they are far too complex and become analytically intractable when inertial effects come into play. At that stage, our only recourse is to rely on numerical techniques which can be computationally expensive. In our past work, we have realized that the MEPP is a reliable tool to help predict mechanical equilibrium states of free falling, highly symmetric bodies such as cylinders, spheroids and toroidal bodies. We have been able to show that the MEPP correctly helps choose the stable equilibrium in cases when the system is slightly out of thermodynamic equilibrium. In the current paper, we expand our analysis to examine bodies with fewer symmetries than previously reported, for instance, a half-cylinder. Using two-dimensional numerical studies at Reynolds numbers substantially greater than zero, we examine the validity of the MEPP. Does the principle still hold up when a sedimenting body is no longer isotropic nor has three planes of symmetry? In addition, we also examine the relation between entropy production and dynamical quantities such as drag force to find possible qualitative relations between them.

Keywords: maximum entropy production; flow past cylinder

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1. Introduction

Homogeneous bodies of revolution around an axis, a, with fore-aft symmetry, when immersed in a quiescent liquid, orient themselves in certain ways with respect to the direction of gravity which depend upon the shape, size, density of the rigid body and the nature of the surrounding fluid [1–3]. In our earlier work on this subject, we analytically explained experimental observations concerning the terminal states of symmetric rigid bodies in Newtonian and non-Newtonian fluids at very small Reynolds numbers[4,5], Re, which is defined as $Re = \frac{Ud}{\nu}$, where U is the uniform velocity, d is the characteristic length and ν is the kinematic viscosity. The same problem, however, becomes much more complicated as the Reynolds number is increased. The effect of inertia is seen to give rise to several interesting Hopf-like bifurcations from the steady orientation to periodic oscillations [6,7] and beyond. Experiments on terminal orientation have come in two forms: (i) sedimentation, where the body falls through a quiescent fluid under gravitational force or as (ii) a horizontal setup with the body being hinged at the center of a flow tank. In this latter case, the body is fixed in space, though allowed to rotate, while the fluid moves past it. Both scenarios are qualitatively similar and will not be distinguished in this work.

Unsteady problems in fluid-solid interaction, in recent years, have seen a revival in interest in the fluid mechanics community. The immense mathematical complexity of the problem and the advent of fast computing has resulted in more problems being solved numerically, where analytical arguments are no longer possible. While these methods effectively capture the dynamical process, they are computationally expensive and often difficult to implement. The fact that fluids are inherent dissipative systems and the events described are out of equilibrium, allows us to apply thermodynamic tools towards these problems. Thermodynamics can reveal the underlying energetics of the system and provide more fundamental explanations for problems involving pattern formation/selection.

2. The Maximum Entropy Production Principle

Optimality principles have long been popular in physics and enjoyed much successes in various branches of theoretical physics. The principle attributed to Ziegler, essentially states that *complex systems which are out of thermodynamic equilibrium settle to a steady state corresponding to maximum entropy production*[8,9]. A more popularly known version of the extremum principle is due to Prigogine[10] and Onsager [11] which holds in the near equilibrium regime and states that steady states correspond to one of minimum entropy production. A parallel statistical mechanics approach due to Shannon and Jaynes based upon the Boltzmann's and Gibbs' interpretations of entropy has yielded noteworthy results and has been shown to be related to Ziegler's principle[9]. A thorough discussion of this subject is presented in the review by Martyushev and Seleznev[8] and it is also shown here that the MEP principle and Prigogine's principle are not contradictory; the former, in fact, subsumes the latter and can therefore be considered the more general principle. While the MEPP has been successfully applied in different contexts [8], there have also been some objections to it (see [12], for instance). Supporters of the MEP however, argue [13] that counter arguments provided are outside the range of applicability of the MEPP. Since fluids are dissipative by nature, they are apt systems for application of such a theory. In fluid mechanics, the MEP argument has been used very sparsely and mostly to understand the transition from laminar to turbulent with varying degrees of success[9,14,15]. Based on our previous work [16–18], we feel that the MEP promises to be a valuable pattern selection principle for the fluid structure interaction problems and gives us insight into the possible dynamics of the complex coupled system which has so far eluded us.

