Article:

Pasha, M, Hassanpour, A, Ahmadian, H et al. (3 more authors) (2015) A comparative analysis of particle tracking in a mixer by discrete element method and positron emission particle tracking. Powder Technology, 270 (Part B). 569 - 574. ISSN 0032-5910

https://doi.org/10.1016/j.powtec.2014.09.007

A Comparative Analysis of Particle Tracking in a Mixer by Discrete Element Method and Positron Emission Particle Tracking

M. Pasha[a], A. Hassanpour[a,*], H. Ahmadian[b], H. S. Tan[c], A. Bayly[c], M. Ghadiri[a]

[a] Institute of Particle Science and Engineering, School of Process, Environmental and Materials Engineering, University of Leeds, Leeds, LS2 9JT, UK
[b] P&G Technical Centre Ltd., Newcastle Upon Tyne, NE12 9BZ, UK
[c] P&G, Beijing Innovation Centre, Beijing. P.R. China

* Corresponding author
Dr Ali Hassanpour
Tel: +44 (0) 113 343 2407
Fax: +44 (0)113 343 2405
Email address: a.hassanpour@leeds.ac.uk

Abstract.

Characterisation of particle flow using Positron Emission Particle Tracking (PEPT) is based on tracking the position of a single particle in a dynamic system. Recent developments in PEPT have facilitated tracking multiple particles aiming at improvements in data representation. Nevertheless for systems with a wide residence time distribution and/or dead zone, the conditions for getting representative data which could reflect the bulk behaviour of the powders need to be analysed and specified. In the present work, an attempt is made to simulate PEPT experiments for a paddle mixer using Discrete Element Method (DEM), with a view to investigate the effect of increasing the number of tracers on their time-averaged velocity distribution and whether it can represent the data on whole population of particles. The time averaged velocity distribution of the individual tracer particles (resembling simulated PEPT) is obtained and compared with the time averaged data on entire particle population. The DEM results indicate that for the investigated paddle mixer, it takes 251 seconds for one tracer to travel adequately in all the active space of the system. The instantaneous tracer velocity fluctuates around the average value obtained for all the particles, suggesting the average tracer velocity is adequately representative of the average particle velocity in the system. The data of PEPT experiment with one tracer with those of DEM with one tracer are in good agreement, however DEM

simulation suggests that increasing the number of tracers in the paddle mixer system does not influence the average velocity distribution. Furthermore, the velocity for all particles in the DEM shows a smooth distribution with a peak frequency of the velocity distribution that is lower than PEPT and DEM tracer. When tracking a single tracer in DEM or PEPT, it may not be detected to have zero velocity at any instant of time, while the data for all particles show that about 0.3% of particles are stagnant.

Keywords: Discrete Element Method (DEM), Positron Emission Particle Tracking (PEPT), Paddle mixer, Number of Tracers

1. Introduction

In industries such as detergent, cosmetic, food and pharmaceutical manufacturing, powder mixing is a common process. Optimisation and control of mixing are critically important but very challenging. A key step in optimising the mixing process is to understand the powder kinematic behaviour (flow fields, mixing patterns, etc.) to enable efficient process design and control [1]. However it is difficult to obtain an insight into the internal flow field during mixing processes and to address the kinematic behaviour of powders using experimental approaches, particularly at large scales. Advances in experimental measurements of internal flow based on Positron Emission Particle Tracking (PEPT) have made it possible to get detailed information on the rate of mixing, but are limited to small scales [2, 3]. In PEPT, the motion of an irradiated tracer particle is tracked using appropriate sensors, from which the temporal and spatial information about the particle is deduced [4]. A natural question which emerges is to what extent the data from a single particle are representative and how such information could be applicable to larger scales. For this purpose Hassanpour et al. [5] simulated a paddle mixer using the Distinct Element Method (DEM) and compared the results to those of PEPT. A qualitative comparison between the time-averaged velocity profiles of a representative case from PEPT measurements and corresponding DEM simulations showed a good qualitative agreement on the internal flow patterns. In order to make quantitative comparisons, the particle dynamics were analysed in terms of normalised velocity distributions (i.e. magnitude of particle velocity normalised to paddle tip speed). Due to the computational limitations, DEM simulations were carried out for a maximum of 10 s of real time only. Within this short period, the data were insufficient for one single particle relating to comparison with PEPT measurements; therefore the data from all particles in the DEM simulations were used in the calculations. The time-averaged normalised velocity distribution obtained from DEM analysis was compared with that from PEPT measurements for representative process conditions. It was found that the DEM model predicted a smooth distribution of particle velocities while the PEPT data showed more scatter or fluctuation in the frequency plot. This difference was attributed to the fact that the PEPT analysis was based on data from only one particle, i.e. the tracer, while the DEM results were from the velocity profiles of the whole population of particles. Overall there was a reasonable agreement in the velocity distribution, but the comparison was not rigorous.

