The effect of particle size on flow in a continuous oscillatory baffled reactor using CFD

Guillermo Jimeno1 | Yeaw Chu Lee2 | Xiong-Wei Ni1

1EPSRC, Centre for Continuous Manufacturing and Crystallisation (CMAC), Centre for Oscillatory Baffled Reactor Applications (COBRA), School of Engineering and Physical Science, Chemical Engineering, Heriot Watt University, Edinburgh, UK
2School of Engineering and Physical Science, Mechanical Engineering, Heriot Watt University, Edinburgh, UK

Abstract
Experimental and numerical characterizations of flow in continuous oscillatory baffled reactors (COBR) have mainly been based on single phase in past decades. By coupling a primary Eulerian liquid phase with a secondary discrete Lagrangian phase consisting of solid particles of given density and size, this work investigates the effects of particle size on axial dispersion, evaluates residence times and velocities of particles, and quantifies the oscillation dampening caused by the presence of solid particles in a COBR.

KEYWORDS
axial dispersion of solids, Eulerian–Lagrangian, oscillatory baffled reactor, RTD

1 | INTRODUCTION
A continuous oscillatory baffled reactor (COBR) is a tubular reactor with periodical restrictions. Each restricted cell behaves as a perfect mixed mini-reactor; the accumulation of many such cells enables plug flow with its unique capability of suspending solids along the reactor. Its predictable scale-up in mixing from lab to production scale has earned worldwide academic research and industrial applications in both synthesis and separation (e.g., crystallization).

In order to characterize flows in a COBR, residence time distribution (RTD) has widely been used both experimentally1–7 and numerically.8–15 These studies were performed mainly in single phase using trackable liquid tracers. Baptista et al.16 studied the behaviour of suspended solid particles of different sizes and densities in a reactor containing baffles without oscillation, but their findings were inconclusive, as the interactions among particles were too significant for the effects of sizes and densities to be evaluated. Mazubert et al.17 employed numerical discrete particle tracking of a secondary phase to measure concentration profiles and analyze the performance of different geometric designs; however, their secondary phase consisted of massless particles that essentially followed the velocity field of the continuous Eulerian phase. Recent work by Ejim et al.18 highlighted the differences and the knowledge gap in the design of COBRs for multi-phase flow processes using correlations obtained from single phase work; this was further manifested by Kacker et al.19 who reported that not only were the optimal operating conditions for minimal axial dispersion involving solids different from that of single phase, but also longer times were spent by solids in a COBR, underlining the need to properly address the effect of different solid particles on axial dispersion and mean residence times. These are the exact objectives of this computational fluid dynamics (CFD) work. The novelty of this work includes examining the effect of particle size on axial dispersion, residence times, and velocities, and identifying and
evaluating the dampening effect to oscillatory amplitudes due to the presence of solids.

2 | GEOMETRY AND OPERATING CONDITIONS

The target device of this study is a NiTech DN15 COBR reactor (www.nitechsolutions.co.uk), the geometric dimensions of the DN15 and all design details were provided by the manufacturer, Alconbury Weston Ltd. (http://www.awl.co.uk). The total length of interest is 752 mm, containing 32 baffled cells, as shown in Figure 1.

For consistency with the vast majority of literature on OBRs and COBRs, the net flow velocity at the inlet is taken in this work as $u_{net}$. This should not be confused with the mean net velocity of the system, termed as $U$ in this work. The net volumetric flow rate, $Q_{in}$, is constant and $u_{net}$ is calculated from $Q / A$. However, while both $Q$ and $u_{net}$ are constant, the net flow velocity does change along the length of the reactor due to the presence of orifice baffles. It should also be noted that while sharp-edged baffles were employed in previous studies, smooth-edged baffles are used in this work (see Figure 1), where $V \neq L \cdot A$. Subsequently, the velocity through orifices ($u_{net-baffle}$) is defined as $Q / A_{b}$ and the mean net velocity ($U$) of the system is within the range of $Q / A \leq U \leq Q / A_{b}$, where $A_{b}$ is the cross-sectional area of the baffle orifice ($\frac{2D_{b}^{2}}{4}$). When the volume of the DN15 reactor is known, $U$ is calculated as $Q L / V$.