3. Theoretical Framework

In our earlier work we have shown that [16] the expression for entropy production, for the case of a sedimenting body in a viscous fluid, is of the functional form

$$\mathcal{P} \;=\; \frac{1}{T_0}\int_{\Omega} \mathbf{T} : \mathbf{D} - \frac{m_e}{T_0}\mathbf{g}\cdot\mathbf{U} = \frac{2\mu}{T_0}\int_{\Omega} \mathbf{D} : \mathbf{D} - \frac{m_e}{T_0}\mathbf{g}\cdot\mathbf{U} \tag{1}$$

where T_0 is the constant ambient temperature, $\mathbf{T}$ is the Cauchy stress tensor, $\mathbf{u}$ is the fluid velocity field and $\mathbf{D}$ is the symmetric part of the velocity gradient $\mathbf{D} = \frac{1}{2}(\nabla\mathbf{u} + \nabla^T\mathbf{u})$. In the above equation, we decompose the stress tensor in general into $\mathbf{T}_N = -p\mathbf{I} + 2\mu\mathbf{D}$, p being the isotropic pressure and μ is the viscous coefficient. Also, $m_e = (\rho_b - \rho_f)|\mathcal{B}|$ is the effective mass, where $|\mathcal{B}|$ represents the volume of the body. For the case of hinged body in a horizontal flow, the gravitational term is neglected which does not contribute to the extrema of entropy production even in the case of sedimentation[16]. The equation (1) is not merely a mathematical construct but based on physically sound reasoning[19] and consistent with previous literature.

3.1. Orientation of an ellipse/spheroid in a flow at slow speeds

In order to put equation (1) to the test, we consider a rigid body moving in a fluid, in its steady state. In our earlier work we have shown that for the problem of sedimentation of a rigid body of any shape in a Newtonian fluid at $Re = 0$, $\mathcal{P} = 0$. This is consistent with the balance of linear momentum and angular momentum equations[20]. The zero entropy production case is therefore identified with the creeping flow regime and the vanishing of $\mathcal{P}$ indicates that sedimentation, if slow enough, is a reversible process[14]. Therefore, in the case of very slow fall speeds (or high viscosities), the sedimenting body can fall with any orientation which is consistent with the observations of Leal [3].
If we restrict the geometry of the body to one possessing 3 planes of reflection symmetry and one axis of rotational symmetry, such as in a prolate spheroid, then for non-zero and small Re when inertial effects become prominent, $\mathcal{P} > 0$ and we can write[16]

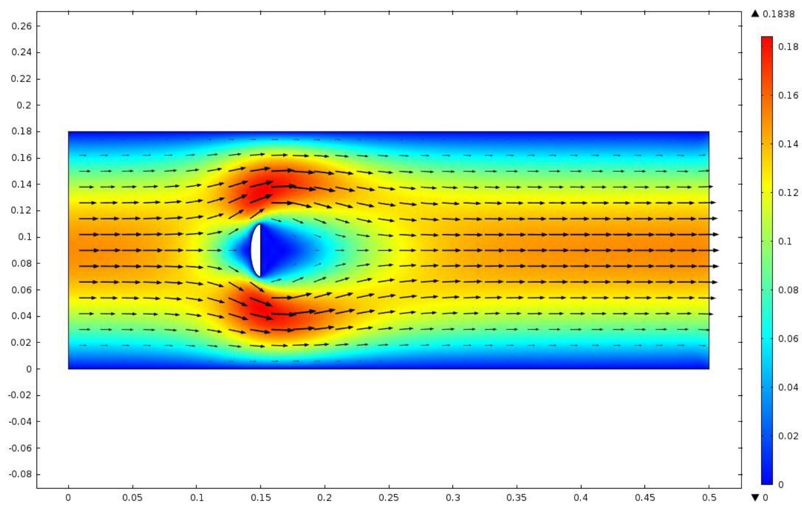
$$T_0\,\mathcal{P} \;=\; U^2(K_{11}\cos\phi^2 + K_{22}\sin\phi^2) - m_e\mathbf{g}\cdot\mathbf{U}. \tag{2}$$

where ϕ is the angle of orientation of the spheroid and K_{11}, K_{22} are positive coefficients. The derivative of $\mathcal{P}$ with respect to ϕ gives us

$$T_0\frac{\partial\mathcal{P}}{\partial\phi} \;=\; U^2(K_{22} - K_{11})\sin 2\phi \tag{3}$$

yielding two possible extrema for $\mathcal{P}$, namely, $\phi = 0$ and $\phi = \pi/2$ [16,17]. Numerical computations for prolate spheroids indicate that $K_{22} > K_{11}$ [16], indicating that $\mathcal{P}$ has a maximum at $\phi = \pi/2$. This angle is known to coincide with the experimentally observed stable terminal state of the spheroid. This result is true for a variety of other bodies which belong to the same symmetry class, such as oblate spheroids,

Figure 1. Numerical simulation of velocity field vectors past a half-cylinder oriented at 90° with respect to the uniform flow direction. The color scheme represents the magnitude of the flow.



