Evaluation of inhomogeneous model and the LCS based investigation in multiphase flows

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Abstract. In this paper, an evaluation of inhomogeneous model for computations of gas-liquid two-phase flow is presented, and the mechanism of gas-liquid two-phase flow in a bubble column is studied based on Finite-Time Lyapunov Exponents (FTLE) and Lagrangian Coherent Structures (LCS). The simulation is conducted with the homogeneous and inhomogeneous models respectively, and the numerical results are compared with the experimental data. It is shown that the inhomogeneous model can calculate the force of the gas more accurately and simulates the details of transient flows well due to the consideration of the interaction between the two phases. With inhomogeneous model, the periodic fluctuation of the bubble hose is captured and the velocity distribution coincides exactly with the experimental data. For the gas-liquid two-phase flow in the bubble column, the process of gaseous flow injected into water can be divided into two stages: the gas rising and gas fluctuation. The Lagrangian Coherent Structures (LCS) which consist of the ridges of the FTLE field can capture the boundary of vortex and the interface between the forward and backward flows in the liquid region, and the LCS have unique value for representing the divergence extent of neighboring particles in regions with different dynamics characteristics.

1. Introduction
It is known that multiphase flows often involve complex interactions between turbulent flow structures, mass transfer between phases, compressibility and unsteady characteristics with phase changing and interface forming and moving. Multiphase flows are ubiquitous in our daily life, and are closely related to many important technologies, including environment protection, aerospace technology, medical treatment and many industry applications. The multiphase flow model is crucial in the calculation of multiphase flows. The multiphase flow models can be divided into several categories. In homogenous model, a common flow field and one set of governing equations are shared by all fluids, which is based on the theory of homogeneous equilibrium flow. However, it is difficult to capture the details of transient flows for the homogeneous model. The researchers have developed a number of methods to modify the turbulence model based on homogeneous equilibrium flow, such as the research of Johansen[1], Biao Huang, Guo-yu Wang[2]. In recent years, with the development of computer technology, inhomogeneous model is gradually applied to the calculation of multiphase flows. This method solves the governing equations for each phase in the flow system and regard the interface as a moving boundary. Meanwhile, it takes the interaction between the phases into account to capture the details of transient multiphase flows. N. Boisson[3] utilized the model to simulate turbulent, two-phase gas-liquid flows in a 2D bubble column, part of the results coincided with the
experimental data, however the unsteady flow characteristic was un conspicuous as the three-dimensional flow effects were ignored. J. Chahed[4] proposed an Eulerian-Eulerian model and the turbulent correlations associated with the added mass force are taken into account in the expression of the force exerted by the liquid on the bubbles.

For the multiphase flow, it is important to investigate their flow structures to predict the dynamical behaviors effectively. In the previous studies, there are two ways to identify flow structures, one is the Eulerian approach aiming at partitioning the flow based on the instantaneous distribution of a velocity field, and there are quantitative criterions used, including $Q$ criterion [5], $\Delta$ criterion [6], $\lambda_2$ criterion [7], $\lambda_{ci}$ criterion [8] and so on. Another is the Lagrangian approach which is concerned with patterns emerging from the advection of passive tracers. Finite-time Lagrangian exponents (FTLE) and Lagrangian Coherent Structures (LCS) were introduced by Haller and Yuan [9] and further defined by Shadden et al. [10].

As to the complex multiphase flows, O’Farrell and Dabiri [11] have proposed a criterion for identifying vortex ring pinch-off in the axisymmetric jet flow based on the LCS. They have found out that the appearance of a new LCS is indicative of the initiation of the vortex pinch-off. Green et al. [12] have studied the three-dimensional flows via the LCS method. It is shown that the LCS can define structure boundaries without relying on a preselected threshold and present greater visible details without the requirement of velocity derivatives. Tang and Tseng[13] utilizes the FTLE and the LCS to get a better understanding of the flow dynamics and underlying physics of the gaseous jet injected into water and time-dependent turbulent cavitating flows. The results indicate that the FTLE field has the potential to identify the structures of multiphase flows, and the LCS can capture the interface/barrier or the vortex/circulation region.