In PEPT the tracking process is carried out for a few minutes to generate sufficiently accurate time-averaged data. However, the total length of experiment for reliable and statistically representative data is based on trial and error and there is no solid evidence confirming the tracer could represent the data for all particles. It has recently been shown [6] that using manipulated algorithms, multiple tracers can be used in PEPT, however its effect on providing better representative data for all the particles has yet to be critically evaluated. In the present work, an attempt is made to simulate PEPT experiments for a paddle mixer using DEM, with a view to investigate the effect of increasing the number of tracers on the time-averaged velocity distribution. The velocity information is available for all individual particles in DEM; therefore, the average particle velocity and velocity distribution of the whole population of particles could be compared with those of individual tracers in the simulation. The results of DEM are also compared to those of PEPT experiment using a single tracer.

2. DEM simulation of the paddle mixer

DEM simulations provide dynamic information of transient forces acting on individual particles throughout the simulations, which is otherwise difficult to obtain. The interactions between the constituent particles are based on theories of contact mechanics. More details on the methodology of the DEM and its applications are presented elsewhere [7, 8]. The simulations were conducted using EDEM® software provided by DEM Solutions, Edinburgh, UK. The calculation of the contact forces of the particles is based on the Hertz-Mindlin model [9]. The experimental work using PEPT was carried out on dry, free-flowing particles; hence the contact model did not include adhesive term. Due to the limitation of computer power, it is not possible at this stage to simulate the actual number of particles (around 50 millions) within a reasonable time. Therefore, the simulation was carried out with a smaller number but larger particles. In this case particle density is adjusted to maintain a similar momentum exchange between particles as of the real case [10]. In the previous work by Hassanpour et al. [5] it was shown that the steady state average velocity magnitude slightly decreased as the particle size was reduced in the same paddle mixer system. This shows that the average particle velocity is slightly sensitive to the particle size, but the effect is not very significant. Here, the same particle size similar to that used by Hassanpour et al. [5] is used. The geometry of the simulated paddle mixer is the same as the previous work, for which a CAD drawing was imported into the EDEM computer code (Figure 1).

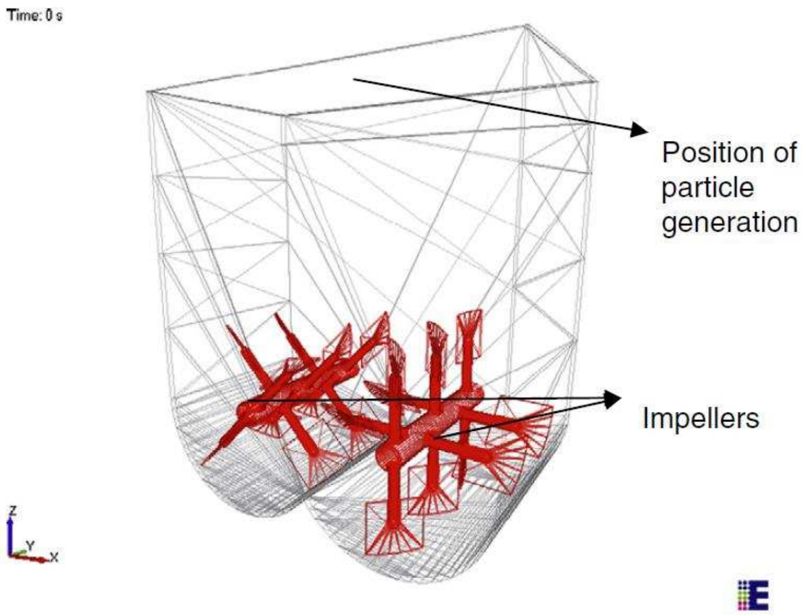

Figure 1: The imported geometry of the paddle mixer simulated by the DEM.

As it can be seen, the mixer consists of two intersected semi-cylinders of the same span and two counter-rotating impellers, each with 10 paddles positioned pair-wise along 5 axial positions.

Properties of the particles are also the same as the previous work [5], which can be seen in Table 1 and 2. Particles were generated randomly at spatial locations above the impellers (the position shown in Figure 1).