The operating conditions of $Q = 100 \text{ ml min}^{-1}$, $f = 2 \text{ Hz}$, and $x_{o} = D_{b}$ (7 mm) were chosen in this CFD work, based on the characteristics of the simulated particles, the CFD domain, and the literature.\[5,19,20]\n
The dimensionless numbers that govern the conditions of flow in a COBR are the net flow Reynolds numbers ($Re_{n} = u_{net} D / \mu$), the oscillatory Reynolds number ($Re_{o} = \omega x_{o} D / \mu$), the Strouhal number ($St = D / 4 x_{o}$), the ratio of the area of the orifice over the area of the tube (known as the restriction ratio, $\alpha = D_{b}^{2} / D^{2}$), and the velocity ratio ($\Psi = Re_{o} / Re_{n}$), where $\rho$ and $\mu$ are, respectively, the fluid density ($\text{ kg m}^{-3}$) and dynamic viscosity ($\text{ kg m}^{-1} \text{ s}^{-1}$); $D$ is the diameter of the tube (m); $D_{b}$ the diameter of the baffle hole (m); $W_{b}$ is the baffle width; $L_{b}$ is the baffle spacing; $L$ is the total length of the device; $\omega = 2 \pi f$ is the oscillation angular frequency (rad s$^{-1}$); $x_{o}$ is the oscillation centre-to-peak amplitude (m); $f$ is the oscillation frequency (Hz); and $u_{net}$ is the net inlet velocity (m s$^{-1}$).

3 | COMPUTATIONAL SIMULATION SETUP

All numerical simulations were performed using ANSYS Fluent 15.0 CFD package over 32 baffled cells, which discretizes the computational domain using finite volume to solve the flow field of a continuous phase. Additionally, Fluent allows for Lagrangian particle tracking by implementing a so-called discrete phase model (DPM) as an add-on to an existing Eulerian phase; this capability was utilized to model tracer and solid particles.

3.1 | Numerical model for Eulerian phase

The fluid selected for this study was water ($\rho = 998.2 \text{ kg m}^{-3}$, $\mu = 1.003 \cdot 10^{-3} \text{ kg m}^{-1} \text{ s}^{-1}$) and the time-dependent incompressible 3D Navier–Stokes equations were solved:

$$\nabla \cdot \vec{u} = 0$$

(1)

$$\rho \left( \frac{\partial \vec{u}}{\partial t} + \vec{u} \cdot \nabla \vec{u} \right) = -\nabla p + \mu \nabla^2 \vec{u}$$

(2)

All simulations were performed utilizing a pressure-based segregated solver along with the SIMPLE pressure-
velocity coupling algorithm. Spatial discretization of the momentum equation was performed using a second-order upwind scheme; pressure at faces of the grid was interpolated using a second-order scheme and time was discretized using a first-order implicit scheme. The time-step was set to 2 ms, ensuring a good number of time-steps per oscillatory cycle of 250, which is higher than the norm reported in literature.\textsuperscript{[5, 17]} The average and maximum values of the Courant–Friedrichs–Lewy coefficient were consistently kept below 2 and 20, respectively.

Because of laminar lows in NiTech DN15 reactors, a laminar solver was selected, which is in agreement with existing literature.\textsuperscript{[5, 14, 17, 21–25]} The impact of inlet boundary conditions on the main flow was minimized by imposing a fully developed parabolic profile: 
\[ u_{inlet}(r, t) = 2u_{net} + \alpha x \sin(\omega t) \left(1 - \frac{r^2}{R^2}\right), \]
where \( R \) is the COBR outer radius and \( r \) is calculated as \( r = \sqrt{y^2 + z^2} \). A constant gauge pressure of 0 Pa was set for the outlet boundary; operating temperature and pressure conditions were set at 300 K and 101 325 Pa, respectively.

### 3.1.1 Mesh sensitivity test

Two tests were performed to ensure independences of both mesh and the number of particles. For the former, a five-baffle-cell tube geometry as illustrated in Figure 2 was employed with a time-step of 0.5 ms for 24 oscillatory cycles, each cycle with a total 250 time-steps. The variables compared between meshes consist of the following: (a) profiles of pressure drop versus time, (b) pressure drop \( \Delta p(t) = p_1(t) - p_2(t) \), and (c) profiles of velocity magnitude versus time extracted at lines 1 and 2 and planes 1 and 2 as shown in Figure 2. These profiles were cycle-averaged and the resultant profiles (of the duration of an oscillatory cycle) were compared using the coefficient of determination:

\[
R^2 = 1 - \frac{SS_{res}}{SS_{tot}} = 1 - \frac{\sum_{i=1}^{n} (\phi_{1,i} - \phi_{2,i})^2}{\sum_{i=1}^{n} (\phi_{1,i} - \bar{\phi}_1)^2}
\]

where \( SS_{res} \) is the sum of squares of residuals between the reference profile and the profile under evaluation (from mesh \( j \)) and \( SS_{tot} \) is the total sum of squares of the target profile. Subscripts \( i \) and \( n \) represent a single data point and the total number of data points in a profile, respectively, while \( j \) is the mesh index and \( \phi \) is the property under evaluation.