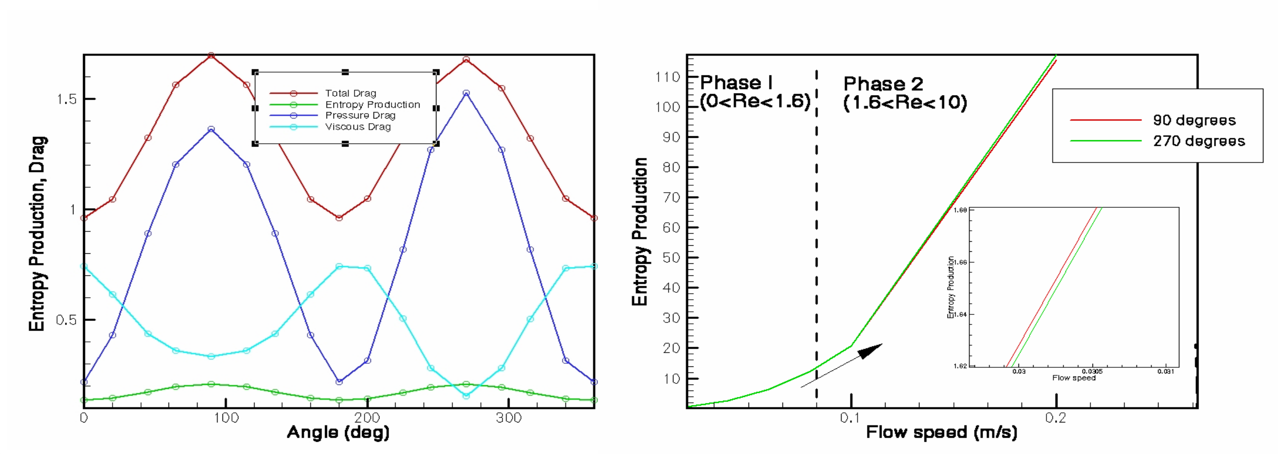
cylinders and torus [16,17]. The MEP principle therefore appears to serve as a selection principle to find the stable terminal configuration. Previous analytical work was performed for $Re << 1$ and the analysis holds in the near-creeping flow regime. We can summarize the results of our analysis in terms of the following proposition:

Proposition 1. *Bodies possessing isotropic symmetry or containing three planes of reflection symmetry with one axis of rotational symmetry, align themselves such as their long axis is perpendicular to the uniform flow direction, in their terminal stable states. This configuration coincides with the (i) maximum entropy production, (ii) maximum total drag, (iii) maximum pressure drag and (iv) minimum viscous drag.*

3.2. Impact of body shape and flow speed

We have been working to test the validity of these principles for bodies with varying symmetry classes. In our recent work, we have considered the case of a half-cylinder in a horizontal flow(see figure 1). This body possesses lesser symmetry than those previously studied. In order to test the validity of the MEPP on this body, we make two observations: (i) the flow past such a body cannot be analytically determined and must be ascertained by numerical computations; (ii) it is easier and qualitatively the same (as the sedimentation case) to consider the problem with the body clamped in different orientations and have the fluid move past the body. With these in mind we used the software, Comsol[21] to perform a two dimensional numerical simulation of flow past the half-cylinder, placed at the center of the domain (see figure 1). The domain height and length in the simulation are 0.18m and 0.5m, respectively. The walls of the domain are the upper and lower sides, and no-slip boundary conditions have been imposed. The front end of the domain is the channel inlet, at which we prescribe a uniform inflow velocity, and the back end of the domain is the channel outlet, at which zero pressure, no viscous stresses are prescribed. The half-cylinder, has dimension of 0.02m (semi-major axis) and 0.0078m (semi-minor axis). We fixed

Figure 2. Panel (a) shows the entropy production, drag force, viscous drag and pressure drag as a function of orientation angles for a half-cylinder at the $Re = 1.20$. Figure (b) shows the entropy production versus flow speed for the case of $\theta = 90°$ and $\theta = 270°$. The boundary between phase 1 and 2($U = 0.08m/s$ and $Re = 1.6$) is determined based on the observation switching of maxima in our data.



(a) (b)

the half-cylinder at its center exactly 0.15m away from the channel inlet and at 0.09m from the bottom to eliminate numerical inlet effects. *Physics-controlled mesh* was selected consisting of 7776 elements. We conduct a parametric sweep with the half-cylinder rotating counterclockwise at different velocities in the viscous fluid to obtain the results being discussed. The mesh density and parameters of the code have been tested for numerical convergence [22].

