A method for simulating the cross-sectional sampling measurement of a contrast fluid evolving in a tube

Joseph Majdalani [a*], David H. Richardson [a], Christopher A. Dawson [b], Steven T. Haworth [b]

[a]*Department of Mechanical and Industrial Engineering, Marquette University, Milwaukee, WI 53233, USA*
[b]*Department of Physiology, Medical College of Wisconsin, Zablocki V. A. Medical Center, Milwaukee, WI 53295, USA*

Abstract

This work describes a numerical methodology for simulating the behavior of two immiscible fluids traveling back-to-back in a tube. The problem arises in the context of a bolus of contrast fluid being suddenly appended to a primary fluid intended for use in x-ray angiography. Several characteristic parameters are identified including the length of tubing and time required for a slug of contrast fluid to evolve into a fully-developed state prescribed by a given Reynolds number. Geometric parameters include the tip volume of contrast fluid and the location of its center of gravity at a given instant of time. These parameters help ascertain the dynamic distribution of contrast fluid throughout the tube. Two other parameters are used to reproduce the line and area fractions of contrast fluid present at an arbitrary location. These fractions, obtained numerically, are shown to agree favorably with experimental x-ray data and theoretical simulations of the problem at hand. Theoretical validation is accomplished by using an exact solution that exists for the special case in which the two immiscible fluids are given identical physical properties. Experimental verification includes sample comparisons to time-dependent concentration curves acquired at a fixed x-ray site.

Keywords: Biomedical optics, data processing, distortion, image evaluation, phase contrast, x-ray simulations

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[*]To whom all correspondence should be addressed. Address: Professor J. Majdalani, Department of Mechanical & Industrial Engineering, Marquette University, 1515 W. Wisconsin Ave., Milwaukee, WI 53233.

Telephone: (414) 288-6877 Facsimile: (414) 288-7082 Email: maji@mu.edu

1. Introduction

The use of contrast agents in optical [1], x-ray [2-6], ultrasound [7, 8], and MRI [9, 10] angiography for tracking vessel flows and transit times is generally based on the assumption that the contrast fluid faithfully traces the mainstream independently of the geometric shape or orientation of the vessel. This idealized assumption may be violated if the contrast agent exhibits different physical properties (e.g., density and/or viscosity) than the mainstream (e.g., blood) to which it is introduced. The problem involving two dissimilar fluids traveling in tandem has been recognized in diverse fields [11-17], but no general approach to its resolution has been advanced. One approach for quantifying the deviations from the ideal tracer assumption under various flow conditions is possible via computational fluid dynamics (CFD). From the CFD results, a transformation is yet required to convert the simulated data to a form that can be compared to experimental measurements based on cross-sectionally sampled concentrations.

The purpose of this study is to introduce a numerical methodology that can be used to simulate x-ray output measurements by converting CFD data to the experimentally observable form of cross-sectionally averaged concentrations. The focus is placed on the joint motion of two viscous fluids in a constant diameter tube containing a primary fluid (representing the mainstream), and a secondary fluid that simulates the contrast agent [2-4]. The ensuing analysis requires identifying dimensionless parameters that can be used in characterizing the pertinent flow conditions. A method for calculating absorbency profiles from simulation results can then be described to allow direct comparison with experimentally obtained x-ray image data. As one test of the validity of the numerical algorithm, computational results will be compared to the exact analytical solution for the limiting case in which the two fluids are assigned identical thermostatic properties.

2. Method

Figure 1 sketches the apparatus in which the contrast fluid can be released from a cylindrical capsule at time zero into the mainstream. The ensuing motion is mechanistically modeled by the start-up flow of a secondary slug of contrast fluid that is suddenly immersed into a primary fluid. The focus of this work will be on simulating the evolution of the secondary fluid.