In this research, the gas-liquid two-phase flow in the bubble column is simulated with the homogeneous and inhomogeneous model respectively, and the numerical results are compared with the experimental data. The Lagrangian Coherent Structures (LCS) is utilized to get better understanding of the flow dynamics and underlying physics of gas-liquid two-phase flow in the bubble column.

2. Inhomogenous model

2.1. Homogenous model

A common set of governing equations are shared by all fluids in homogenous model, the continuity equations are presented below:

$$\frac{\partial}{\partial t}(\rho_m) + \frac{\partial}{\partial x_j}(\rho_m u_j) = S^m$$

(1)

$S^m$ describes mass sources, and it is set to 0 in flows without mass transfer.

The momentum equations are presented below:

$$\frac{\partial}{\partial t}(\rho_m u_j) + \frac{\partial}{\partial x_j}(\rho_m u_i u_j) = -\frac{\partial p}{\partial x_j} + \frac{\partial}{\partial x_j} \left[ (\mu_m + \mu_t) \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3} \frac{\partial u_k}{\partial x_k} \delta_{ij} \right) \right] + \rho_m f_i$$

(2)

$$\rho_m = \sum_{\alpha=1}^{N} (\rho_{\alpha} \gamma_{\alpha}) \quad \mu_m = \sum_{\alpha=1}^{N} (\gamma_{\alpha} \mu_{\alpha})$$

(3)

$\gamma_{\alpha}$ is the volume fraction of phase $\alpha$, $\mu_{\alpha}$ is the dynamic viscosity of phase $\alpha$, and $\mu_t$ is the turbulent viscosity. $\rho_m f_i$ describes momentum sources due to external body forces. It should be noted that momentum transfer induced by interphase mass transfer and interfacial forces are neglected.

2.2. Inhomogenous model

The inhomogenous model solves the governing equations for each phase and takes the interaction between the phases into account. The continuity equations for phase $\alpha$ are presented below:
\[
\frac{\partial}{\partial t} \left( \gamma_a \rho_a \right) + \frac{\partial}{\partial x_j} \left( \gamma_a \rho_a u_{aj} \right) = \gamma_a S^m_k + \sum_{\alpha=1}^{N} S^m_{\alpha} \tag{4}
\]

\( S^m_k \) describes mass sources in phase \( \alpha \), \( S^m_{\alpha} \) is the mass flow rate per unit volume from phase \( \alpha' \) to phase \( \alpha \).

The momentum equations for phase \( \alpha \) are presented below:

\[
\frac{\partial}{\partial t} \left( \gamma_a \rho_a u_{\alpha i} \right) + \frac{\partial}{\partial x_j} \left( \gamma_a \rho_a u_{\alpha i} u_{aj} \right) = -\gamma_a \frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_j} \left[ \gamma_a (\mu_a + \mu') \left( \frac{\partial u_{\alpha j}}{\partial x_j} + \frac{\partial u_{\alpha j}}{\partial x_i} - \frac{2}{3} \frac{\partial u_{\alpha k}}{\partial x_k} \delta_{ij} \right) \right] + \gamma_a \rho_a f_i + M_{\alpha i} + \sum_{\alpha=1}^{N} S^m_{\alpha} \tag{5}
\]

\( \gamma_a \rho_a f_i \) describes momentum sources due to external body forces for phase \( \alpha \). \( M_{\alpha i} \) describes the interfacial forces acting on phase \( \alpha \) due to the presence of other phases. \( \sum_{\alpha=1}^{N} S^m_{\alpha} \) represents momentum transfer induced by interphase mass transfer.

To closure the equations, the original \( k-\varepsilon \) turbulence model is used in this study, which is proposed by Launder and Spalding.[14]

3. Lagrangian coherent structures

The Lagrangian system based criterions based on trajectories and even invariant to rotation of the frame of reference. The finite time Lyapunov exponent (FTLE) is a typical representative of these criterions, which is introduced below.

