Application of Nonequilibrium Thermodynamics to Pattern Selection in Fluid Solid Interaction

Blas J. Ortega
Montclair State University

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MONTCLAIR STATE UNIVERSITY

/ Application of Nonequilibrium Thermodynamics to Pattern Selection in Fluid Solid Interaction /

by

Blas J. Ortega

A Master's Thesis Submitted to the Faculty of
Montclair State University
In Partial Fulfillment of the Requirements
For the Degree of
Master of Science, Pure and Applied Mathematics Concentration

May 2016

College of Science and Mathematics

Department of Mathematical Science

Thesis Committee:

Thesis Sponsor
Ashwin Vaidya

Committee Member
Bong Jae Chung

Committee Member
Diana Thomas
APPLICATION OF NONEQUILIBRIUM THERMODYNAMICS
TO PATTERN SELECTION IN FLUID SOLID INTERACTION

A THESIS

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BLAS ORTEGA

Montclair State University

Montclair, NJ

2016
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 the past, it has been shown 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. Physicists 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 this thesis, 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.
Acknowledgements

I would like to express my most sincere gratitude to my supporting family who are the reason why I pursued graduate studies. Yahaira, Grace and Lianna, you are the love of my life and this would not have been possible without your support and understanding. I am very grateful for all my professors throughout this journey, specially for my committee members, Drs. Bong Jae Chung, Diana Thomas, and Ashwin Vaidya for trusting in my capabilities to do research and for the wisdom they have shared with me through out this experience. I am specially thankful to Dr. Ashwin Vaidya for giving me a second chance at doing research when the first project did not work out and for being a true educator. I am in debt with you for the rest of my life. This gratitude is also extended to Dr. Greenstein for his contribution in the fine printing of 3D particles, and therefore, making possible for the experiments to be conducted. Additionally I want to say thank you to Dr. Nita for being the first person to speak to me about doing research and for always having a pair of ears to listen to my infinite number of questions. Thank you all!
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Chapter 1

Introduction

The terminal position of homogeneous bodies of revolution around an axis, $a$, with fore-aft symmetry, depends on the shape, size, and density of the body, and the nature of the fluid in which the body is immersed [1]. In a Newtonian fluid, the body falls with $a$ (longer axis) perpendicular to the direction of the flow [11]. One way to conduct experiments on terminal orientation of a solid is by letting the body fall through the fluid as it sediments due to gravity [21]. Another way is by setting up the experiment horizontally with the body hinged at the center of the flow tank [2]. In this latter case, the body is allowed to rotate around one axis due to being fixed in space while the flow moves pass the body [2]. Both experimental setups hence similar qualitatively results and will not be distinguished in this thesis [20].
Sedimentation of a solid body in a Newtonian fluid has been studied and explained from a force point of view. When the forces acting on the body cancel one another, then the body has reached mechanical equilibrium. Our goal here is to look at this problem of pattern selection and understand it from an energy point of view. In order to do so, we must first define what a dissipative system is, and what is dissipation.

"A dissipative system is a thermodynamically open system which is operating out of, and often far from, thermodynamic equilibrium in an environment with which it exchanges energy and matter" [57].

"Dissipation includes the concept of a dynamical system where important mechanical modes, such as waves or oscillations, lose energy over time, typically due to the action of friction or turbulence. The lost in energy is converted into heat, raising the temperature of the system" [58].

Dissipation is related to entropy in a system. Entropy production can be thought as the speed at which the lost in energy is being converted into heat.

Problems concerning pattern formation are often related to optimal principles and conservation laws. The principle of minimum potential energy, the principle of least action, and Fermat’s principle of least time are some examples of such principles [4]. Since the final orientation of a body in a viscous fluid is a problem of pattern selection, it lends itself for us to study a principle that must be optimized. Further, since fluid systems are essentially dissipative and the events described are out of equilibrium, this allows us to use thermodynamics tools towards these problems [11,20]. In this study, we will test the validity of the Maximum Entropy Production Principle (MEPP) in predicting the terminal orientation of a solid in a Newtonian fluid.
For the purposes of this study we define the \( Re = \frac{Ud}{\nu} \), where \( U \) is the uniform velocity, \( d \) is the characteristic length and \( \nu \) is the kinematic viscosity. In the problem presented in this thesis, \( d = B \sin \theta + H \cos \theta \), where \( B \) is the major axis and \( H \) is the semi-minor axis, \( \nu = 10^{-3} \text{kg/m}^3 \), and \( U = 0.001 \text{m/s} - 0.5 \text{m/s} \). Therefore, we have \( 0 < Re \leq 10 \) in our analysis. It has been shown that the terminal state of symmetric rigid bodies in Newtonian fluids depends highly on the Reynolds number \( (Re) \) and the geometry of the body. At small \( Re \), a steady terminal orientation is observed. However, when the \( Re \) reach certain range of values, the problem becomes more complicated [20]. These details are described in detail in the results section of this study.