2.1. Experimental model

As illustrated in Fig. 1, the experimental setup consists of a flow circuit, an x-ray source, a cylindrical tube test section, and a detector. The 0.00744 m diameter tube is positioned between the x-ray source (Fien Focus FXE-100.20), and the image intensifier/CCD camera detection system [2]. Images on the left are obtained directly from the tube as the contrast fluid passes through the field of view. Flowing through

the tube at a rate of 1.5×10^{-5} m^3s^{-1} (900 ml/min) is a mixture of ethylene glycol and water having a density of $\rho_1 = 1070\ kg\,m^{-3}$, and a viscosity μ_1, similar to the viscosity μ_2 of the contrast fluid ($\mu_1 \approx \mu_2 = 0.00686\ kg\,m^{-1}s^{-1}$). The latter consists of 60% diatrizoate meglumine in H_2O ($\rho_2 = 1250\ kg\,m^{-3}$) with an initial length of $h_0 = 6$ cm. This contrast fluid is introduced into the inlet of the tube via an injection loop with minimal flow disturbance (see Fig. 1). While the mainstream is continuously circulated through tube sections 1, 2, and 4, the contrast fluid is initially contained in section 3, which is separated from the mainstream by means of two solenoid valves. At time zero, the solenoids divert the flow through section 3 while closing off section 2. This enables the contrast fluid to merge into the mainstream flowing into test section 4. As the contrast fluid passes through section 4, x-ray images are acquired at a rate of 30 frames per second. These images provide the means to reconstruct cross-sectional absorbency profiles at discrete time intervals.

2.2. Computational fluid dynamics model

The numerical simulations are conducted using a commercial computational fluid dynamics (CFD) code [18] in which the problem geometry and boundary conditions are readily implemented. The code solves the Navier-Stokes equations using finite volume and finite difference approximations. The software consists of four separate programs that operate as follows. First, the preprocessor program translates input data into a form that can be interpreted by the main processor. Second, the main processor carries out the algorithms necessary for generating solutions under the specified range of physical conditions. The main processor executes a control logic that aids in the selection of convergence criteria and time step sizes intended to eliminate numerical instabilities. Third, the postprocessor enables the user to extract data, perform calculations, and format plots needed to summarize the results. Geometrical configurations are constructed by assembling solid geometric objects which, when added together, define the flow region. The flow geometry is then embedded into the computational grid by defining the fractional areas of grid cells and corresponding fractional volumes that are open to flow. For that purpose, all equations are supplemented with area and volume porosity functions. The scheme is known as the Fractional Area-Volume Obstacle Representation (FAVOR) [19]. It is intended to track complex fluid-fluid interfaces such as the ones encountered here.

To facilitate the simulation of a developing two-phase flow, virtual probes are placed at several positions along the length of the tube. These probes are used to monitor pressures, densities and velocities. The length of the tube is proportional to the flow Reynolds number such that the flow will have reached 99% of its fully developed state before exiting the test section. Using a constant diameter of $D = 0.00744$ m, the operating variables are summarized in the first two columns of Table 1. These

pertain to four different case-studies involving different flow Reynolds numbers, pressure drops (Δp), and tube lengths (L_∞). The flow domain is subdivided into a mesh of fixed rectangular cells (Table 1). Each cell is associated average values of all dependent variables. Variables are located at the centers of the cells except for velocities; these are located at the cell faces. Wall boundaries and other geometric features are embedded in the mesh by specifying the fractional areas and fractional volumes of the cells that are open to flow. These area-volume fractions are time independent.

To construct discrete numerical approximations of the governing equations, control volumes are defined surrounding each variable location. For each control volume, surface stresses and body forces are computed in terms of surrounding variables. These quantities are then combined to form approximations for the conservation equations. Most terms in the equations are evaluated using the current time level value of the local variables. This procedure leads to a simple and efficient computational scheme for most purposes, but requires the use of a limited time step to maintain stability and precision. One important exception to this explicit formulation arises in the treatment of pressure forces. In this code, pressures and velocities are coupled implicitly by using time-accelerated pressures in the momentum equations and time-accelerated velocities in the continuity equation. This semi-implicit formulation of the finite difference equations leads to an efficient solution for the low speed and incompressible flow problem under consideration. Using standard descriptors and an asterisk to denote dimensional variables, the simulated equations include the conservation of mass and momentum equations. The continuity equation used in the program can be written in the general canonical form

$$V\frac{\partial \rho}{\partial t*}+\frac{\partial}{\partial x*}\left(\rho_i u_i A_x\right)+\delta\frac{\partial}{\partial y*}\left(\rho_i v_i A_y\right)+\frac{\partial}{\partial z*}\left(\rho_i w_i A_z\right)+\xi\frac{\rho_i u_i A_x}{x*}=0 \tag{1}$$

