Determining mixing properties of a two-dimensional cavity transfer mixer

A. Woering, W. Gorissen

J.M. Burgers Centre for Fluid Mechanics, Institute of Twente, P.O. Box 217, 7500 AE Enschede, The Netherlands

Abstract

From an engineering point of view mixing is one of only a few situations where chaos can actually be beneficial to the efficiency of a process. However, chaos complicates matters significantly because the process can, and probably will become very sensitive to changes in the governing parameters, meaning that the efficiency of an otherwise good mixing process can decrease considerably when, for example other fluids are used. Consequently, the calculation of the mixing properties is very sensitive to computational errors. The aim of this study is to determine the effect of truncation errors induced by using deformation tables on the analysis and optimization of mixing processes.

1 Introduction

Mixing of viscous fluids is one of the key processes in industry in order to ensure the quality and proper composition of, for example, plastic products. Large efforts have been made in this field by, for example, Chien et al.[1] on the basis of chaotic mixing and by Li and Manas-Zloczower[2] on how to understand and improve existing mixing devices. The two approaches differ very much as the first addresses simple, mostly two-dimensional, model problems, while the latter studies time-dependent complex geometries involving visco-elastic fluids.
As a link between these two situations we study the 2D Cavity Transfer Mixer, which has a time-dependent complex geometry, which is filled with a simple Newtonian fluid. To optimize the mixing in an arbitrary geometry the following steps need to be taken. First the calculation of the velocity fields, second the integration of the particle trajectories from the velocity fields and third the analysis of the trajectories and optimization.

The analysis is based on the use of deformation tables, see section 2.3, which enables fast and low cost determination of the mixing properties at reasonable accuracy. To allow for thorough testing of the proposed deformation table technique the calculation of the velocity fields and the particle trajectories must be very accurate. The required accuracy is obtained by applying the boundary element method to the computation of the velocity fields and a Bulirsch-Stoer integration scheme to the determination of the particle trajectories.

2 Mixing in the 2D Cavity Transfer Mixer

The Cavity Transfer Mixing flow, shown in figure 1, is proposed as a model for mixing in more complex geometries and it consists of a rectangular cavity, which is filled with a highly viscous fluid, such as glycerine. The cavity is driven periodically by a solid wall and by another equally sized cavity, which is filled with the same fluid.

Both the wall and the facing cavity are moving with a uniform velocity $U$. Important additional parameters are the cavity size (width $W \times$ height $H$) and the wall displacement $D$. As both the Reynolds number, $Re = UW/\nu$ and the frequency number, $\beta = W^2/\nu T$ are assured to be small, the flow within the system can be described by the Stokes equation

$$-\nabla P + \mu \nabla^2 u = 0.$$ (1)
Because the Stokes equation only has (quasi-) steady solutions, any time dependency must arise through the boundary conditions.

**Hamiltonian system** From a Lagrangian point of view, the flow or rather the trajectories of advected fluid particles are given by

\[
\frac{d\mathbf{x}}{dt} = \mathbf{u}(\mathbf{x}, t)
\]  

which is a finite dimensional dynamical system. Moreover, because of the incompressibility and two-dimensionality of the flow, the system is Hamiltonian, in which the streamfunction \( \Psi \) represents the Hamiltonian operator. Without time dependency the system is integrable and efficient mixing will not occur as distances between trajectories will only grow linearly in time.

If the system has time dependent boundary conditions, it may become non-integrable and produce chaotic particle trajectories. Chaos in this context means that particle trajectories, which are orbits of the dynamical system, grow apart exponentially fast and thus could lead to "good" laminar mixing.

**Route towards optimization** Optimization of a mixing process is much more complicated than calculating particle trajectories alone. From parameter space \( P \), which in practical situations may be vast, there exists a subspace \( M \) of lower dimension than \( P \), that produces optimal mixing, as regards one or more objective quantities representing mixedness. In the case of the 2D Cavity Transfer Mixer parameter space is spanned by \([W/H, D/H]\).

Although a mixedness number is not available for the time being, it is still possible to exclude bad mixing subspaces from \( P \) by using tools from dynamical system analysis, which can be calculated from the trajectories.

Available tools in order of computational costs, cf. Jana et al.\[3\], are: dye advection, Poincaré sections, position and character of periodic points, manifolds and finally distribution of stretching.

### 2.1 Velocity fields

In order to produce accurate but foremost continuous velocity fields a boundary element technique, see for example Pozrikidis\[4\] and Higdon\[5\], was used. Continuity of the velocity fields is desirable as interpolation of grid velocities gives rise to numerical errors which are too large to use in further analysis of this chaotic system.