The geometry of the solid also plays a big role in the terminal position of the body. So far, all related studies have been performed on very symmetric bodies, such as cylinders and spheroids. If the MEPP proves to be a successful selection criterion to determine the terminal orientation of an ellipse, will it still hold for a shape with less symmetry? In order to test the validity of the MEPP as a pattern selection tool we will (i) verify that it coincides with the known terminal orientation of bodies with fore-aft symmetry (Ellipse), (ii) restrict the symmetry of the body by cutting the ellipse in half to form half-cylinders of various aspect ratios, and (iii) compare the results from the simulations with experiments to solidify the veracity of our findings.

1.1 MEP Principle

Optimality principles have enjoyed popularity in physics due to their successes in various areas of theoretical physics. Ziegler's principle states that complex systems which are out of thermodynamic equilibrium settle to steady state corresponding to maximum entropy production [4, 5]. From a statistical view point, Shannon and
Jaynes, based on interpretations of entropy by Boltzmann and Gibbs, were able to relate their results to Ziegler’s principle. A more popular version of the entropy optimal principle is due to Prigogine [6] and Onsager [7] which works for systems in the near equilibrium regime and shows that the minimum entropy production corresponds with the steady state of the system. In a discussion presented in the review by Martyushev and Seleznev [4], it is clarified that Ziegler’s principle and Prigogine’s principle are not contradictory. In fact, they indicate that the MEP is a more general principle to be applied [4,17].

In 1931, it was shown by Onsager [7], and most recently studied by Chung et al [11], that the local entropy production density equation can be written by the the product of thermodynamic forces1-1 (denoted $X$) and fluxes (denoted $Y$)

$$\rho_s = \sum_i X_i Y_j + \sum_j X_i Y_j + \sum_{kl} X_{kl} Y_{kl}$$

and this product may be represented as scalars, vectors or second order tensors. If we are looking at near equilibrium phenomena, Onsager indicated that a linear function of the forces, $Y_i = \sum_{i,j} L_{ij} X_j$ may be used to represent flux. Here, $L_{ij}$ represent phenomenological constants satisfying the reciprocity relations by Onsager [7,8], $L_{ii} \geq 0, L_{ii} L_{kk} \geq \frac{1}{4}(L_{ik} + L_{ki})^2$. When concerned with an incompressible fluid in motion, $\rho_s$ takes the specific form [11]

$$\rho_s = \frac{1}{T} T : D + j_q \cdot \nabla \left( \frac{1}{T} \right)$$

where $T$ is the temperature, $j_q$ is the heat flux, $T$ is the Newtonian fluid Cauchy stress tensor $T = -pI + 2\mu D$ and $D$ is the symmetric part of the velocity gradient $D = \frac{1}{2}(\nabla u + \nabla^T u)$ [11]. Here, viscous dissipation is the first term on the right hand side, while the second term represents the heat conduction due to a temperature gradient [11].
In our 2D simulation, we ignore gravity, and we assume negligible effect of the heat conduction term, and also, that the ambient temperature \( T = T_0 \) is constant \([11,18,19]\). We then integrate Eq.(1.2) over the entire domain of the unbounded fluid to obtain the net global entropy production as follows

\[
\mathcal{P} = \frac{1}{T_0} \int T : D \, dV
\]  

(1.3)

\[
\mathcal{P} = \frac{1}{T_0} \int 2 \mu D : D = \frac{2 \mu}{T_0} \int D : D \, dV
\]  

(1.4)

\[
\mathcal{P} = \frac{1}{T_0} \int 2 \mu \left[ \left( \frac{\partial v_x}{\partial x} \right)^2 + \left( \frac{\partial v_y}{\partial y} \right)^2 \right] + \mu \left[ \frac{\partial v_x}{\partial x} + \frac{\partial v_x}{\partial y} \right]^2 \, dV
\]  

(1.5)

In order to compute equation (1.5), we first need to solve the velocity field corresponding to the flow past ellipse and half-cylinders. These are then numerically put back into the integral in eq.(1.5) to find \( \mathcal{P} \). Without loss of generality, \( T_0 = 1 \).