The details of the mesh independent test can be found elsewhere\textsuperscript{[15]}; the density of selected mesh is 117 000 notes per baffled cell, which is above the norm reported in the literature.\textsuperscript{[13, 21, 23, 25–28]} The test and discussions for the independence of the number of particles in the simulation are given later in Figure 3.

### 3.2 Numerical model for Lagrangian phase

In this numerical study, paracetamol (\( \rho = 1263 \text{ kg m}^{-3} \)) was selected as the discrete solid phase. While the shape of paracetamol crystals ranges from needle-like to plate-like to octahedral blocks,\textsuperscript{[30–31]} mono-sized spherical particles of diameters \( (D_p) \) of 50, 100, and 150 \( \mu \text{m} \) were modelled for the purpose of simplicity. Liquid phase information was obtained from discrete massless particles that act as a perfect tracer as they move according to the flow field of the continuous liquid phase. The trajectory
of each discrete particle is predicted by integrating the force balance on the particle as follows\[32]:

\[
\frac{d\overline{u}_p}{dt} = \overline{F}_D + m_p \frac{\rho - \rho_p}{\rho_p} + \overline{F}
\]  

\(4\)

where \(m_p\), \(\overline{u}_p\), and \(\rho_p\) are, respectively, the mass, velocity, and density of the particle. The second term in the right-hand side of Equation (4) accounts for the force due to the weight of the particle and the buoyancy effect. The first term, \(\overline{F}_D\), is the drag force, defined as follows\[32]:

\[
\overline{F}_D = \frac{1}{2} \rho C_D A_p \left| \overline{u} - \overline{u}_p \right| \left( \overline{u} - \overline{u}_p \right)
\]  

\(5\)

where \(A_p\) is the cross-sectional area of the particle and \(C_D\) is the drag force coefficient, calculated as the spherical drag law proposed by Morsi and Alexander.\[33\] The third term, \(\overline{F}\), includes the virtual mass force, \(\overline{F}_VM\), and the pressure gradient force, \(\overline{F}_PG\); the former accounts for the force required to accelerate the fluid surrounding the particle and the latter is the resultant force from the pressure gradient along the fluid flow around the particle.\[32\]

\[
\overline{F}_VM = \frac{1}{2} m_p \rho \left( \frac{D\overline{u}}{Dt} - \frac{d\overline{u}_p}{dt} \right)
\]  

\(6\)

\[
\overline{F}_PG = m_p \rho \frac{D\overline{u}}{Dt}
\]  

\(7\)

where \(\frac{D}{Dt}\) is the material derivative. The position of each particle, \(\overline{x}_p\), is governed by the following:

\[
\frac{d\overline{x}_p}{dt} = \overline{u}_p
\]  

\(8\)

Equations (4) and (8) are integrated using a trapezoidal discretization scheme with the same time-step as the Eulerian phase (2 ms). When particles are defined as massless, the particle velocity equals to the velocity of the continuous phase, \(\overline{u}_p = \overline{u}\); hence, only Equation (8) is required to predict their trajectories.\[32\] The ANSYS Fluent DPM is appropriate for solid volume fractions below 10%,\[32\] which is the case in this work. All particles were released along a cross-sectional plane at the middle of a pre-defined baffled cell; this is known as surface injection, which will be further discussed in Section 4.2. In order to cope with the potential computational limitation of modelling too many particles, ANSYS Fluent tracks parcels. A parcel may contain multiple particles; its position is defined by a tracked representative particle and its diameter is that of a sphere whose volume is the ratio of the total parcel mass to particle density. However, in order to model and predict the behaviour of individual particles, the mass of each parcel in this work was set as that of a single particle; that is, each parcel contained one particle and thus the terminologies of parcel and particle are interchangeable in this study. No particle–particle interaction or particle diffusion in the liquid phase were included in the model.

When drag forces balance the weight of the particle and the buoyancy force,\[34\] the terminal (or settling) velocity, \(u_t\), of a particle is determined via the following:

\[
u_t = \sqrt{\frac{4gD_p}{3C_D} \left( \frac{\rho_s - \rho}{\rho} \right)}
\]  

\(9\)

The drag force coefficient \(C_d\) of 0.46 at Re = 1000 was used in this work,\[33\] with terminal velocities being reported in Table 1.