Here V denotes the fractional volume open to flow; ρ_i, $i=1,2$ correspond to primary and secondary fluid densities; (u_i, v_i, w_i) represent the velocity components of the ith fluid; and (A_x, A_y, A_z) symbolize the fractional areas open to flow in the x, y, and z directions. The coefficients δ and ξ change depending on the selected coordinate system. The equations of motion for each fluid are the Navier-Stokes equations augmented by some corrective terms. These are

$$\frac{\partial u_i}{\partial t*}+\frac{1}{V}\left(A_x u_i\frac{\partial u_i}{\partial x*}+\delta A_y v_i\frac{\partial u_i}{\partial y*}+A_z w_i\frac{\partial u_i}{\partial z*}\right)-\xi\frac{A_y v_i^2}{x*V}=-\frac{1}{\rho_i}\frac{\partial p}{\partial x*}+G_x+f_x-b_x \tag{2}$$

$$\frac{\partial v_i}{\partial t*}+\frac{1}{V}\left(A_x u_i\frac{\partial v_i}{\partial x*}+\delta A_y v_i\frac{\partial v_i}{\partial y*}+A_z w_i\frac{\partial v_i}{\partial z*}\right)+\xi\frac{A_y u_i v_i}{x*V}=-\frac{1}{\rho_i}\delta\frac{\partial p}{\partial y*}+G_y+f_y-b_y \tag{3}$$

$$\frac{\partial w_i}{\partial t*}+\frac{1}{V}\left(A_x u_i\frac{\partial w_i}{\partial x*}+\delta A_y v_i\frac{\partial w_i}{\partial y*}+A_z w_i\frac{\partial w_i}{\partial z*}\right)=-\frac{1}{\rho_i}\frac{\partial p}{\partial z*}+G_z+f_z-b_z \tag{4}$$

where (b_x, b_y, b_z) represent flow losses whereas (G_x, G_y, G_z) and (f_x, f_y, f_z) denote body and viscous accelerations. Diffusion between the two fluids is ignored because the primary and secondary fluids remain immiscible over the short time scales over which testing is conducted.

3. Results and discussion

3.1. Output interpretation

A typical output of this code is illustrated in the numerically generated profiles shown in Fig. 2. This run corresponds to a downward flow in a vertical tube of length $L_\infty = 0.38$ m, diameter $D = 0.00744$ m, a Reynolds number of $R = 100$, and a density ratio of 1.17. As shown at several discrete times, the shape of the interface evolves into a gradually more elongated form in the downstream sections of the tube. However, due to the vertical flow orientation, the contrast fluid remains symmetrical about the tube axis.

In order to convert numerical (or analytical) simulation results into a form that can be compared to x-ray image data obtained from cross-sectional sampling techniques, a systematic methodology is needed. This methodology is based on several characteristic parameters that are described next.

3.1.1 Characteristic parameters

Let us consider the two-dimensional representation of the evolving contrast fluid at a given instant of time. As shown in Fig. 3, an orthogonal (x, y, z) reference frame can be used in which all spatial coordinates are normalized by the tube radius a, and where z represents the non-dimensional axial distance in the streamwise direction. The contrast fluid is always bounded by two interfaces whose intersection with the (x, z) plane yields a leading, outer curve, and a trailing, inner curve. The leading and trailing curves delimit the outer and inner interfaces that intersect the axis of symmetry at z_o and z_i, respectively (see Fig. 3). At any other streamwise location, the outer and inner curves may be prescribed by the outer and inner (dimensionless) coordinates r_o and r_i. Note that, at time $t = 0$, $z_i = 0$ and $z_o = h_0 / a = h \simeq 16.1$, where $h_0 = 0.06\,\text{m}$ denotes the length of contrast fluid introduced initially. In the computational model, the initial positioning of the contrast fluid is offset from the tube's leading edge by a small dimensionless distance ε such that $z_i = \varepsilon$, and $z_o = \varepsilon + h$. In the CFD simulations, using $\varepsilon = 1.3$ has helped eliminate edge effects. We have also found it useful to employ a dimensionless time based on $t = \mu_2 t^* / (\rho_2 a^2)$, where t^* is real time. A justification for this choice will be given below.