A dynamical system in its most general form is often expressed by:

\[
\begin{align*}
\dot{x}(t; t_0, x_0) &= v[x(t; t_0, x_0), t] \\
x(t_0; t, x_0) &= x_0
\end{align*}
\tag{6}
\]

Where, \( t \) represents time and is thought of as the independent variable and the dependent variable \( X \) represents the state of the system. The vector function \( v \) typically satisfies some level of continuity.

The finite time version of the Cauchy-Green deformation tensor, \( \Delta \), at the given point \( x_0 \) is defined as:

\[
\Delta_{t_0}^{T_{LE}}(x_0) = \left( \frac{\partial x(t_0+T_{LE}; t_0, x_0)}{\partial x_0} \right)^T \left( \frac{\partial x(t_0+T_{LE}; t_0, x_0)}{\partial x_0} \right)
\tag{7}
\]

Where \( ( \ )^T \) is the transpose of the deformation gradient tensor, \( t_0 \) is the time being considered, \( T_{LE} \) is the integration time.

The FTLE is defined as:

\[
\sigma_{t_0}^{T_{LE}}(x_0) = \frac{1}{T_{LE}} \ln \sqrt{\lambda_{\text{max}} \left( \Delta_{t_0}^{T_{LE}}(x_0) \right)}
\tag{8}
\]

Where \( \lambda_{\text{max}} \left( \Delta_{t_0}^{T_{LE}}(x_0) \right) \) is the max eigenvalue of the finite time deformation tensor \( \Delta_{t_0}^{T_{LE}}(x_0) \), and it represents the maximum stretching of particles, with the corresponding eigenvector providing the direction and vector which \( \delta x_0 \) will aligned to. The FTLE is a scalar value which characterizes the amount of stretching about the trajectory of point over the time interval. Once the FTLE field has been calculated, LCS is defined as ridges in the FTLE field. LCS have proven to be an effective tool for identifying exact vortex boundaries and can even be used to divide a flow into lobes that govern transport, as is done in classical lobe dynamics analysis[15].
4. Results and discussions
The numerical model is originated from Ref. [16], as shown in figure 1. Figure 2 shows the computational domain and boundary conditions of the bubble column, which is the same as the experimental setup in Ref. [16]. The water in the column is still at initial time, with its upper surface being free surface. The diameter of venthole, positioned at the midpoint of the soleplate, is 1cm, with ventilating velocity 48L/h. The mesh is generated with 40,000 structured hexahedron grids, and the O-type orthogonal mesh is adopted around the venthole.

Figure 1. Experimental setup[16]. Figure 2. Domain and boundary conditions.

Figure 3 displays the experimental visualization of the gas-liquid flow in a bubble column[16]. The bubbles are rising in a meandering way, producing a broad bubble size distribution with a mean size of about 5 mm. The bubble hose is growing and slowly moving in lateral direction. The circulation flow of the liquid phase continuously changes the flow direction due to the movement of the bubble hose. Some fine bubbles with diameter of 1 mm and less circulate with the liquid phase.

Figure 3. Transient flows of the bubble hose in experiment.

4.1. Evaluation of Inhomogeneous model
Figure 4 displays the computational gas volume fraction contours and streamlines with homogenous and inhomogenous models respectively, which shows the transient flows of the bubble hose and vortex in simulations. The process of gaseous flow injected into water can be divided into two stages: the gas rising and gas fluctuation. At the rising stage (t=1s, 10s, 20s), the results obtained by the two different multiphase model show the same characteristic of the gas-liquid flow. The bubble hose grows along vertical direction to the outlet. The vortex structures are formed in the liquid phase symmetrically. With the length of bubble hose increasing, the vortex structures move to the outlet. At the end of this stage, the flow tends to be steady and two distinct vortexes are distributed at the left and right side of the bubble hose respectively. However, at the fluctuation stage (t=30s, 40s, 50s and 60s),
the distinction appears between the results obtained by the homogenous and inhomogenous models. In the results with Inhomogenous model, the bubble hose start to wiggle periodicity, and the vortexes formed at the free surface move along the bubble hose to the bottom of column alternately. This phenomenon has been validated in the experiment conducted by Pfleger[16], Becker[17], T.-J. Lin[18], R.F. Mudde[19].