4 | ANALYSIS METHOD AND MODEL VALIDATION

4.1 | Determination of axial dispersion

In a tubular reactor, mixing is commonly quantified by the axial dispersion coefficient (\(D_a\)), which describes the
degree of spread (in the axial direction) of a tracer
injected upstream as a pulse,\textsuperscript{[35]} as follows:

\[
\frac{\partial C}{\partial t} = D_u \frac{\partial^2 C}{\partial x^2} - U \frac{\partial C}{\partial x} \tag{10}
\]

where \(C\) is the tracer concentration as a function of time, 
\(t\), and position, \(x\), and \(U\) is the mean net flow velocity of
the system \((U = u_{\text{net}} = QL/V)\). Although Equation (10)
was originally derived for a single-phase flow, it can also
be used for two-phase (solid–liquid) cases. When the
concentration of a liquid tracer is defined as \(C_L = m_L/V_L\)
and the concentration of solids as \(C_S = m_S/(V_L + V_S)\),
Equation (10) becomes independent of the volume of the sec-
nondary solid phase when \(V_S \ll V_L, V_L + V_S \approx V_L\), which
is the case in the present study. This is also consistent
with the work of Ejim et al.\textsuperscript{[18]} and Kacker et al.\textsuperscript{[19]} If a
perfect input pulse injection is assumed, typical boundary
conditions for Equation (10) are as follows:

\[
C(x, 0) = \frac{n}{A} \delta(x) \tag{11}
\]

\[
\lim_{x \to \pm \infty} C(x, t(t)) \tag{12}
\]

where \(n\) is the volume of tracer/secondary phase injected,
\(A\) is the cross-sectional area of the device, and \(\delta(x)\) is a
Dirac delta function. Thus, the analytical solution to
Equations (11) and (12) at fixed values of \(D_u\) and \(U\) is
given by the following:

\[
C(x, t) = \frac{1}{\sqrt{4\pi D_u t}} \exp \left( -\frac{(x - Ut)^2}{4D_u t} \right) \tag{13}
\]

Under the assumption of a perfect pulse injection, the
plug flow with axial dispersion model can also be solved
based on an inverse Peclet number \((Pe = UL/D_u)\)\textsuperscript{[35]}:

\[
\sigma_0^2 \times \frac{\bar{C}^2}{t^2} = 2 \frac{1}{Pe} + 8 \left( \frac{1}{Pe} \right)^2 \tag{14}
\]

where \(\sigma_0^2\) is the dimensionless variance, \(\bar{C}^2\) is the vari-
ance, and \(t\) is the mean residence time of the tracer con-
centration, defined as follows:

\[
\begin{align*}
\sigma^2 &= \frac{1}{\bar{C}^2} = 2 \frac{1}{Pe} + 8 \left( \frac{1}{Pe} \right)^2 \\
\bar{t} &= \frac{\int_0^\infty t \bar{C}_w(t) dt}{\int_0^\infty \bar{C}_w(t) dt} = \frac{\sum_{i=1}^{N} t C_w(t_i) \Delta t_i}{\sum_{i=1}^{N} C_w(t_i) \Delta t_i} 
\end{align*}
\tag{15}
\]

where \(N\) is the total number of measured concentration
data and \(C_w\) is the concentration of particles (\#particles
m\(^{-3}\)) at time \(t\), weighted by particles’ initial velocity
\((u_{\text{net}})\), and normalized by the maximum velocity in the device
\((u_{\text{o}})\); this approach has successfully been implemented
for the analysis of RTD profiles in micro-channels by
Aubin et al.\textsuperscript{[36]} and in COBRs by Mazubert et al.\textsuperscript{[17]} Equa-
tion (14) is used to evaluate the axial dispersion coeffi-
cient under the perfect pulse method (PPM).

A perfect input pulse is, however, unachievable in
practice and unmeasurable experimentally; subsequently,
an imperfect pulse method (IPM) was proposed\textsuperscript{[37]} where the concentration profile of the tracer/secondary
phase is measured at two points downstream of the tracer
injection (i.e., \(C_I(t)\) and \(C_A(t)\)), making the form of the
impulse irrelevant. This method was firstly implemented
in OBRs by Mackley and Ni\textsuperscript{[38]} who adopted the solution
of Göebel et al.\textsuperscript{[39]} and used a normalized concentra-
tion \((E(t))\)\textsuperscript{[40]} for better comparison among results:

\[
E(t) = \frac{C_w(t)}{\int_0^\infty C_w(t) dt} = \frac{\sum_{i=1}^{N} C_w(t_i) \Delta t_i}{\sum_{i=1}^{N} C_w(t_i) \Delta t_i} \tag{17}
\]