Table 1: The properties of particles and walls used in DEM simulation

Property	Particles	Equipment wall
Particle diameter (mm)	4.52	-
Shear modulus (GPa)	0.1	70
Density (kg/m^3)	1000	7800
Poisson's ratio (-)	0.2	0.3

Table 2: The contact properties used in DEM simulation

Property	Particle-particle	Particle-wall
Coefficient of sliding friction	0.3	0.3
Coefficient of rolling friction	0.01	0.01
Coefficient of restitution	0.4	0.4

The filling of 60000 particles was carried out while the mixer impellers were stationary similar to previous work [5]. The particles were subjected to gravitational acceleration and gradually settled toward the bottom of the mixer. The simulations were carried out under a constant rotational speed of impellers for 10 minutes of real time which took three months to complete. For confidentiality reasons it is not possible to disclose the impeller rotational speeds.

3. PEPT experiments

The experimental results of PEPT are taken from the previous work of Hassanpour et al [5]. In their work, the Positron Emission Particle Tracking (PEPT) facility of the University of Birmingham (Birmingham, UK) was used to track particle motion. In a typical experiment, particles were loaded into the mixer which was then started and run for a couple of minutes to ensure that the steady state was reached before starting the data requisition process. Radioactive particles (0.7 mm in diameter with 1200 kg/m^3 density) were used as tracers, which were activated by an ion exchange method with radioactive water produced in a cyclotron [4]. For each experiment one tracer was used and the data acquisition was performed for at least 15 min for each run which gave at least 20,000 data points in the form of spatial locations in the Cartesian coordinate as a function of time.

4. Results and discussion

Figure 2 shows the streamlines of the tracer from three different viewing angles as well as a view of all the particles in the system, all coloured based on the normalised speed (i.e. ratio of tracer particle speed to paddle tip speed): red being the maximum (i.e. 1) and blue being the minimum (i.e. 0).