Theory has been used to explain these problems but with limitation on the value of \( Re \). Previous theoretical calculations are based on expansions of flow velocity, and they are only valid in a extremely small range of \( Re \). Also, the theory is limited to highly symmetric bodies. On the other hand, experiments have shown auto rotation and oscillatory motion of the solid at high values of \( Re \), but the production of entropy has not been captured in such experiments. This leaves us with the theory having its limitation due to being only useful for small value of \( Re \) and experiments showing us the behavior of solids at any value of \( Re \) without being able to use the entropy production to explain the behavior of the system. In this study we use computations on these problems to be able to test the MEPP with more precision than theory or experiments can offer. Numerical simulations gives us the freedom to compute the entropy production for any values of \( Re \).
According to a review by Martyushec and Sleznev [4], the MEPP can "pretend to be an universal principle governing the evolution of nonequilibrium dissipative systems". Part of their review deals with the use of the MEPP in different scientific disciplines such as: hydrodynamics [22–37], crystal growth and and other solid state transformations [38–43], transfer of electrical charge, radiation, etc [44–48], and chemistry and biology [49–53,55,56].

We can clearly see that the Maximum Entropy Production Principle has been applied in many different fields with success. Is this a fundamental law of nature? Have we discovered a 4th law of thermodynamics? Could all pattern selection in nature be explained by the Maximum Entropy Production? Our goals are less lofty here, In this study we explore modest goals of testing the robustness of MEP for complex geometries and in far from equilibrium simulations.

1.2 Sedimentation Experiments (Newtonian)

Perhaps the easiest way to determine the terminal orientation of a solid in a fluid is by letting the solid sediment in a tank that allows for observation of the body in motion. These type of experiments have been performed abundantly in the past, and we will design such an experiment to compare with the results from our simulations. One example of sedimentation experiment was performed by D.D.Joseph [21]. In his work, he showed how elliptical bodies with round ends, when immersed in a Newtonian fluid, orient themselves such that their longer axis is perpendicular to the direction of the flow [21]. A picture of the cylindrical body as it sediments in the fluid is shown below.
Figure 1.2: Snapshot of aluminium cylinders sedimenting in a Newtonian liquid (60% glycerine in water) [21].

1.3 Experiments in Flow Tanks

An alternative to sedimentation experiments is to set up the experiment in a flow tank. Experiments in flow tanks are set up horizontally in a recirculating water tunnel, in which the inlet channel velocity can be controlled (see figure 1.3). In doing so, the behavior of the solid can be observed for long periods of time and exposed to higher values of $Re$ (higher velocity) compared to sedimentation studies [13]. This type of experiments have been successful in exploring the steady state of solids, and it is the inspiration for our simulation.

Figure 1.3: The Panel (a) shows a schematic of the experimental setup for the time dependent experiments. The arrows indicate the flow direction of water in the flow chamber. The Panel (b) shows the details of the particle suspension mechanism which restricts the motion of the body (cylinder or prolate spheroid) to rotation about the suspension axis alone. (Picture taken from [13]).

In a later study, this type of experimental setup was used to study and classify the vortex-induced oscillation and the wake structure of flow past finite cylinders [3]. The
experimental setup and the results can be seen in figure 1.4 and figure 1.5 respectively. In these type of experiments, the body is suspended in the flow tank by using a wire inserted in the walls of the tank to prevent the solid from displacement. This allows the body to rotate in one direction.

Figure 1.4: Schematic a shows how the angle $\theta$ is defined in our study. The dashed lines indicate a frame attached to the body. The angle $\theta$ can be thought of as the inclination of the body frame with respect to an inertial frame with the same origin. The mathematical analysis reveals that the equilibrium states correspond to $\theta=0, \pi/2$ with the former being the stable state. We define the angle $\zeta=\pi/2-\theta$ to allow for a more convenient description of the cylinder’s dynamics in our mathematical model. b-d show various perspectives of the experimental setup, b and c from the sides and d from the rear of the flow tank. (Picture taken from [3]).
Figure 1.5: This phase diagram shows the varying dynamics of the cylinder as a function of Reynolds number ($Re$) and the non-dimensional inertia $I^*$ of the body. These include steady orientation (S), small, random oscillations (O), periodic oscillations (P) and autorotation (A). The image is prepared by color interpolation of a discrete data set. The variation in colors gives us an indication of the threshold of bifurcation. The cartoons of the cylinder in the plot are meant to represent the dynamics displayed by the hinged cylinder, and the arrow to the left is indicative of the flow direction. (Picture taken from [3]).