A geometric feature of particular interest is the 'tip' volume of secondary fluid upstream of the plane $z = z_i$. We find it convenient to normalize this tip volume V_T^* by the initial slug-volume of contrast fluid

$V_0 = \pi a^2 h_0$. The resulting dimensionless tip volume can be written as $V_T = V_T^* / V_0$. This ratio measures the level of dispersion of the original slug throughout the tube. While V_T can be used to quantify the bulk amount of secondary fluid at a given axial station, the asymmetry of the tip volume can be extrapolated from the spatial position of its center of gravity. We hence find it useful to define the position of the tip's center of gravity by its three principal coordinates x_C, y_C, and z_C. In symmetric flow, only z_C is needed to locate the tip volume.

A plot of V_T and z_C versus non-dimensional time t illustrates in Fig. 4 the evolution of the tip volume and its center of gravity with the passage of time. This graph corresponds to several Reynolds numbers and the axisymmetric geometry for which the ratio of primary to secondary fluid densities is set equal to unity. The figure illustrates the faster decay of the tip volume in higher Reynolds number flows. This behavior reflects the faster motion in the streamwise direction inferred from the z_C-graph. The latter illustrates the ability of the tip's center of gravity to cross longer distances in the same period of time with each successive increase in R. In asymmetric flows, similar plots can be used to quantify V_T, x_C, y_C, and z_C at different density ratios.

3.1.2 The line fraction of fluid

Since x-ray imaging detects the fraction of contrast fluid in a cross-sectional plane, it is desirable to obtain a comparable representation of the simulation results at the same downstream location. For that purpose, one may first consider an (x, y) plane intersecting the tube at a fixed point z. Within that plane, one may choose the x-axis to represent the line intersection of the x-ray beam with the detection plane. Subsequently, as x is varied from -1 to $+1$ in the numerical domain, the segment swept across the tube can be used to mimic the x-ray diameter along which experimental data are recorded.

It is helpful to note that the $z = z_i$ plane shown in Fig. 3 divides the contrast fluid into two zones: the tail, wherein the cross-section of the contrast fluid has an annular 'doughnut' shape, and the tip V_T where the cross-section is that of a solid disk. The algorithm for quantifying the fraction of fluid in a constant z plane (i.e., isosurface) depends on the zone under consideration.

In the tail section, we find it convenient to define the two angles θ_o and θ_i that subtend r_o and r_i as the line of detection is swept across $(-1 \le x \le 1)$. At any fixed point x, the thickness of the contrast fluid in the y direction is equal to a given length l^* that can be calculated from the geometric profile. Since the x-ray imaging technique senses the mass density at a given point x, this mass density becomes directly proportional to the thickness of the contrast fluid l^* and, therefore, the local absorbency. It is expedient to define the non-dimensional length $l(x) = l^* / a$ to be the line fraction of secondary fluid at

fixed time (Fig. 3). Having normalized all spatial dimensions by the radius of the tube, it can be seen from Fig. 3 that, in the tail zone, one must have

$$l(x)=\begin{cases}2\ \left(r_o\sin\theta_o-r_i\sin\theta_i\right), & 0\le|x|<r_i\\ 2\ r_o\sin\theta_o, & r_i\le|x|\le r_0\\ 0, & |x|>r_0\end{cases} \tag{5}$$

In like fashion, the line fraction in the tip zone can be determined from

$$l(x)=\begin{cases}2\ r_o\sin\theta_o, & 0\le|x|\le r_0\\ 0, & |x|>r_0\end{cases} \tag{6}$$

In order to reproduce the x-ray absorbance curve across the width of the tube at a given instant of time, $l(x)$ is evaluated for $-1\le x\le 1$ at the corresponding time and z location. Using same density fluids, two sample cases at $z=100$ and $z=252$ are shown in Fig. 5 for a Reynolds number of 400 and a specific instant of time ($t=0.81$). Recalling that the x-ray beam is pointing in the y direction, this figure illustrates the ability of Eq. (5) to capture the ring-shaped contrast fluid in the tail zone along with its U-shaped line fraction. Being directly proportional to the density of contrast fluid, the line fraction $l(x)$ can be used to approximate the U-shaped absorbency curve at that point in time. Figure 5 also illustrates the disk-shaped contrast fluid in the tip zone and its corresponding semi-elliptic line fraction.