Lorentz’ reciprocal identity, applied on a two dimensional bounded flow, yields for the velocity of an internal point \( \mathbf{x}_0 \)

\[
4\pi \mu u_i(\mathbf{x}_0) = \oint_{\mathcal{L}} (\mathbf{S}_{ij} f_j - T_{ijk} u_j n_k) \, dl
\]
with the fundamental solutions

\[
S_{ij} = \delta_{ij} \log r - \frac{\hat{x}_i \hat{x}_j}{r^2} \quad (4)
\]

\[
T_{ijk} = 4\mu \frac{\hat{x}_i \hat{x}_j \hat{x}_k}{r^4} \quad (5)
\]

and

\[
\dot{x} = x - x_0,
\]

\[
r = (\dot{x}^2 + \dot{y}^2)^{\frac{3}{2}}
\]

**Boundary Elements** Applying the boundary integral method to the 2D Cavity Transfer Mixer, the integral (3) was evaluated at N collocation points, while the boundary \( L \) is approximated by N straight elements, i.e.

\[
u_i(x) = \frac{1}{4\pi \mu} \left[ \sum_{j=1}^{N} A_{ij}(x, x_n) f_j(x_n) + \sum_{j=1}^{N} B_{ij}(x, x_n) u_j(x_n) \right] \quad (6)
\]

The velocities on the boundaries are known and are chosen to vary linearly over each element while the unknown forces are taken constantly to ensure consistency with the Stokes equation. The contributions of the elements to the boundary integral are calculated both numerically and analytically. With a view to the accuracy and the efficiency of the computations the elements are distributed non-uniformly over \( L \) to arrange for a larger density near corners and sudden changes of the boundary velocities.

As the problem of the Cavity Transfer Mixer is posed in terms of boundary velocities, the vector of 2N boundary forces must be calculated to complete the righthand side of eq. (6) by solving the set of 2N linear equations which are constructed from \( A_{ij} \) and \( B_{ij} \):

\[
A_{kl} \dot{f}_l = \tilde{v}_k \quad (7)
\]

using a collocation method with the collocation points positioned at the centres of the elements.

**Non-uniqueness of the solution** Matrix \( A_{kl} \) will be singular as the problem is not unique with regard to the level of static pressure. In some cases this can be eliminated by simply imposing a reference pressure on one of the boundary elements by choosing a certain normal force vector and subsequently eliminating a column from \( A_{kl} \).

However, in most cases, for example in asymmetrical geometries, imposing a pressure on one particular element leads to a rank deficient system:

\[
\text{rank} [A \mid \tilde{v}] \neq \text{rank} [A] \quad (8)
\]

Because of the singularity of eq. (7) and the difference in rank, as in eq. (8), only approximating solutions can be found, for instance by applying:
**a)** A perturbation method in which a small vector $\epsilon$ is added to the right-hand side of eq. (7) to enforce solvability of the system.

**b)** A least squares method in which the sum of the squared residuals, $\sum r_k^2 = \mathcal{R}$, is minimized:

\[
A_{kl} f_l - \tilde{v}_k = r_k \quad \text{with} \quad f_l = \tilde{f}_l + \delta_l
\]

\[
A^T A \mathbf{f} = A^T \tilde{\mathbf{v}}
\]

Both methods, of which the first is less time consuming and the latter somewhat more accurate, provide force vectors that adequately represent the flow after fixing the ambient pressure.

**2.2 Particle trajectories**

The velocity fields calculated with the boundary element method were used to compute the trajectories of arbitrary fluid particles by integrating

\[
\frac{dx}{dt} = \mathbf{u}(\mathbf{x}; t)
\]

\[
\mathbf{x}_i = \mathbf{X}_i + \int_0^t \mathbf{u}(\xi_i; \tau) \, d\tau
\]

The number of time-steps $M = T/\Delta \tau$ in computing the trajectories and the number of boundary elements were chosen such that both of the induced truncation errors are of the same order of magnitude over one period $T = (2W + D)/U$ of the flow.

The accuracy with which the trajectories need to be determined is fairly high, as even with modest chaotic behaviour one could easily gain an order of magnitude of the truncation error every few periods. Therefore the accuracy must be at least $O(10^{-5})$ per period to enable calculation up to ten periods.

To guarantee the required accuracy for the time-integration 1024 velocity fields were used when the two cavities are in mutual contact and one for the two driven cavities situation. The position $\mathbf{x}_i$ after one period of forcing $T$ is computed using the Bulirsch-Stoer integration method, see Press et al.[6] on the sequence of velocities $\mathbf{u}(\xi_i)|_{t=nT}$ plus a series of interpolated velocities

\[
\tilde{\mathbf{u}}(\xi_i) = 0.5 \left( \mathbf{u}(\xi_i)|_{t=nT} + \mathbf{u}(\xi_i)|_{t=(n+1)T} \right)
\]

The same accuracy can be obtained by using approximately 500 elements on average for the calculation of the velocity fields.

**2.3 Deformation tables**

As the analysis of the system is not confined to this particular problem a disconnection between the calculation of the trajectories and the analysis
of the flow was made in the form of deformation tables.