We will conduct our 2D simulations using COMSOL by employing this horizontal setup of a solid body hinged at the center of a channel and letting the flow pass the body. The specifics of this simulation will be discussed in the next chapter.
Chapter 2

Computations

2.1 Numerical Method

The software COMSOL Multi-physics [15] was used to create and conduct our 2D simulations. The COMSOL module of Fluid Structure Interaction (FSI) was used to set up the simulation.

Our attempt is to simulate flow past a solid in different positions and compute the entropy production and drag forces produced by the system as COMSOL gives the solution to the fluid field in the system. In doing so, COMSOL solves the following coupled equations:

\[ \rho \left( \frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} \right) - \mu \nabla \cdot (\nabla \mathbf{u} + \nabla^T \mathbf{u}) + \nabla p = 0 \]  
\[ \nabla \cdot u = 0 \]

(2.1)  
(2.2)

where \( \rho \) is the density of the fluid, \( \mathbf{u} \) is the incompressible fluid velocity field, \( t \) is time, \( \mu \) is the kinematic viscosity, and \( p \) is the pressure.
After the flow field was computed, the net drag, pressure drag, viscous drag and entropy production on the solid as a function of the flow velocity were evaluated.

The net drag computed is given by

$$F_D = \hat{u} \cdot \int_s \mathbf{T} \cdot \hat{n} \, ds$$

(2.3)

If we decompose equation (2.3), we obtain the components of drag, namely, pressure drag and viscous drag which are as follows:

$$F_{PD} = \hat{u} \int_s -p \hat{n} \, ds$$

(2.4)

$$F_{VD} = \hat{u} \int_s 2\mu \mathbf{D} \cdot \hat{n} \, ds$$

(2.5)

Similarly, entropy production (see equation (1.5)) is computed in the simulation.

The simulations for our study were performed on a two-dimensional domain with length 0.5 m and height 0.18 m (see figure 2.1).

Figure 2.1: Ellipse hinged in the center of the two-dimensional domain.

The channel inlet was set to be the front wall of the domain, at which a uniform inflow velocity was prescribed. The channel outlet was set to be the end wall of the domain, at which zero pressure, no viscous stresses were prescribed. The top and
bottom walls of the domain were set to have slip boundary conditions. Having slip boundary conditions is equivalent to conducting the study in a fluid with infinite volume, that is, the behavior of the body and the flow itself is not be influenced by wall effects. The bodies were each fixed exactly 0.15 m away from the channel inlet and at 0.09 m from the bottom to avoid possible numerical inlet effects (see figure 2.1).

We designed an ellipse and several half-cylinders with different aspect ratios. The aspect ratio of the half cylinders was defined in the following manner. For half-cylinders with aspect ratio greater than 2, it was defined as the ratio of the major axis and the semi-minor axis. For half-cylinders with aspect ratios less than 2, it was defined as the ratio of the minor axis and the semi-major axis (see figure 2.2). In addition to the ellipse, we studied half-cylinders with aspect ratio 0.1(AR0.1), 0.25, 0.5, 1, 1.5, 2, 3, 4, and 5(AR5).

![Diagram showing a half-cylinder with AR5 at the left, and a half-cylinder with AR0.1 at the right.]

Figure 2.2: The figure above shows a half-cylinder with AR5 at the left, and a half-cylinder with AR0.1 at the right.

A fine mesh was chosen for all simulations (see figures 2.3, 2.4, 2.5). COMSOL uses the finite element method (FEM) to generate a mesh for the study. Several convergence tests to verify the accurateness of the computational results were performed on the meshing by a previous thesis student whose work was on [54]. COMSOL used the PARADISO solver, which was run for 5 seconds in increments of 0.01 of a second,
to solve for the time dependent variables. The Navier-Stokes equations for the flow past the body were solved by the FSI module in COMSOL. Once the velocity field was solved, the solution was put back into the integrals for entropy production, total drag, pressure drag and viscous drag.

Figure 2.3: *Fine* mesh in the domain for the ellipse consisting of 5662 elements.
Figure 2.4: *Fine* mesh in the domain for the half-cylinder (AR5) consisting of 5742 elements.

