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A simplified approach to compute distribution matrices for the mapping method

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ABSTRACT

The mapping method has proven its efficiency as an analysis and optimization tool for mixing in many different flow devices. In this paper, we present a new approach to compute the coefficients of the distribution matrix, which is, both in terms of computational speed and complexity, more easy to implement as compared to the original approach developed in our group. The new approach is of the same accuracy as the original approach as is demonstrated by studying mixing in the standard two-dimensional cavity flow. The power of the new approach is that it can easily be implemented to analyze mixing in complex geometries where the original approach fails. This is demonstrated by analyzing mixing in a static Sulzer SMX mixer. To enhance the availability of the mapping method for general users of CFD in commercial packages like Fluent, CFX, Star CD, etc., we finally add an example of an implementation of the new approach in Matlab, applying it to study mixing in a time periodic sine flow (TPSF).

1. Introduction

Numerous mixing studies using the mapping method applied to various industrial flow devices as well as to a number of microfluidic devices have shown that the method is an efficient tool to perform fast analyses and, more important, make a real optimization possible of various designs or mixing protocols (Anderson & Meijer, 2000; Fard, Famili, & Anderson, 2008; Galaktionov, Anderson, & Peters, 1997; Galaktionov, Anderson, Peters, & Meijer, 2002, 2003; Kang, Singh, Kwon, & Anderson, 2008; Kruijt, Galaktionov, Anderson, Peters, & Meijer, 2001; Kruijt, Galaktionov, Peters, & Meijer, 2001; Singh, Anderson, Speetjens, & Meijer, 2008; Singh, Kang, Meijer, & Anderson, 2008). Chaotic mixing of viscous liquids in laminar flows is based on repetitive stretching and folding, the so-called bakers transformation. Spencer and Wiley (1951) suggested that the distribution of material in such flows can be handled quite well by the use of matrix methods. The mapping method is based on their suggestion and describes the transport of a conservative quantity from one state to another by means of a discretized mapping stored as a matrix. In the standard mapping method the quantity is the local concentration, in the extended mapping method it is the area tensor describing the structure of the dispersed phase in a mixture of two fluids. In both cases, we need the matrix describing the transport of fluid from an initial cross-section to a final one (for spatially periodic flows) or from an initial time to a final time (for time-periodic flows). The coefficients of the matrix, the distribution coefficients, contain the fraction of material from part of the domain that is transferred to various parts of the domain when a specified flow is applied. In the original approach of mapping, adaptive tracking of boundaries is applied to obtain the fraction by determining intersections of a deformed cell with a original one. However, this interfacial tracking approach is not always feasible and it fails in mixers with complicated geometries. Apart from that the method requires lots of additional book keeping and necessitates time to time insertion of markers on the edges that are stretched or curved, it requires renumbering of surfaces, flipping of surfaces, restructuring surfaces, etc. (Galaktionov et al., 1997; Galaktionov, Anderson, Peters, & Van De Vosse, 2000). Therefore, a simpler approach of mapping to compute the coefficients of the mapping matrix would allow for a much wider use of the method. Here, we present a new approach for mapping based on straight forward particle tracking, an option that is readily available in most CFD packages. Accuracy of the new approach is demonstrated by analyzing mixing in a standard two-dimensional lid-driven cavity flow. The ability to analyze complicated shaped geometries is demonstrated by studying mixing in a Sulzer SMX static mixer, which contains complex mixing elements. To show user-friendliness we implemented the new approach of mapping in Matlab, applying it to a well-known time periodic sine flow (TPSF) (Cerbelli, Vitacolonna, Adrover, & Giona, 2004; Franjione & Ottino, 1992; Liu, Muzzio, & Peskin, 1994), where velocity field as

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well as the particle trajectories are analytically known. The Matlab code is downloadable from www.mate.tue.nl/~anderson.

2. Mapping method: the original interfacial tracking approach

A distribution matrix $\boldsymbol{\varphi}$ is formed to store information about the distribution of fluid from one discretized cross-section to the next due to a specified flow. To obtain the coefficients of $\boldsymbol{\varphi}$, the initial cross-section of the flow domain is subdivided into a large number of discrete cells (N) of identical size. During flow, the material from a donor cell is transferred to different recipient cells. The fraction of material that is transferred from the donor cell to a recipient cell gives the distribution coefficient of the donor cell with respect to the recipient cell. Thus, in total N cells form a distribution matrix of the order $N \times N$.

The original mapping method (Anderson & Meijer, 2000; Galaktionov et al., 1997, 2002, 2003; Kruijt, Galaktionov, Anderson et al., 2001; Kruijt, Galaktionov, Peters et al., 2001) used tracking boundaries of cells by putting tracers on the boundaries of cells and applying interfacial tracking (adaptive front tracking) to obtain the accurate deformed boundaries of the cells (see Fig. 1). In this way, the discrete coefficient φ_{ij} equals the fraction of deformed cell Ω_j at $z = z_0 + \Delta z$ (or $t = t_0 + \Delta t$) that is found in the original cell Ω_i at $z = z_0$ (or $t = t_0$):

$$\varphi_{ij} = \frac{\int_{\Omega_j|_{z=z_0+\Delta z} \bigcap \Omega_i|_{z=z_0}} dA}{\int_{\Omega_j|_{z=z_0}} dA}. \tag{1}$$

Tracking all interfaces of all N cells during a flow over a distance Δz can be done, as previously demonstrated for different flows (Anderson & Meijer, 2000; Galaktionov et al., 1997, 2002, 2003; Kruijt, Galaktionov, Anderson et al., 2001; Kruijt, Galaktionov, Peters et al., 2001), but it is cumbersome to track interfaces experiencing complicated deformation patterns. Generally, in mixing devices producing complicated mixing patterns or in mixing devices which have complex geometries, the interfacial tracking to do adaptive tracking of boundaries fails. Therefore, here we propose a new straight forward way to compute the mapping coefficient.