In principle, the outer and inner radii of the secondary fluid needed in Eqs. (5)–(6) can be determined, at any location z and time t, by reverse interpolation of the displacement function $z(r,t)$. The latter can be obtained by integrating the velocity field. Once $z(r,t)$ is determined, one can extrapolate for $r_i=r_i(z,t)$ and $r_0=r_0(z-h,t)$ where r_i and r_o correspond to particles originating at $t=0$ from the trailing and leading interfaces given by $z=z_i=0$ and $z=z_o=h$, respectively (see Fig. 2). In asymmetric flows, the azimuthal coordinate θ is also considered in correlating these functions.

3.1.3 The area fraction of fluid

Another figure of merit is the total fraction of contrast fluid that appears in a plane of cross-section area $A_c(z)$ at a given instant of time. This fraction can be realized from

$$s(z,t)=\frac{A_{\text{bolus}}}{A_c(z)}=\frac{\pi(a^2r_0^2-a^2r_i^2)}{\pi a^2}=r_0^2-r_i^2 \tag{7}$$

The geometric parameter $s(z,t)$ can be used to account for the total area fraction of radiopaque contrast fluid in an (x,y) plane. By generating plots of $s(z,t)$ versus time at fixed z one is able to emulate the local decay of secondary fluid concentration. This behavior is illustrated in Fig. 6 at several Reynolds

numbers. From the graph, one may infer that, for lower Reynolds numbers, the time $t = 0.81$ is not sufficient for any contrast fluid to reach a selected z-plane.

Conversely, by plotting $s(z,t)$ versus z at fixed time, one is able to assess the instantaneous distribution of the secondary fluid over the tube length. The resulting behavior is illustrated in Fig. 6 as well. In both cases the availability of contrast fluid at any downstream location is seen to diminish more rapidly at higher speeds.

For fixed z, both $l(x)$ and $s(t)$ for simulation case 2 are plotted in Fig. 7 and compared to the experimentally acquired concentration curves sampled over time at the location of the viewing site. The comparison demonstrates graphical agreement between simulated and experimentally acquired results using the two-density fluids described in §2.1. Differences in detail will be the subject of additional work using the tools developed herein. Taking into consideration discretization errors and imperfections in tube shape and alignment, the simulated predictions appear to be in fair agreement with experimental samples.

3.2. Analytical verification

In addition to the sample comparison with laboratory measurements in Fig. 7, an analytical model can be used to provide a theoretical confirmation of the technique used earlier to track the primary-to-secondary fluid interface. This can be accomplished by assigning to both primary and secondary fluids identical thermostatic properties; in this case the problem reduces to the single phase flow development of a cylindrical contrast fluid in a tube. Although numerical simulations treat each of the two fluids separately, computational results can be compared to the exact solution. Despite its sole applicability to the benchmark problem for which $\rho_2 \approx \rho_1$ and $\mu_2 \approx \mu_1$, this solution enables us to verify the validity of the proposed methodology.

The solution for the idealized start-up flow of an incompressible fluid with constant transport properties is described in [20]. The problem considers a fluid that is initially contained in a long horizontal tube of length L and radius a. At $t = 0$, a pressure gradient $\Delta p / L$ is impressed upon the system. Using the axisymmetric $u(r,t)$ to denote the axial velocity, the solution to this problem can be written as

$$u(r,t) = u_{\max}\left[\left(1-r^2\right) - 8\sum_{n=1}^{\infty}\frac{J_0\left(\alpha_n r\right)}{\alpha_n^3 J_1\left(\alpha_n\right)}e^{-\alpha_n^2 t}\right];\; u_{\max} \equiv \frac{a^2\Delta p}{4\mu L} = \frac{\mu R}{\rho a},\; t \equiv \frac{\mu t^*}{\rho a^2} \tag{8}$$

where α_n denotes the n^{th} root of the zeroth order Bessel function, and $u_{\max}$ refers to the maximum centerline velocity realized after a sufficiently long time. Here $R = 2\rho U a / \mu = \rho a^3 \Delta p / (8\mu^2 L)$ is based

on the average mainstream velocity U and corresponds to the same Reynolds number introduced previously.