Deformation tables relate the positions of an initial grid of points to their positions after a full period of forcing $T$ yielding the overall deformation of the system. Subsequently a table can be used to calculate the position of any particle $x$ at any time $t = nT$ with $n = 1, 2, \ldots$ by interpolating between grid points.

Important features of the tables are the relatively compact manner of storing the behaviour of the flow while the interpolations take place relatively late in the calculations and the tables enable very fast computation of the trajectories and moreover of the chaotic quantities derived from the trajectories.

However, the main reason for using these tables is to have a method of optimization at our disposal that can be applied to 'any' mixing process, regardless of how the velocities and trajectories have been computed.

2.4 Reducing the parameter space

The final step in determining the mixing properties before actual optimization can take place is to calculate Poincaré sections, dye advection patterns and stretching function distribution. From a practical point of view one would want to obtain as much useful information as possible about the behaviour of the system at a large number of parameter settings using as little computational time as possible. It is therefore important to focus solely on the mixing performance instead of on detailed information of the dynamical system itself.

In that respect some of the quantities proposed earlier are not feasible in all cases. For instance it can be shown, see Jana et al.[3] and Swanson and Ottino[8], that the analysis of periodic points becomes a tedious and costly process when there is no symmetry in the mapping, which in general applies to industrial mixing processes. Investigating the behaviour of manifolds is not preferable either, because one needs detailed knowledge of the exact location of (hyperbolic) periodic points, which either originates from the analysis of periodic points or a very dense stretching function distribution. The more sophisticated stretching distribution carries this information about the system also, thus making the manifold tool more or less redundant. Some of the above quantities were tested on the Journal Bearing Flow, see section 4 using both deformation tables and regular integration of trajectories.

3 Results

Regarding the 2D Cavity Transfer Mixer optimization of mixing with respect to the possible parameter settings is carried out as described in section 2. The obvious method, which is also applied here, is to keep one parameter constant while optimizing the other. Considering a cavity with
an aspect ratio of $W/H = 1.66$ the wall displacement ratio $D/H$ was varied. The velocity fields, see figure 2 are generated with an element density of approximately 60 elements per unit length ($H = 1.00$) using a (cosine) condensed grid. This results in a total number of 450 elements on average and the accuracy with which the velocities are calculated is typically $\mathcal{O}(10^{-7})$ in this situation.

Time integration, with an accuracy comparable to the one from the boundary element method, requires 1024 time steps for the upper cavity to pass the lower one plus an equally large number during the forcing by the solid wall. This results in a rather large number of calculations taking up a large amount of CPU time to provide a deformation table. From this table the tools such as its Poincaré sections and dye advection patterns, as shown in figures 3 and 4 can be determined. Next the optimization of this choice of settings must be completed with a stretching function analysis.

**4 Implementation of deformation tables**

To determine the effects of using deformation tables, as described in section 2.3, instead of complete trajectories the *Journal Bearing Flow*, see
Figure 4: Dye advection at two different wall displacements after 0, 1, 2 and 3 periods of forcing.

Figure 5: The Journal Bearing Problem

tested by assessing the deviations in the Poincaré sections and in the dye advection patterns, compared with those computed from integrating the analytical solution of the velocity fields.
4.1 Poincaré sections and dye advection

The evaluation of Poincaré sections and dye advection patterns, using linear interpolation of numerical data, implies larger truncation errors. This causes the numerical system to behave more chaotically than the actual system would, as these errors will grow rapidly, see for example the reduction in size of the regular islands in figure 6. Note that the differences in the dye advection patterns after four periods are still small and hardly noticeable. So in that respect the method will be rather too optimistic with regard to the mixing performance, but it will generally characterize the system properly.

Figure 6: Poincaré sections (A,B,C,D) and dye advection patterns (E,F,G,H) for two different forcings (A,C,E,G) and (B,D,F,H) using regular integration (C,D,G,H) and deformation tables (A,B,E,F).

5 Discussion

The velocity fields in the 2D Cavity Transfer Mixer are adequately calculated using the boundary element technique accompanied by the least squares method to resolve the rank deficiency. Although the solution does not satisfy the boundary conditions completely, important properties such as the skew-symmetry of the velocities is preserved. Furthermore, it is shown by means of the Journal Bearing Flow that numerical errors need not necessarily stand in the way of optimizing a mixing process and that in principle the method of deformation tables is feasible. Especially dye advection patterns up to ten periods or more closely resemble the patterns obtained by the full calculation of the trajectories the points of the advected line. Poincaré sections are somewhat more sensitive to disturbances as a very large number of periods must be computed. Nevertheless their main features are still present using deformation tables.

The optimization of the 2D Cavity Transfer Mixer will be continued by
514 Boundary Elements

using the deformation table technique extensively on Poincaré sections and dye advection patterns, and on the computation of stretching function distributions also. The optimization will be completed with the development of practical analysis tools for the computed quantities.

References