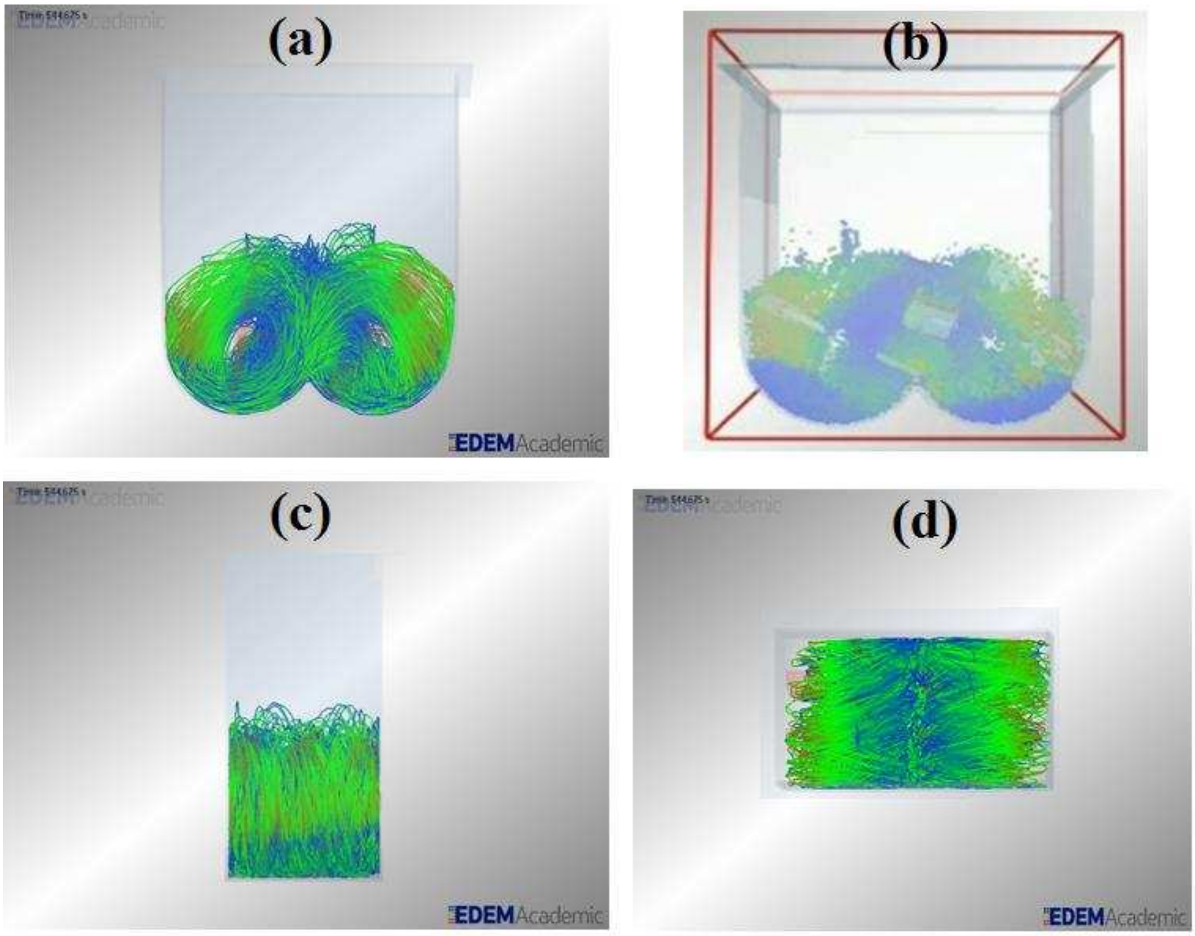

Figure 2: The tracer streamlines and particles view: (a) front view streamlines (b) front view of the particles (c) right view streamlines and (d) top view streamlines in the system. The colour scheme is based on the normalised speed of the tracer/particles.

Figure 2 qualitatively shows that the tracer particle has been present almost in all active locations of the mixer space, which was occupied by the particles. The velocity distribution, which can be qualitatively seen by the colour scheme used in the figure, matches with that of the whole population of particles in the simulation. This has been analysed quantitatively and will be shown in the next section.

Figure 3 shows the development of tracer streamlines at four different simulation times: 1, 13, 52 and 384 s. The trace is coloured based on the normalised speed of the tracer particle: red being the maximum (i.e. 1) and blue being the minimum (0).