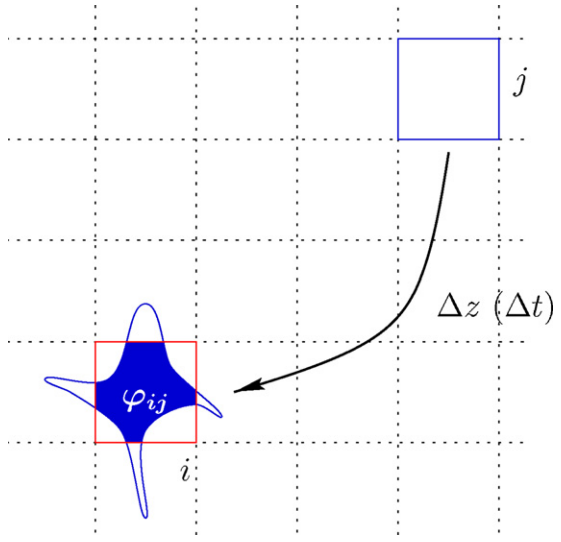

Fig. 1. Mapping using the interfacial tracking approach: depiction of cell advection and computing the coefficient φ_{ij}; φ_{ij} is the fraction of the area of Ω_j that is donated to Ω_i during the specified flow.

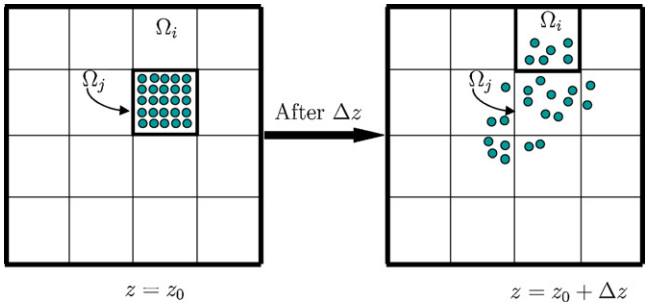

Fig. 2. Mapping using the particle tracking approach: illustration of the computation of the coefficients Φ_{ij} of the mapping matrix $\boldsymbol{\Phi}$. The cell Ω_j at $z = z_0$ is covered with a number of markers that are tracked during flow in Δz (to arrive at the final cross-section $z = z_0 + \Delta z$). The ratio of the number of markers received by the recipient cell Ω_i to the initial number of markers in Ω_j is determined (in this example Φ_{ij} is 6/25).

3. Mapping method: the new particle tracking approach

Fig. 2 depicts how the mapping coefficients are calculated in the new formulation of the method. To approximate the coefficients of the mapping matrix (or distribution matrix), K markers inside all cells are tracked. The markers are uniformly distributed in the cells without touching the boundaries. Then, to determine the final distribution of markers, they are advected during the flow from $z = z_0$ to $z = z_0 + \Delta z$. If the number of markers in the donor cell Ω_j is M_j at $z = z_0$ and the number of markers found after tracking in the recipient cell Ω_i is M_{ij} at $z = z_0 + \Delta z$, then the mapping coefficient Φ_{ij} is calculated as

$$\Phi_{ij} = \frac{M_{ij}}{M_j}. \tag{2}$$

In other words, the coefficient Φ_{ij} is again the measure of the fraction of the total flux of cell Ω_j donated to cell Ω_i. If the number of markers tracked is large enough, then Φ_{ij} approaches φ_{ij}. As demonstrated later in this article, here, it is advantageous to use backward particle tracking to track the particles: particles originally filling the recipient cell are tracked backward against the flow direction to find their parent cells. The advantage is that all the recipient cells (at the outlet) receive an equal number of particles, while in forward tracking there is no guarantee that all the recipient cells have equal number of particles. This is due to the fact that any ordered array of particles at the inlet becomes disordered at any downstream position.

4. Mapping the concentration and defining a measure of mixedness

Once the mapping matrix $\boldsymbol{\Phi}$ (or $\boldsymbol{\varphi}$) is computed, the concentration distribution, denoted as a column vector with length N, $\boldsymbol{C}^1$ after the deformation from $z = z_0$ (or $t = t_0$) to $z = z_0 + \Delta z$ (or $t = t_0 + \Delta t$) can be obtained by multiplying the mapping matrix $\boldsymbol{\Phi}$ with the initial concentration vector $\boldsymbol{C}^0$:

$$\boldsymbol{C}^1 = \boldsymbol{\Phi}\boldsymbol{C}^0. \tag{3}$$

Note that concentration vector $\boldsymbol{C}$ represents the coarse-grained description of volume fraction (dimensionless concentration) of a marker fluid in a mixture of two marker fluids with identical material properties, and its component C_i describes the concentration (volume fraction) locally averaged in the cell Ω_i. For n-times repetitive mixing (from $z = z_0$ to $z = z_0 + n\Delta z$), the same operation is repeated n times on the same mass and, hence, the concentration evolution after n steps is given by $\boldsymbol{C}^n = \boldsymbol{\Phi}^n\boldsymbol{C}^0$. For sufficiently large n, the matrix $\boldsymbol{\Phi}^n$ will not be sparse and it becomes that large that it