Figure 2.5: *Fine* mesh in the domain for the half-cylinder (AR0.1) consisting of 6768 elements.
We set COMSOL to conduct a parametric sweep (see figures 2.7 and 2.8) for the parameters $Re$ and $\theta$ (see figure 2.6). $Re$ took the values of 0.02, 0.06, 0.1, 0.16, 0.2, 0.4, 0.8, 1, 1.2, 1.6, 2, 4, 6, 8, and 10. $\theta$ ranged from $20^\circ$, $45^\circ$, $65^\circ$, $90^\circ$, $115^\circ$, $135^\circ$, $160^\circ$, $180^\circ$, $200^\circ$, $225^\circ$, $245^\circ$, $270^\circ$, $295^\circ$, $315^\circ$, $340^\circ$, to $360^\circ$.

Figure 2.6: Angle at which the solid is fixed in the system. In the figure $\theta = 45^\circ$.

A parametric sweep for each value of the $Re$ was performed. For $Re = 0.02$, the sweep simulated the flow past the ellipse at each angle $\theta$. Then, the sweep was performed for next value of $Re$ and all angles $\theta$. This procedure was done until the results were collected for all values of $Re$, all angles $\theta$, and for the ellipse and half-cylinders of different aspect ratio. We computed the results for entropy production, total drag, pressure drag and viscous drag.

Figure 2.7: Ellipse in the parametric sweep. At each angle $\theta$, the simulation runs and the results are recorded by COMSOL [15]. The particle rotated in a counterclockwise direction.
Figure 2.8: Half-cylinder (AR5) in the parametric sweep. At each angle $\theta$, the simulation runs and the results are recorded by COMSOL [15]. The particle rotated in a counterclockwise direction.

2.2 Results

2.2.1 The Ellipse

Figure 2.9: Numerical simulation of velocity field vectors past an ellipse oriented at 90° (terminal position) with respect to the uniform flow direction. The color scheme represents the speed of the flow.
We first began testing the validity of the MEPP as a pattern selection principle in a Newtonian fluid by running our simulation with the very well known case of an ellipse. Bodies with fore-aft symmetry orient themselves with the longer axis perpendicular to the direction of the flow. With this in mind, we design an ellipse in our 2D simulation and execute the parametric sweep. The ellipse has dimensions 0.02 m (major axis) and 0.0078125 m (minor axis). The terminal orientation of the ellipse known from previous cases, (see figure 2.9), is where $\theta = 90^\circ$ in our simulation.

Our results showed that at this angle of $\theta$ the system coincided with (i) maximum entropy production, (ii) maximum total drag, (iii) maximum pressure drag and (iv) minimum viscous drag. Note that two maximums are observed in the figure 2.10. However, there is only one unique terminal position, since the two maxima observed correspond to $\theta = 90^\circ$ and $\theta = 270^\circ$, which are identical positions with respect to the incoming flow.

Figure 2.10: Entropy production, drag force, pressure drag and viscous drag as a function of orientation angles for the ellipse at $Re=1.6$
2.2.2 The Half-Cylinder: Aspect Ratio 5 (AR5)

Figure 2.11: Numerical simulation of velocity field vectors past a half-cylinder (AR5) oriented at 90° (terminal position) with respect to the uniform flow direction. The color scheme represents the speed of the flow.

Now that we know that the maximum entropy production coincides with the terminal orientation of an ellipse in a Newtonian fluid, we will investigate this further by reducing the symmetry of the body. The half-cylinder is a perfect modification to the problem and serves to further investigate the validity of the MEPP in more complicated cases. The AR5 half-cylinder we designed has dimensions of 0.02 m (major axis) and 0.0039 m (semi-minor axis). It was clamped at the center of the domain as specified in the numerical method. Contrary to the ellipse, we found that for the half-cylinder, in the range $0.02 < Re < 1.6$, there are two distinct maxima for the entropy production to choose from. Those correspond to the flow being perpendicular to the parabolic and flat side of the half-cylinder respectively. Similarly, there are two extrema for total drag, pressure drag and viscous drag. These extrema are observed at $\theta = 90°$ and $\theta = 270°$ (see figures 2.12, 2.13, and 2.14).
Figure 2.12: Entropy production, drag force, pressure drag and viscous drag as a function of orientation angles for the half-cylinder AR5 at $Re=0.1$

Figure 2.13: Entropy production, drag force, pressure drag and viscous drag as a function of orientation angles for the half-cylinder AR5 at $Re=1$
We carefully proceed to analyze the results and note that as the $Re$ increase the system is pushed further from thermodynamic equilibrium, and there is a switch from the entropy production being a maximum when $\theta = 90^\circ$ to being a min-max. In figure 2.15 we see that the switch occurs for $Re > 1.6$. In phase 1, corresponding to $0 < Re < 1.6$, the system is the near equilibrium state which corresponds to stokes like flow where inertial effects are negligible. In this phase, the selection of the terminal position coincides with (i) maximum entropy production, (ii) maximum total drag, (iii) min/max pressure drag and (iv) max/min viscous drag.