| t  | 1s | 10s | 20s | 30s | 40s | 50s | 60s |
|----|----|-----|-----|-----|-----|-----|-----|
| Inhomo-genous | ![Image](image1.png) | ![Image](image2.png) | ![Image](image3.png) | ![Image](image4.png) | ![Image](image5.png) | ![Image](image6.png) | ![Image](image7.png) |
| Homo-genous | ![Image](image8.png) | ![Image](image9.png) | ![Image](image10.png) | ![Image](image11.png) | ![Image](image12.png) | ![Image](image13.png) | ![Image](image14.png) |

**Figure 4.** Transient flows of the bubble hose and vortex in simulations.

Figure 5 shows the long-time-averaged velocity distributons of the liquid phase which is drawn as a vector plot for the centre plane of the rectangular bubble column. Contours of gas void fraction are shown in the figure. In the results of inhomogenous model, the bubble hose distribute symmetrically along the wide direction. We recognize the centre upflow of the bubble hose and the circulation of the fluid on both sides of the hose. In the results of homogenous model, the bubble hose deviate from the centre line as well as the upflow region, and the circulation region appear on single side of the hose.

**Figure 5.** Time-averaged velocity distribution in height direction.
Figure 6 shows a comparison of long-time-averaged simulation results with the experimental data. Vertical fluid velocity distributions versus the column width are drawn in detail for the three heights of 13cm, 25cm, 37cm, which are showed in figure 5. The velocity distribution predicted by inhomogenous model coincides well with the experimental data, which describe the strong upflow with the maximum velocity in the centre range above the venthole and the downflow with negative velocity at the column walls. However, the velocity distribution predicted by homogenous model shows exaggerated maximum values for all three heights, and the maximum velocity deviate from the centre line. Meanwhile, the downflow with negative velocity appear on single side of the column walls, which is incompatible with the experimental data.

Figure 7 shows the transient flow structures at the gas rising stage when $t=1s$. Figure 7(b) show the FTLE field at the rising stage ($t=1s$), with integration time $T_{LE}=1.5s$ (30 numerical time steps). The corresponding bubble hose and vortex at given moment is presented in figure 7(a). The distribution and shape of LCS can be clearly seen in figure 7(b). We can observe that the LCS highlights the main flow passage of the fluid excluding the reverse flow, meaning that the interfaces between the forward and backward flows are captured by the LCS. Combined with the particle trace shown in figure 7(c), the particles inside the LCS (Region B), flowing downstream with the bubble hose, highlight the main flow region, while the particles outside the LCS (Region A) represent the reverse flow region. It is noted that this boundary is hard to be distinguished in the Eulerian methods.

Figure 8 shows the transient flow structures at the gas fluctuation stage when $t=30s$. The integration time $T_{LE}$ used to compute the FTLE is 4.5s (90 numerical time steps). Compared to the Euler-system based identification of a vortex, the FTLE field presents the boundary of a vortex by

4.2. The Lagrangian Coherent Structure Based Investigation
In the Lagrangian Coherent Structure (LCS) based investigation, two typical moments are selected to elaborate the mechanism of the gas-liquid two-phase flow.
substance line with Lagrangian characteristics without any threshold defined, to ensure its objectivity. Notice that the flow behavior will be dissymmetric with the time passing and the dynamic tendency of the flow, instead of the current flow field, is expressed by FTLE field. The regions with high and low value of FTLE are continuously curling and staggering, and then the ridges of FTLE, LCS, are formed. It has unique value for representing the divergence extent of infinite neighboring particles, which are subjected to the plucking of the flow. Furthermore, LCS are curling nearby the vortex centers, rather than stretching to them. In figure 8(c), we now superimpose four set of fluid particles, which are initially located on either side of the LCS, with the evolution of the LCS. It demonstrates how the LCS acts as a time-dependent separatrix. The particles in region A, D basically keeps the relative position and the space between them changes slightly, which is matched along with the low value of FTLE region. However, the particles in region B, C is scattered to the bilateral of the vortex centers, corresponding to the high value of FTLE region. So that the results reflected by LCS can be validated.