Mackley and Ni\textsuperscript{[38]} suggested that the normalized
concentration measured at an upstream point (1) during
a short time interval, \(\Delta t\), can be regarded as a perfect
pulse injection with an injected volume \(E(t_i)\Delta t\) at time
\(t = t_i\). Taking the limit \(\Delta t \to 0\) and integrating over all
possible injection times, \(t_i\), the normalized concentration

\begin{table}[h]
\centering
\caption{List of all simulated conditions}
\begin{tabular}{|c|c|c|c|c|c|c|c|c|}
\hline
Run \# & \(Q\) (ml min\(^{-1}\)) & \(f\) (Hz) & \(x_o\) (mm) & \(Re_n\) & \(Re_o\) & Material injected & \(D_p\) (\(\mu\)m) & \(u_r\) (m s\(^{-1}\)) \\
\hline
1 & 100 & 2 & 5 & 141 & 938 & Tracer (massless) & – & – \\
2 & 100 & 2 & 7 & 141 & 1313 & Tracer (massless) & – & – \\
3 & 100 & 2 & 7 & 141 & 1313 & Paracetamol & 50 & 0.019 \\
4 & 100 & 2 & 7 & 141 & 1313 & Paracetamol & 100 & 0.027 \\
5 & 100 & 2 & 7 & 141 & 1313 & Paracetamol & 150 & 0.034 \\
\hline
\end{tabular}
\end{table}
at point (2) can be estimated by the convolution integral equation:

$$E_2'(t) = \int_0^t E_1(t_1)TR(t-t_1)dt_1 = \sum_{i=1}^N E_1(t_{1,i})TR(t-t_{1,i})\Delta t_{1,i}$$

(18)

where $TR(t)$ is the transfer function for open-open boundary conditions; the formulation by Westerterp et al.\[^{[41,42]}\] is used in the current work as follows:

$$TR(t) = \frac{1}{\sqrt{4\pi Da}} \exp\left(-\frac{(L-Ut)^2}{4Da t}\right)$$

(19)

where the distance from the injection point, $L$, is essentially the distance between measuring points (1) and (2). The normalized concentration predicted at point (2), $E_2'(t)$, is compared with the measured normalized concentration at such point, $E_2(t)$, and the axial dispersion coefficient is fitted in order to satisfy the target function:

$$\Delta E = \sum_{i=1}^N \{E_2(t_i) - E_2'(t_i)\}^2$$

(20)

where $N$ is the total number of normalized concentration data. The optimal axial dispersion coefficient is obtained when the target function (20) is minimized. While the value of the mean net flow velocity, $U$, can be assumed as $U = QL/V$, a more accurate method, making use of the available upstream and downstream RTD profiles, is to calculate the time it takes for the tracer/secondary phase to travel from measuring points (1) to (2) as follows:\[^{[42]}\]:

$$U = \frac{L}{\int_0^\infty tE_2(t)dt - \int_0^\infty tE_1(t)dt} = \frac{L}{\sum_{i=1}^N tE_2(t_i)\Delta t - \sum_{i=1}^N tE_1(t_i)\Delta t}$$

(21)

Equation (21) significantly increases the accuracy of results, especially involving tracer and solids whose velocity may differ from that of the primary liquid phase ($QL/V$). Both the IPM and the PPM have been used to quantify axial dispersion in this work, enabling comparison and final selection.

4.2 Injection of discrete particles

Due to the nature of oscillatory flow in COBRs, forward and backward motions are generated during oscillations, resulting in particles flowing in and out of a control domain. It is thus crucial to select the injection point as well as subsequent measuring locations so that that open boundary effects on particles are minimized. In terms of the particle injection point, it was set at the baffle-cell number 15 (i.e., 352.5 mm from the inlet) to ensure that less than 0.1% of the injected particles would leave the system through the inlet for all the simulated conditions listed in Table 1. Note that each simulated scenario only modelled mono-sized particles, all of which left the domain of interest by the end of each run (i.e., no particles remained in the domain).