A similar numerical computation for the entropy production for the flow past an ellipse was also performed for flow speeds ranging between $0.02m/s$ - $0.5m/s$ which correspond to Reynolds numbers, $0.4 \leq Re \leq 10$. In the computation of the Re, d was chosen to be twice the major axis and ν was set to be $10^{-3}m^2s/$. The results of the computation are consistent with proposition 1. The calculations for the half-cylinder are seen to be more complex than that of an ellipse (or spheroid). Let us define a set $\mathcal{S}$ which contains the maxima of $\mathcal{P}$. Therefore, in the case of the half-cylinder, $\mathcal{S}$ contains two states corresponding to two local maxima, at 90° and 270° (see figure 2(a)), the former of which is the experimentally observed stable configuration. The total drag force and pressure drag, also reveal extrema at these angles. How, then, do we choose the stable state from set $\mathcal{S}$? Proposition 1 does not help since the ellipse possesses only one extremum. To formulate the appropriate, more general selection principle, we refer to the figure 2(b) which shows the values of the entropy production with respect to the flow speed for the case of 90° and 270° orientation. In Phase 1, corresponding to $Re < 1.6$, the stable state appears to correspond to max $\mathcal{S}$ (where the difference between the two entropy production extrema is extremely small), while in Phase 2, the stable state switches to min $\mathcal{S}$. There is no contradiction with Proposition 1 where set $\mathcal{S}$ contains only one element. As the flow speed increases and pushes the system farther away from thermodynamic equilibrium, the selection principle appears to reveal more complexity.

Proposition 2. *In the near equilibrium state, corresponding to* $0 < Re \leq 1.6$*, bodies possessing one axis of reflection symmetry, such as half-cylinders, with sufficiently large aspect ratio, align themselves* *such that their flat sides become perpendicular to the uniform flow direction. These bodies possess two equilibria corresponding to orientation angles* $90°$ *and* $270°$*, with the former corresponding to the terminal stable state. This stable configuration coincides with (i) the maximum entropy production; (ii) maximum total drag;(iii) min-max of pressure drag and (iv) max-min of viscous drag, over all angles. When the system is sufficiently far from thermodynamic equilibrium, corresponding to flow speeds* $1.6 < Re \leq 10$*, the half-cylinders, with sufficiently large aspect ratio, continue to align themselves with* $\theta = 90°$ *in the stable state. This stable configuration coincides with (i) the min-max of entropy production; (ii) min-max total drag;(iii) min-max of pressure drag and (iv) max-min of viscous drag.*

Note that the upper limit of Re in Phase 2 is limited by the range of flow speeds explored studied here and is not an indication of the limits imposed by thermodynamic effects.

4. Conclusions

In all of the cases explored thus far[16,17,19], the MEPP holds for sufficiently small flows. However, our study indicates that geometric effects are significant and allow us to test the validity of MEPP as a selection principle. What makes the case of the half cylinder particularly challenging is that an analytical expression for the flow field is not available. We therefore perform numerical simulations to solve for the velocity field. The advantage of this approach, however, is that velocity field is also no longer restricted to the linear regime but can be used to study cases where inertial effects of the fluid are significant. Our simulations consider Reynolds number in the range $0.4 < Re < 10$, advancing our analysis, possibly into a regime which is beyond the near-equilibrium regime. Also to be noted is that the general case of the half-cylinder geometry is a complex problem and the results also depend on the aspect ratio of the body, i.e. the ratio of major axis to the semi-minor axis (denoted γ). The current study only reports the case $\gamma = 5$. Analysis for $\gamma = 4$ displays similar results. Additional cases, especially for smaller γ will be conducted in the future. Our preliminary work on the half-cylinder indicates that MEPP is capable of capturing the equilibrium states of a body in a flow and is a sufficient requirement in the near-equilibrium state ($0 < Re \leq 1.6$). However, when $Re > 1.6$, the MEPP needs to be bolstered by additional constraints to serve as a valid selection principle. Propositions 2 reveals that the pressure or viscous drag are more uniform predictors and the *min-max of pressure drag* or *max-min of viscous drag* can also work as a selection principle for bodies with one plane of symmetry. Entropy production and total drag both dislpay similar extrema and switching properties. The shift in the entropy production (figure 2(b)) beyond $Re \approx 2$ coincides with the critical regime where flow separation is thought to occur and wake vortices become more prominent [23] in the flow past a cylinder. Interestingly, the same critical Re also shows up in our thermodynamic analysis of flow past a half-cylinder. This change is also remarkably similar to the results by Hubler et al. [24] on the entropy production during the self-assembly of nanotubes. They also observe a switching from a maximum to a minimum entropy production with increasing dissipative effects. The fluid-solid interaction problem discussed here serves as a perfect testing ground for the MEPP. A more thorough investigation of these cases and for additional symmetry classes and higher Re are currently being pursued.

Acknowledgements

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Author Contributions

Authors AV and BC planned and designed the study. Author BO performed the numerical computations.

Conflicts of Interest

The authors declare no conflict of interest.

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