In phase 2 ($Re > 1.6$), the system is pushed farther from thermodynamic equilibrium. So far, theory has not been able to explain what happens when a system is out of thermodynamic equilibrium. This is the first study where we now have an idea of what it means to go out of thermodynamic equilibrium, and it coincides with the onset of vertexes. MEP is still a local maximum, but no longer a global maximum. It is now a min-max for the system out of equilibrium. The terminal position coincides with (i) min-max entropy production, (ii) min-max total drag, (iii) min-max pressure drag and (iv) max-min viscous drag.
The results obtain in phase 2 represent a description of pattern selection in a system that is far from thermodynamic equilibrium. This is very powerful result since for the first time we have an idea how the entropy production describe the system. Although this is only one example, the results show that a system that is far from equilibrium will settle to a steady state corresponding to the min-max of entropy production. Is this a new principle? We are intrigued by these results and efforts in generalizing it will be pursued.

![Graph showing entropy production versus flow speed for the case of θ = 90° and θ = 270°. The boundary between phase 1 and 2 (U = 0.08 m/s and Re = 1.6) is determined based on the observation switching of maxima in our data.]

Hubler et al also observed a switching in entropy production in their study of the self-assambly of nanotubes [16]. As the system is pushed further and further from thermodynamic equilibrium, the selection principle becomes more and more complex. This is in part due to the development of vortexes in the flow. (see figure 2.16)
2.2.3 The Half-Cylinder: Aspect Ratio 0.1 (AR0.1)

The next case we considered in our research was a half-cylinder with a short horizontal axis and a long vertical axis. Cutting such a cylinder in half will also be a modification to a long ellipse and serves as the next body to test the MEP principle. The AR0.1 half-cylinder we designed has dimensions of 0.027951 m (semi-major axis)
and 0.0027951 m (minor axis). Since in our simulation the body is clamped, we do not account for gravity in the study and the results for our AR0.1 half-cylinder revealed only one possible terminal position. Namely, the maximum entropy production occurred at the angles $\theta = 0^\circ$ and $180^\circ$, (see figure 2.18) which are identical positions with respect to the direction of the flow. This make sense, since if we consider a much longer and thinner body, infinitely stretching it, then the center of mass will be at the middle of the body, and it will be similar to what our simulation produced, and similar to the ellipse. Keeping this in mind, and using the maximum entropy production as a pattern selection principle, we arrived at the conclusion that a significantly long body, with its horizontal axis much shorter that its vertical axis, will orient itself such that the longer axis is perpendicular to the direction of the flow (see figure 2.17). This position coincides with (i) maximum entropy production, (ii) maximum total drag, (iii) maximum pressure drag and (iv) minimum viscous drag.

![Figure 2.18](image_url)

Figure 2.18: Entropy production, drag force, pressure drag and viscous drag as a function of orientation angles for the half-cylinder AR0.1 at $Re=1.2$

The analysis of the entropy production as a function of $Re$ for the angles $\theta = 0^\circ$ and $180^\circ$ was done, and the results were as expected. Since both angles are mirror images of one another about the $x-axis$, the entropy production at each of this
angle is the same (see figure 2.19).

![Graph showing entropy production versus flow speed for the case of $\theta = 0^\circ$ and $\theta = 180^\circ$.

Figure 2.19: entropy production versus flow speed for the case of $\theta = 0^\circ$ and $\theta = 180^\circ$

2.2.4 Half-cylinders with aspect ratios between 0.5-3

In addition to the extreme cases, we also studied half-cylinders with other aspect ratios. Our initial studies indicated that half-cylinders in this range of aspect ratio displayed interesting transitional behaviors that have not been noticed before. The half-cylinder with AR0.25 produced similar results to the half-cylinder AR0.1. Likewise, the half-cylinder with AR4 produced similar results to the half-cylinder AR5. For half-cylinders with $0.5 \leq AR \leq 3$, the results were more complex and yet to be completely explained from the MEP perspective (see figures 2.20, 2.21, and 2.22 for sample calculation results). The geometry of the solid body seems to play an important role in the pattern selection, and the results of these half-cylinders will be analyzed meticulously in future studies.
We can observe from the figure on the left, that the entropy production behaves the same as in the extreme case of AR0.1. However, the figure on the right displays a maximum of entropy production at $\theta = 20^\circ$, which was not expected for this half-cylinder and future analysis of these results is currently being pursued.