The position and velocity of every injected particle are extracted and stored at every simulated time-step; this information is post-processed to calculate concentration profiles at any given measuring point. Effectively, measuring cells act as laboratory concentration probes, monitoring the number of particles present within their baffles. In the present study, the sensitivity of results on the number of particles was tested by examining and comparing two injections of 4050 and 8100 particles, respectively. These numbers are significantly larger than what is reported in literature, for example, 2484 massless particles.\[^{[17]}\] Surface injection of 4050 discrete particles was implemented into a cross-sectional plane in the middle of a baffle-cell containing 4050 computational cells (i.e., one particle per computational cell). For 8100 particles, it involved simultaneous surface injections at two cross-sectional planes at 0.75 mm apart. The operating conditions of run #2 in Table 1 were used for the tests. Figure 3 (left) displays the profiles of $E(\theta)$ versus $\theta$ measured at the baffled cell (27) for both numbers; the degree of agreement between profiles is very good as both profiles overlap one another. The axial dispersion coefficients calculated using the PPM, Equation (14), and the IPM, Equations (18)–(21), at different lengths of the reactor for both particle numbers are presented in Figure 3 (right). Again, the agreement between results is remarkable, reporting an average percentage error of 2.8%. On the balance of accuracy and computing time, 4050 particles were selected for this work.

The optimal measuring points for the conditions tested in this study were identified as the baffled-cell numbers between 17–27, as shown in Figure 4, ensuring that over 99.9% of the injected particles pass through these points as they propagate downstream.

4.3 Comparison of perfect and imperfect pulse methods

Figure 5 shows the axial dispersion coefficients obtained from both the PPM and IPM as a function of length for all runs (refer to Table 1). Results provided by IPM were calculated with baffled cell (17) as $C_1$ and baffled cells (19)–(27) as $C_2$. 
The axial dispersion coefficient \((D_a)\) obtained by PPM (open diamonds) clearly changes with the length at which RTD curves were measured; as a matter of fact, the length of the device may not be sufficient for \(D_a\) to reach its asymptotic value. On the other hand, constant \(D_a\) values close to the asymptotic line (straight solid line) are seen for all IPM simulated runs (Figure 5). As a result, the IPM method is used for the determination of the axial dispersion coefficients for all the subsequent presentation in the following sections.

### 4.4 Validation of simulated results

Experimental data of methylene blue (single phase) and melamine-water (two phases) by Kacker et al.\(^{[19]}\) are used to validate our CFD simulations, as shown in Figure 6 (left—single phase, right—two phases).

We see that axial dispersion coefficients for the single-phase case in this work follow the same trend and have the similar magnitude as data of Kacker et al.\(^{[19]}\) (Figure 6, left). The RTDs in Figure 6 (right) are also
remarkably close both in magnitude and shape, which validates our model. In our study, a $D_a$ of 0.0006 m$^2$ s$^{-1}$ was obtained from run #4. By taking the density difference between the two studies into consideration and using the correlation from Ni et al.,$^{[7]} D_a$ is multiplied by a density ratio ($\rho_{\text{melamine}}/\rho_{\text{paracetamol}}$), giving a value of $D_a = 0.000 748$ m$^2$ s$^{-1}$, which is within the range of 0.0006–0.001 m$^2$ s$^{-1}$ suggested by Kacker et al.$^{[19]}$

The validity was also tested by comparing axial velocity of the continuous liquid phase with that of the tracer (massless particles) as shown in Figure 7. The velocity of the Eulerian liquid phase was calculated as the volume-weighted average, $\bar{u}_x$, of the whole simulated domain. The average velocity in the axial direction, $\bar{u}_x$, experienced by particles (tracer and/or solid) at any given time, $t$, was calculated as follows:

$$\bar{u}_x(t) = \frac{\sum_{i=1}^{N(t)} u_{xi}(t)}{N(t)}$$ (22)

where the index $i$ represents a specific particle and $N(t)$ represents the total number of particles present in the system at time $t$. The degree of agreement between profiles is exceptionally good, further verifying the methodology.

5 | RESULTS AND DISCUSSION

5.1 | Flow patterns of solids and solid suspension

The flow patterns of massless particles and paracetamol particles in water are shown in Figures 8–11 with particles projected into a 2D plane. Suspension of particles looks good visually along the whole length of the tube, even with particles of 150 μm diameter.

Quantitatively, the suspension of particles was analyzed by monitoring their positions in the vertical axis, $y$, throughout all simulated time-steps and averaging it over...
the total number of particles present in the entirety of the system, \( N \), for each condition as follows:

\[
\bar{y}(t) = \frac{\sum_{i=1}^{N(t)} y_i(t)}{N(t)}
\]  

(23)

From Figure 11, we see that the average positions of liquid phase particles and small solid particles (50 \( \mu \)m) stayed at the centre of the device (\( y = 0 \)), it denotes good suspension of solids. For particles of size 100 and 150 \( \mu \)m, they moved away from the centreline due to the effect of the gravitational force, but were still in upper quartile of the tube, with the bottom wall of the reactor being \( y = -7.5 \) mm. All particles were suspended, and no settlement of particles was observed at all, even for the largest particles considered in this study.