![Figure 8. Flow structures at the fluctuation stage (t=30s).](image)

5. Conclusions
In this research, an evaluation of inhomogeneous model for computations of gas-liquid two-phase flow is presented, and the mechanism of gas-liquid two-phase flow in a bubble column is studied based on Finite-Time Lyapunov Exponents (FTLE) and Lagrangian Coherent Structures (LCS). Three main conclusions are achieved:

1. Compared to the homogenous model, the inhomogeneous model can simulate the details of transient flows more accurately due to the account of the interaction between the two phases. The periodic waggle of the bubble hose at the fluctuation stage is captured and the velocity distribution predicted by the inhomogeneous model coincides well with the experimental data.

2. For the gas-liquid flow in a bubble column: The process of gaseous flow injected into water can be divided into two stages: the gas rising and gas fluctuation. The bubble hose grows along vertical direction and the vortex structures form in the liquid phase symmetrically at the rising stage. The bubble hose wiggle periodicity and the vortex move along the bubble hose to the bottom of column alternately at the fluctuation stage.

3. The ridges of the FTLE field can form LCS to highlight the main flow passage of the fluid excluding the reverse flow and to capture the boundary of vortex. The LCS have unique value for representing the divergence extent of neighboring particles in regions with different dynamics characteristics.

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References
[1] Johansen S T, Wu J and Shyy W 2004 *International Journal of Heat and Fluid Flow* **25**(1)
[2] Huang B, Wang G Y, Yuan H T and Wang F F 2010 Transactions of Beijing Institute of Technology 30(10) 1170-1174
[3] Boisson N and Malin M R 1996 International Journal for Numerical Methods in Fluids 23(12) 1289-1310
[4] Chaheh J, Roig V and Masbernat L 2003 International Journal of Multiphase Flow 29(1) 23-49
[5] Hunt J C R, Wray A A and Moin P 1988 Eddies, stream, and convergence zones in turbulent flows Center for Turbulence Research Report CTR-S88 pp 193-208
[6] Chong M S, Perry A E and Cantwell B J 1990 Physics Fluids A 2 765-777
[7] Jeong J H and Hussain F 1995 Fluid Mechanics 285 69-94
[8] Zhou J, Adrian R J, Balachandar S and Kendall T M 1999 Fluid Mechanics 387 353-396.
[9] Haller G and Yuan G 2000 Physica D 147 352-370
[10] Shaddlen S C, Lekien F and Marsden J E 2005 Physica D 212 271-304.
[11] O’Farrell C and Dabiri J O 2010 Chaos 20 017513
[12] Green M A, Rowley C W and Haller G 2007 Journal of Fluid Mechanics 572 111–120
[13] Tang J N and Tseng C C Lagrangian-based investigation of multiphase flows 11th Int. Conf. on Fluid Control (Keelung, Taiwan, 5-9 December 2011)
[14] Launder B E and Spalding D B 1974 Computational Methods in Applied Mechanics and Engineering 3(2) 269-289
[15] Rom-Kedar V, Leonard A and Wiggins S 1990 Journal of Fluid Mechanics 214 347–358
[16] Pfleger D, Gomes S and Gilbert N 1999 Chemical Engineering Science 54 5091-5099
[17] Becker S, Bie H and Sweeney J 1999 Chemical Engineering Science 54 4929-4935
[18] Lin T J, Reese J, Hong T, and Fan L S 1996 AIChE Journal 42(2) 301-318
[19] Mudde R F, Lee D J, Reese J and Fan L S 1997 AIChE Journal 43(4) 913-926