It should be noted that the evolution of the profile into its final form takes place within the time interval $0 \le t \le 0.81$. In particular, at $t_\infty = 0.81$, one finds $u(r,t_\infty) = 0.99u(r,\infty)$, indicating that the flow will have reached 99% of it final fully-developed form. The distance traveled by a given particle as a function of time is obtained by integrating Eq. (8) from 0 to t to obtain the displacement function which, when normalized by a, becomes

$$z(r,t) = \frac{\rho a u_{\max}}{\mu}\left[\left(1-r^2\right)t - 8\sum_{n=1}^{\infty}\frac{J_0\left(\alpha_n r\right)}{\alpha_n^5 J_1\left(\alpha_n\right)}\left(1-e^{-\alpha_n^2 t}\right)\right] = R\left[\left(1-r^2\right)t - 8\sum_{n=1}^{\infty}\frac{J_0\left(\alpha_n r\right)}{\alpha_n^5 J_1\left(\alpha_n\right)}\left(1-e^{-\alpha_n^2 t}\right)\right] \quad (9)$$

Based on Eq. (9), the minimum length of tubing traveled by the fastest centerline particle originating at $z = 0$ until full development can be calculated to be

$$z(0,t_\infty) = R\left[t_\infty - 8\sum_{n=1}^{\infty}\frac{1-e^{-\alpha_n^2 t_\infty}}{\alpha_n^5 J_1\left(\alpha_n\right)}\right] \quad (10)$$

To track a particle originating at the leading surface of the contrast fluid, this distance must be augmented by $z = h + \varepsilon$; the latter combines the dimensionless length of the contrast fluid and the edge offset needed in the CFD model. Consequently, the optimal length of tubing L_∞ needed for meaningful and time-efficient simulations is found to be $L_\infty = z(0,\tau_\infty) + h + \varepsilon$. Being directly proportional to the flow Reynolds number, L_∞ must be increased with successive increases in R to allow for the desired flow development to occur within the computational domain.

As explained earlier, it is often necessary to calculate the inner and outer radii of contrast fluid situated in a given z plane at a prescribed time. Despite the apparent usefulness of Eq. (9), it is not possible to find an inverse solution of the type $r = r(z,t)$. Instead an interpolation function for $r_i = r_i(z-\varepsilon,t)$ and $r_0 = r_0(z-h-\varepsilon,t)$ must be generated by discretizing Eq. (9) at several spatial locations and times. The leading and trailing interpolation functions can be curve fitted using least-squares. The resulting functions will then contain the geometric information needed to reproduce the various figures of merit described previously.

The data gathered from the analytical model can be used to quantify key parameters such as $l(x)$, $s(z,t)$, z_C, and V_T. For the sake of brevity, we only compare the analytically derived V_T^A to the numerically approximated V_T^N at the four Reynolds number cases presented in Table 1. Therein, the maximum discrepancy between theory and simulation is calculated at several different times and shown to be very small. Generally, this discrepancy does not exceed 10%. A similar level of agreement is

realized with the other characteristic parameters. Table 1 also gives the number of cells, optimal length of tubing L_∞, and pressure drops, Δp, used in both analytical and numerical models. Note that the pressure drop calculated analytically from Eq. (8) can be used to estimate, for each Reynolds number, the corresponding pressure boundary condition needed in the numerical model.

4. Conclusions

A numerical approach is presented for simulating the motion of two dissimilar fluids in a tube and for parameterizing results that are equivalent to experimentally obtainable cross-sectional samples. Several useful parameters are identified including:

- The optimal length of tubing (L_∞) that must be used in a numerical model to capture 99% of the time-dependent evolution of the secondary fluid.
- The dimensionless time $(t_\infty = 0.81)$ needed for the secondary fluid velocity to reach 99% of its fully-developed value.
- The tip volume of secondary fluid (V_T) that can be used to measure the degree of fluid dispersion in the tube.
- The tip volume's center of gravity (x_C, y_C, z_C) that can be used to locate the contrast fluid and determine the amount of offset from the axis of symmetry in the presence of gravitational bias.

In addition to the above, two relevant quantities are needed for the numerical estimation of absorbency profiles obtained by cross-sectional sampling; specifically, one may cite:

- The line fraction of fluid (l) that reproduces the concentration of secondary fluid along a line of detection normal to the flow motion.
- The area fraction of fluid (s) that totals in a given isosurface normal to the flow and enables quantification of both temporal and spatial distributions of contrast fluid throughout the tube.

The last two fractions (l, s) are reproducible from a reverse interpolation function that locates the outer/inner radii (r_o, r_i) of the leading/trailing surfaces that envelope the secondary fluid. Having determined the procedural parameters for emulating cross-sectional sampling techniques, further experimental and numerical simulations are necessary to explore the effects of gravity under various orientations, density ratios, and flow Reynolds numbers.

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