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ON THE DESIGN OF 3D MICROMIXERS HAVING THE BERNOULLI PROPERTY

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Summary In dynamical systems theory a hierarchy of characterisations of mixing exist Bernoulli -> mixing ->ergodic, ordered according to the quality of mixing (the strongest first). We consider micromixers whose flows take one of two forms: 2D "blinking flows", or 3D duct flows. We show that these types of flows can be reduced to so-called linked twist maps (LTMs). LTMs can be shown to possess the Bernoulli property of mixing under certain conditions. Hence, conditions can be specified for a large class of micromixers guaranteeing the best quality mixing. Extensions of these concepts lead to first principle-based designs without resorting to lengthy computations.

INTRODUCTION

Microfluidics is the recently coined term to describe the study of fluid flows in devices having dimensions ranging from millimeters to micrometers . The volumes of fluid involved range from nanoliters (10^{-9} liters) to picoliters (10^{-12} liters). The applications of such fluid flows have literally exploded on the past few years.
Because of the length scales associated with the flow of fluids in microchannels the flow is characterized by a low Reynolds number (Re), and is therefore laminar (smooth in space, as opposed to turbulent). Hence, there is a need to understand transport, stirring, and mixing, in low Reynolds number, laminar flows. From the point of view of fluid mechanics, many aspects of this subject are well-developed and quite mature. However, the problems posed by applications at the microscale introduce some new difficulties. The channel lengths and flow speeds in “micromixers” are not sufficient to allow for the mixing effects of molecular diffusion. In this case, it is critical to understand the details of particle paths in the fluid flow over relatively short time scales (compared to the molecular diffusive time scale). This is precisely the subject area of what has been broadly termed “chaotic advection” ([1], [2]).

OPTIMAL DESIGN OF 3-DIMENSIONAL MICROMIXERS HAVING THE BERNOULLI PROPERTY

A dynamical system having the *Bernoulli property* on some invariant set of its domain possesses the “mathematically optimal” form of mixing on that domain. The obvious question then is "how do we design a mixer so that it has the Bernoulli property on as large a domain as possible?" To a mathematician, this might seem a naïve question since rigorous proofs that maps possess the Bernoulli property on regions of nonzero volume are notoriously difficult. Few examples are known, the Baker’s transformation being one of them. To a physicist or engineer, the known examples have a rather artificial flavour, epitomized by the Baker’s transformation, and consequently, tend not to provide inspiration for digging out "useful" concepts from the difficult and often less than user-friendly mathematics. The situation is not bleak however; we describe a new (from the point of view of applications to fluid mixing) type of map, or advection cycle, that has been rigorously shown to possess the Bernoulli property. Most surprisingly (and very fortuitous for the design purposes) many previously built micromixers, as well as a variety of potentially new micromixers, can be optimised for the Bernoulli property if they are designed so that the flow patterns give rise to a linked twist map (LTM). In order to show how this can be done we begin by describing precisely what a LTM is and, most importantly, its mixing properties. The material presented here is based on a series of papers by [3], [4], [5] published in the pure mathematics literature.