Furthermore, by dividing the tube plane into the top, middle, and bottom regions as \( x_1 \), \( x_2 \), and \( x_3 \) as sketched in Figure 12, the fractions of particles in each region can then be monitored and plotted with time in Figure 13.

For the liquid phase (massless tracer) and small particles, around 45% of the particles stay consistently in the middle region, while the rest stay in the top (27.5%) and bottom...
(27.5%) areas of the device. As particles increase in size, the percentage of the particles present in the bottom regions increased while suspended. Table 2 summarizes the distributions of the fractions in the three regions. For industrial applications, adjusting the intensity of the oscillatory velocity according to the target particle sizes would move larger particles back to the central regions for better suspension.

5.2 | Effect of particle size on axial dispersion and residence time

The effect of particle size on axial dispersion is presented in Figure 14 (left), plotting $E(\theta)$ versus $\theta$ of the baffled cell (27) for all runs performed (see Table 1). While the
impact of particle size on RTDs is qualitatively minimal (Figure 14, left), the mean residence time required for particles to reach baffled cell (27) from the injection cell (15) becomes longer as particle size increases, displaying a noticeable shift in the profiles of \( E(\theta) \) versus \( t \) (Figure 14, right). These findings are consistent with the work of Ejim et al.\([18]\) and Kacker et al.\([19]\) Table 3 compares both the axial dispersion coefficient \( (D_a) \) and the mean residence time \( (t) \).

### 5.3 Effect of particle size on their velocity—the dampening phenomenon

The average velocity in the axial direction, \( \bar{u}_x \), experienced by tracer and/or particles at any given time, \( t \), was calculated as per Equation (22), averaging over all particles present in the entirety of the system. Because the total number of particles is a function of time, results for each simulated run are only reported until the mean residence time measured at baffled cell (27) is reached (i.e., \( t = \bar{t}_{\text{baffle-cell-27}} \)), ensuring that the open boundary effect is avoided. Figure 15 plots \( \bar{u}_x \) with time for particles of different sizes. For the liquid phase plot (top left), the peak of the forward velocity (0.12 m/s) is larger than that of the backward one (0.9 m/s); this is because the forward motion is a sum of net and oscillatory flows, while there is only backward motion in flow reversal. The presence of solid particles reduces the magnitudes of peak axial velocities in both directions, but more in the forward direction. In addition, flat velocity profiles for liquid and small particles (top left and right) have gradually changed to exponential decays (bottom left and right) for larger particles 100 and 150 \( \mu \)m in diameter. This is the dampening phenomenon to the oscillation amplitude caused by the presence of large particles. Table 4 shows the percentage of dampening with respect to the liquid-phase case.

The minimum transport velocity required for the suspension of slurry in a horizontal tube \( (u_{\text{min-h}}) \) is given by the modified Durand equation\([43,44]\):

\[
u_{\text{min-h}} = C_{mh} \left[ 2g \left( \frac{\rho_s}{\rho_l} - 1 \right) D \right] \left( \frac{d_p}{D} \right)^{1/6} \tag{24}
\]

where \( D \) is the diameter of the tube, \( d_p \) is the diameter of the particle and \( C_{mh} \) is an empirical constant that ranges

| TABLE 2 | Asymptotic values for the fraction of particles present at different regions of the DN15 \( (Q = 100 \text{ ml/min}, f = 2 \text{ Hz}, \ x_o = 7 \text{ mm}) \) |
|---|---|---|---|
| \( x_1 \) (%) | \( x_2 \) (%) | \( x_3 \) (%) |
| Tracer (massless) | 27.5 | 45 | 27.5 |
| Paracetamol 50 \( \mu \)m | 26 | 43 | 31 |
| Paracetamol 100 \( \mu \)m | 19 | 35 | 46 |
| Paracetamol 150 \( \mu \)m | 11 | 24 | 65 |

**FIGURE 13** Fraction of particles present at different regions of the DN15 as a function of time \( (Q = 100 \text{ ml/min}, f = 2 \text{ Hz}, \ x_o = 7 \text{ mm}) \)
Figure 14  $E(\theta)$ versus $\theta$ (left) and $E(\theta)$ versus $t$ (right) profiles for different particle sizes ($Q = 100 \text{ ml/min}$, $f = 2 \text{ Hz}$, $x_0 = 7 \text{ mm}$)

Table 3  $D_a$ and $\bar{t}$ values for different particle sizes ($Q = 100 \text{ ml/min}$, $f = 2 \text{ Hz}$, $x_0 = 7 \text{ mm}$)