We can observe from the figure that the local maxima of entropy production occur at angles for which no experiments have been designed to compare with. A more
careful analysis of these results will be pursued in the future.

Figure 2.22: Entropy production, drag force, pressure drag and viscous drag as a function of orientation angles for the half-cylinder AR3 at $Re=1.2$ (on the left) and $Re=8$ (on the right).

We can observe from the figure that even though the entropy production behaved as expected, the drag force in the system needs to be more carefully interpreted. We will rigorously analyze these results in the future.
Chapter 3

Experiments on Half-cylinders

In order to compare the results from our simulation, we designed 3D particles to conduct a sedimentation experiment. In the past, scientists have designed sedimentation experiments with cylinders and simple geometric shapes, but for half-cylinders nothing has been done. In our work, however, half-cylinders is the focus of the study.

3.1 Experimental Method

For our experiment we used a glass tank with dimensions 24 in high and 4.8 in $\times$ 4.8 in base (see figure 3.1).

Figure 3.1: Tank used for the sedimentation experiment.
The liquid of this experiment consisted of water and corn syrup. We carefully mixed the water and the corn syrup in order to be able to observe a slow descend as the particle were released. The volume of water to syrup used was $\frac{3}{5}$ to $\frac{2}{5}$. The volume of the mixture in the tank was approximately 6308 mL$^3$. We inserted the particles at the top of the tank, immersed in the fluid, and released them to observe the terminal orientation.

We designed 3D particles for the ellipsoid, and the half-cylinders with aspect ratio 5 and 0.1, using www.tinkercad.com (see figure 3.2). We used a MakerBot Mini 3D printer to print the particles. The MakerBot Replicator Mini takes plastic (PLA filament), melts it, and squeeze it to build a 3D solid object layer by layer with the touch of one button using a method called fused deposition modeling.

Figure 3.2: a) is the 3D shape produced by rotating our 2D half-cylinder (AR5) about its semi-minor axis, b) is the 3D shape produced by expanding our 2D half-cylinder (AR5) into the z axis, c) is the 3D shape produced by rotating our 2D half-cylinder (AR0.1) about its semi-major axis, d) is the 3D shape produced by expanding our 2D half-cylinder (AR5) into the z axis, and e) is the 3D shape produced by rotating the 2D ellipse about its longer axis.
3.2 Experimental Results

When the experiment was set in motion, each particle was released from different initial orientations and the final orientation was documented each time. Snapshots of the particles were taken as they descended to the bottom of the tank. Movies of the particles sediments were recorded to document the time the particles took to hit the bottom of the tank. Each particle took approximately 10 seconds to reach the bottom of the tank.

3.2.1 The Ellipsoid

![Figure 3.3: In the figure above, a-c show the possible initial and terminal position for the ellipse.

<table>
<thead>
<tr>
<th>Run</th>
<th>$\theta_i$</th>
<th>$\theta_f$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>a</td>
<td>a</td>
</tr>
<tr>
<td>2</td>
<td>b</td>
<td>a</td>
</tr>
<tr>
<td>3</td>
<td>c</td>
<td>a</td>
</tr>
<tr>
<td>4</td>
<td>a</td>
<td>a</td>
</tr>
<tr>
<td>5</td>
<td>b</td>
<td>a</td>
</tr>
<tr>
<td>6</td>
<td>c</td>
<td>a</td>
</tr>
<tr>
<td>7</td>
<td>a</td>
<td>a</td>
</tr>
<tr>
<td>8</td>
<td>b</td>
<td>a</td>
</tr>
<tr>
<td>9</td>
<td>c</td>
<td>a</td>
</tr>
<tr>
<td>10</td>
<td>a</td>
<td>a</td>
</tr>
</tbody>
</table>

Table 3.1: The table shows 10 runs for the ellipse for different initial positions $\theta_i$ and the observed terminal position $\theta_f$. 
Figure 3.4: Experiment set in motion for the ellipse, particle e) (see figure 3.2). The terminal orientation of the ellipsoid coincided with the terminal orientation predicted by the simulation. The initial orientation for the case of the ellipse is shown in figure 3.3.

3.2.2 Half-Cylinder AR5

- Figure 3.5: In the figure, a-e show possible initial and terminal position for the AR5 particle.