Linked Twist Maps

Let $S_1(r,\theta) = (r, \theta + g_1(r))$ be a twist map defined on the annulus A_1 (see Fig. 1) with $\frac{dg_1}{dr} \neq 0$ and $g_1(r_i^1) = 2\pi n$, for some integer n. Then r_o^1 is chosen such that $g_1(r_o^1) = 2\pi n + k_1$, where k_1 is an integer whose value will be discussed shortly.
Let $S_2(r,\theta) = (r, \theta + g_2(r))$ be a twist map defined on A_2 (see Fig. 1) with and $g_2(r_i^2) = 2\pi m$, for some integer m, and $g_2(r_o^2) = 2\pi m + k_2$. Furthermore, we suppose that the annuli intersect transversally in two disjoint components in the sense that $r_i^1 \cap r_i^2 \neq \emptyset$ and $r_o^1 \cap r_o^2 \neq \emptyset$ (see Fig. 1). The map defined by $S_2 \circ S_1$ on $A_1 \cup A_2$ is referred to as a *linked twist map* (LTM). Let $\alpha_i = \sup_{r_i^i \leq r \leq r_o^i} \frac{dg_i}{dr}$. The value of α_i is a measure of the strength of the differential winding of the map. $\alpha_i > 0$ is just referred to as the "twist condition". Regarding the annuli as chosen and fixed, there are four important parameters for the linked twist map: k_1 and k_2, which describe the number of twists for each twist map, and α_1 and α_2 , which describe the strength of each twist.
We can now state the main results on mixing. There are two cases to consider. One is where the annuli rotate in the same sense. This corresponds to k_1 and k_2 having the same sign (the co-rotating case). In this case if each map is at least a double twist ($|k_i| \geq 2$) and $\alpha_1\alpha_2 > 0$, then on $A_1 \cup A_2$ the linked twist map has the Bernoulli property.
Interestingly, if the annuli rotate in the opposite sense, i.e., k_1 and k_2 have opposite signs (the counter-rotating case), then the conditions that the linked twist map has the Bernoulli property on $A_1 \cup A_2$ are more restrictive. If the product of

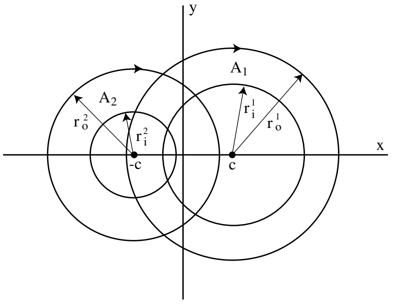

Figure 1. Geometry of the annuli from each half cycle of the advection cycle that make up the linked twist map.

α_1 and α_2 are negative then we must have $\alpha_1\alpha_2 < C_0 \approx 17.24445$. These results also indicate that, all things being equal, it is easier to achieve the Bernoulli property in the co-rotating case, as opposed to the counter-rotating case. It is then apparent that in designing a flow for optimal mixing the key quantities we need to understand are $g_i(r)$, $i = 1, 2$, on the annuli of choice, since these functions determines the rotation properties of the annuli, the radii of the annuli, and the strength of the twist. This is significant because the design of a mixer with the Bernoulli property boils down to the properties of one function describing closed streamlines in each half cycle of the advection cycle.

How to Make a LTM from a Duct Flow

Now we describe how to obtain a linked twist map (LTM) from a duct flow. By *duct flow* we mean a three-dimensional, steady, spatially periodic flow where the axial flow does not depend on the axial coordinate. We refer to each spatial period as a *cell*, and the flow is described by a mapping from the beginning of a cell to the end of a cell. This mapping is the composition of two mappings, each a twist map. The first twist map is the mapping of particles from the beginning of the cell to the half cell. The second twist map is the mapping of particles from the end of the half cell to the end of the cell. The cell to cell LTM obtained in this way will be discontinuous in the sense that each twist map is computed separately and continuity at the half cell is not enforced. Details of the computations required to go from a duct flow of this type to a linked twist map can be found in [6] and [7].

EXAMPLES OF MIXERS THAT CAN BE ANALYZED AS LTMS

Many mixers fit within the linked twist map framework. This is significant because LTMs provide an analytical approach to the design of devices producing a mathematically optimal, and precisely defined, type of mixing, depending on the geometry of the streamlines in the cross-section of the flow at the end of each half cell. Two comments first. The first example of a chaotic flow, the blinking vortex flow [1], is also the most transparent and the most immediately analyzable example of a flow that can be put in the form of a LTM. In this case the flow itself is already in the form of a linked twist map and the functions can be controlled at will. It is remarkable that, in some sense, this example encompasses, if not all, a large number of other examples. It is also important to stress that the most conceptually efficient way to think about mixing is in terms of maps and not in the terms of deviations for integrability. The most useful heuristic, is "streamline crossing", i.e. streamlines in a bounded domain at two different times must intersect. This precisely the central message of the LTMs.

Recently there have been a number of studies of micromixers appearing in the literature that can be analyzed in terms of LTMs. Two examples are the 2D electroosmostically driven “blinking flow” in [8] and the 3D pressure driven micromixer in a channel with patterned walls in [9].

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