Table 4  Percentage of oscillatory dampening and minimum transport velocity for paracetamol solids of different sizes ($Q = 100 \text{ ml min}^{-1}$, $f = 2 \text{ Hz}$, $x_0 = 7 \text{ mm}$)

With respect to the values provided by the liquid phase (massless tracer).
from 0.4–1.5. A $C_{mh}$ of 1.5 was used in the present study. Table 4 shows the $u_{min-h}$ required by each condition, along with the percentage of the time that the oscillatory axial velocity at the inlet and in the tube is higher than the minimum transport velocity, that is, $|\dot{u}_{x-inlet}(t)| > u_{min-h}$ and $|\dot{u}_{x-ELP}(t)| > u_{min-h}$, respectively.

The minimum transport velocity required for slurry suspension in a horizontal tube increases by 20% as particles grow from 50–150 μm in diameter; however, the magnitudes of the oscillatory velocities or the fluid mechanical forces exerted by eddies at both the inlet and within the tube are greater than the minimum terminal velocity for the majority of the time for all simulated particles. Hence, it is expected that all particles remain suspended throughout their journeys in the reactor. In industrial operations, the reduction in the degree of suspension as particles grow in size would be dealt with by an according increase in oscillatory velocity.

6 | CONCLUSIONS

In our work, solid–liquid fluid flow in a COBR was modelled by the combination of a primary Eulerian liquid phase with a secondary discrete Lagrangian phase; the effect of particle size on axial dispersion, residence times, and velocities was examined. Our data agree with the works by Ejim et al. and Kacker et al. In this work, we have identified and evaluated the dampening effect to oscillatory amplitudes due to the presence of solids. While mono-size spherical particles are used in this work, the understanding of dispersion of a solid phase in liquid and its associated effect is much needed in order to fill the knowledge gap in the area of COBR research and development.

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PEER REVIEW

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NOMENCLATURE

- $A$: reactor’s cross-sectional area (m$^2$)
- $A_p$: cross-sectional area of a particle (m$^2$)
- $C$: concentration (kg m$^{-3}$)
- $C_{D}$: orifice discharge coefficient
- $C_d$: drag force coefficient
- $D$: tube diameter (m)
- $D_a$: axial dispersion coefficient (m$^2$ s$^{-1}$)
- $D_b$: baffle hole diameter (m)
- $D_p$: diameter of a particle (m)
- $E$: normalized concentration
- $F$: force (N)
- $F_D$: drag force (N)
- $F_{PG}$: pressure gradient force
- $F_{VM}$: pressure gradient force
- $f$: oscillation frequency (Hz)
- $g$: gravity (m s$^{-2}$)
- $L$: reactor’s length (m)
- $L_b$: spacing between baffles (m)
- $m$: mass (kg)
- $N$: total elements in a summation
- $n$: number of baffles in the system
- $Pe$: Peclet number
- $Q$: volumetric flow rate (ml min$^{-1}$)
- $R$: tube radius (m)
- $R^2$: coefficient of determination
- $r$: radial position (m)
- $\bar{r}$: position of each infinitesimal particle (m)
- $Re_o$: oscillatory Reynolds number
- $Re_n$: net flow Reynolds number
- $St$: Strouhal number
- $t$: time (s)
- $\bar{t}$: mean residence time (s)
- $TR$: transfer function for open-open boundary conditions (s$^{-1}$)
- $U$: mean net velocity (m s$^{-1}$)
- $u$: velocity (m s$^{-1}$)
- $u_{inlet}$: inlet velocity (m s$^{-1}$)
- $u_{min}$: minimum velocity required for the suspension of slurry in a horizontal tube
- $u_{net}$: net inlet velocity (m s$^{-1}$)
- $u_t$: terminal velocity (m s$^{-1}$)
- $W_b$: baffle width (m)
- $x$: position in the horizontal axis (m)
- $x_o$: oscillatory centre-to-peak amplitude (m)
- $x_p$: piston’s position (m)
- $y$: position in the vertical axis (m)
- $z$: position in the depth axis (m)
- $\alpha$: the ratio of the area of orifice to the area of tube (the restriction ratio)
- $\Delta x$: control volume size (m)
- $\theta$: normalized time (\bar{t})
- $\mu$: viscosity (kg m$^{-1}$ s$^{-1}$)
- $\rho$: density (kg m$^{-3}$)
- $\sigma^2$: variance
- $\sigma_{\theta}^2$: dimensionless variance
- $\phi$: property under evaluation
ψ velocity ratio (Re_o/Re_n)

ω oscillation angular frequency (rad s^{-1})

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