Table 3.2: The table shows 10 runs for our AR5 particle for different initial positions \( \theta_i \) and the observed terminal position \( \theta_f \). The table on the left shows the results for AR5 particle a), and the table on the right shows the results for AR5 particle b) (see figure 3.2).
The terminal orientation for the half-cylinder coincided with the terminal orientation predicted by the simulation. The exception was for particle b) (see figure 3.2). As shown on table 3.2, the terminal orientation of particle b) was different in two of the runs of the experiment. The length of particle b) was 2 in and it showed initial swinging oscillation motion before it reached a steady state. Since the length and width of the tank were 4.8 in respectively, particle b) found itself forcing its way to the walls of the tank and not being able to turn upside down and sediment with the curved side down as expected.

Figure 3.6: Experiment set in motion for the AR5 particle a) (see figure 3.2). Towards the bottom of the tank, very little to no oscillations were observed.

Figure 3.7: Experiment set in motion for the AR5 particle b) (see figure 3.2). Towards the bottom of the tank, some, but small oscillations were observed.
3.2.3 Half-Cylinder AR0.1

The AR0.1 particles c) and d) gravitated towards the walls of the tank each time they were released (see figure 3.8). This was due to particles c) and d) being heavier towards the thicker end of each particle. Therefore, the center of mass of each of these particles changed compared to our 2D simulation due to our simulation not accounting for gravitational effects.

![Image](image.png)

Figure 3.8: Experiment set in motion for the AR0.1 particles c) and d) (see figure 3.2).

In the figure above (top left), we observe the 3D version of the AR0.1 particle that results from rotating the AR0.1 half-cylinder about its longer axis. The other three particles shown are the 3D version that result from extending the AR0.1 half-cylinder into the z-axis. More rigorous experiments are currently being designed to verify the results from our 2D simulation.
Chapter 4

Conclusion

In previous work, scientists have studied the MEP principle and have found it to be a valuable tool to predict pattern selection. However, studies had only been conducted for very symmetric bodies and in extremely small $Re$. We want to understand if this is a general principle and if it can be used to study other fluid dynamics patterns. We designed a problem to test if the MEP works when the solid solid body is not highly symmetric (half-cylinders) and for high values of $Re$, in the regime when the system is "far from thermodynamic equilibrium".

The main results of this study are:

1) We found that bodies possessing isotropic symmetry or containing two planes of reflection symmetry with one axis of rotational symmetry (ellipse), align themselves such as their long axes is perpendicular to the uniform flow direction, in their terminal stable states. The results were verified for $0 < Re \leq 10$ in our simulation and also through experiments. This configuration coincides with (i) maximum entropy production, (ii) maximum total drag, (iii) maximum pressure drag, and (iv) minimum viscous drag.
2) In the near equilibrium state, corresponding to $0 < Re < 1.6$, 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.

3) 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. It was also observed in the experiments that regardless of the initial orientation of the AR5 half-cylinder, its final orientation was with the curved side facing the flow. 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*.

4) We found that bodies possessing one axis of reflection symmetry, such as half-cylinders, with sufficiently small aspect ratio, align themselves such as their long axes is perpendicular to the uniform flow direction, in their terminal stable states. The experiments to verify these result are currently being carefully designed. This configuration coincides with (i) *maximum entropy production*, (ii) *maximum total drag*, (iii) *maximum pressure drag*, and (iv) *minimum viscous drag*.
Table 4.1: 2D simulation results for $Re = 0.1$ and $Re = 10$ for all aspect ratios. Data in yellow represent results that are being carefully analyzed.

The MEPP proved to be a useful tool to predict the terminal orientation of a homogeneous body with fore-aft symmetry as it sediments in a newtonian fluid. The MEPP also proved to be valid as a pattern selection tool for a half-cylinder sedimenting in a newtonian fluid, a body with less symmetries. For the range $Re, (0 < Re < 1.6)$ for the half-cylinder AR5, the terminal position of the solid body coincided with that of Maximum Entropy Production. For $Re > 1.6$, the terminal position of the half-cylinder AR5 coincided with that of Min-Max Entropy Production. Experiments are currently being designed to compare with the results from the simulation for the half-cylinder AR0.1. More research and rigorous experiments are necessary to fully understand the behavior of half-cylinders with aspect ratios $0.5 \leq AR \leq 3$. 
Bibliography


[51] K. Matin’on, UFN (PHYSICS-USPEKHI) 8 (1) (1928) 1.

[52] V.F. Luginin, Brief Course of Thermochemistry, Moscow, 1903 (in Russian).


[58] https://simple.wikipedia.org/wiki/Dissipation