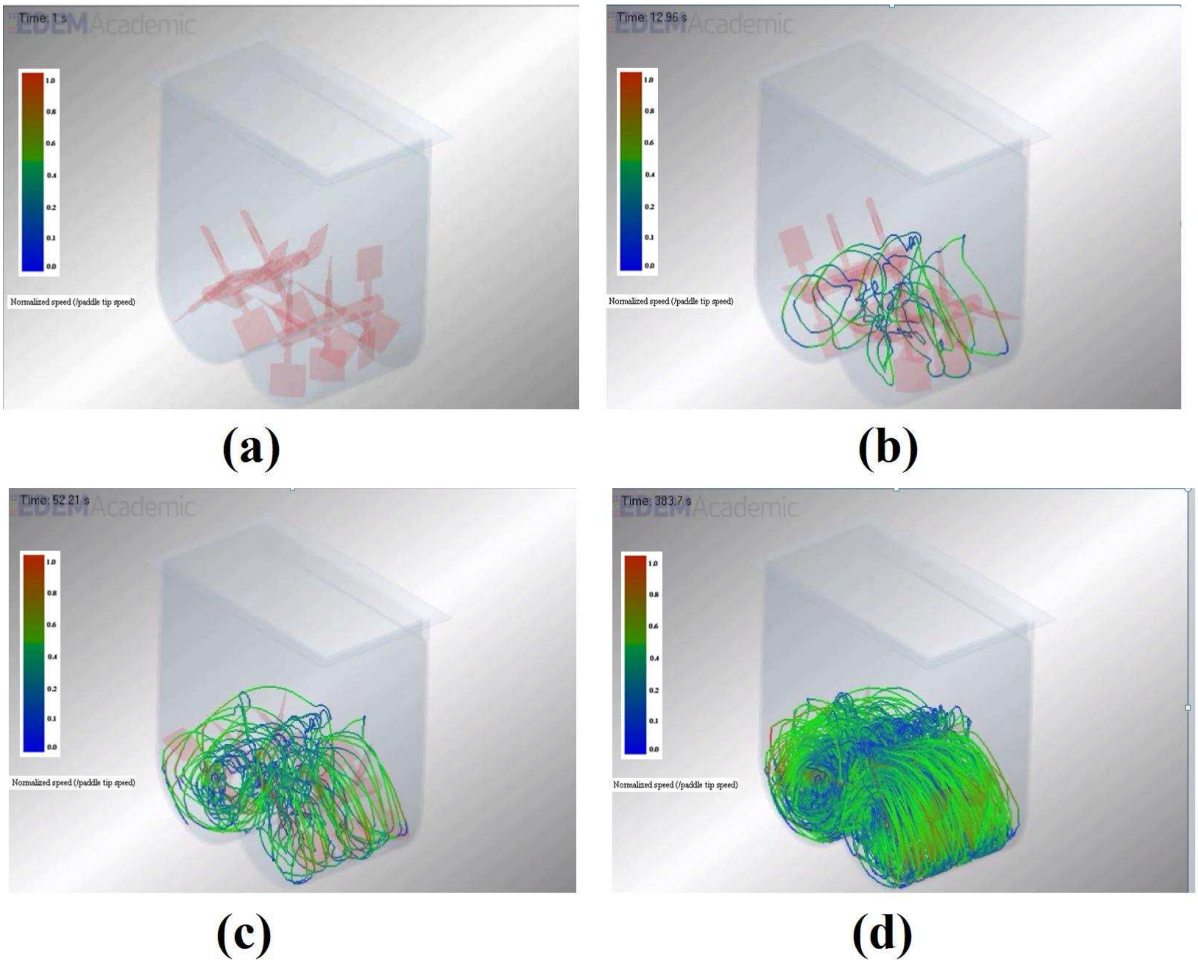

Figure 3: Tracer streamlines development at four different simulation times: (a) 1, (b) 13, (c) 52 and (d) 384 s. The trace is coloured based on the normalised speed of the tracer particle.

Figure 3 qualitatively shows the streamlines gradually develop and after about 384 seconds of simulation time shows presence in almost all the dynamic space of the geometry.

Figure 4 shows the average velocity (magnitude of velocity) of the whole particle population as compared to the tracer velocity for the first 100 seconds of the simulation.

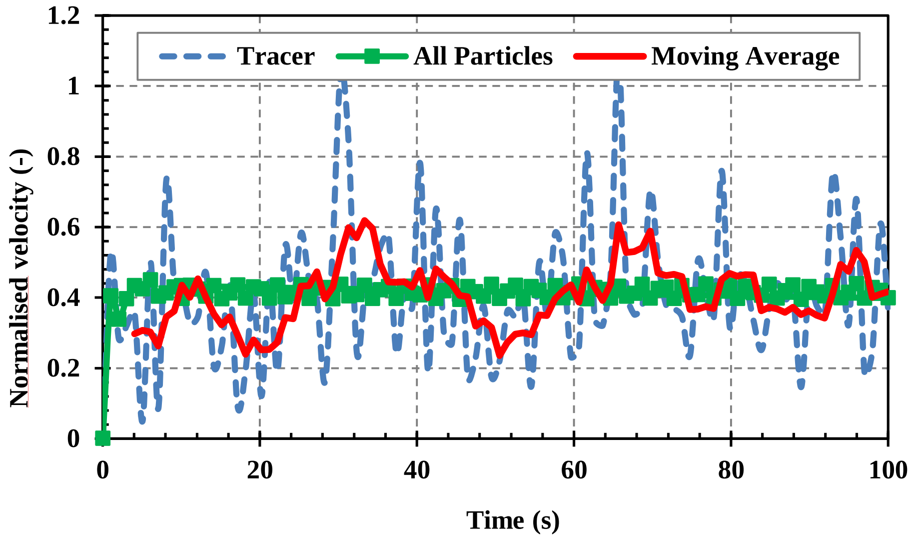

Figure 4: Average velocity of the whole particle population, tracer velocity and its moving average for the first 100 seconds of the simulation.

The figure shows the tracer velocity fluctuates over the average value obtained for all the particles in the system. In order to better compare the tracer velocity with the average velocity of all particles, the fluctuations of tracer particle were reduced by arithmetically averaging the tracer velocity for every 5 data points (i.e. every 0.05 seconds instead of every 0.01 seconds) which is also plotted as a function of time. The moving average trend of the tracer velocity demonstrates fewer fluctuations, suggesting that the average tracer velocity could be representative of the average particle velocity in the system.

In order to quantitatively investigate the time needed for the tracer to develop its streamlines, the normalised tracer velocity distribution is evaluated at different simulations times and is plotted in Figures 5 and 6. To do so, the active region of the geometry was divided into cuboid bins each of which had dimensions of 0.0205, 0.02 and 0.02 m in x, y and z direction, respectively. In each recorded time-step, based on the position of the tracer, the bin in which the tracer existed was determined. This spatial discretisation is similar to PEPT analysis. The normalised tracer velocity in each bin which was then evaluated and its distribution among bins is plotted (as seen in Figures 5 and

6). Throughout the present paper, the velocity distributions for DEM tracer(s) are obtained based on recording sample rates of 0.01 seconds.

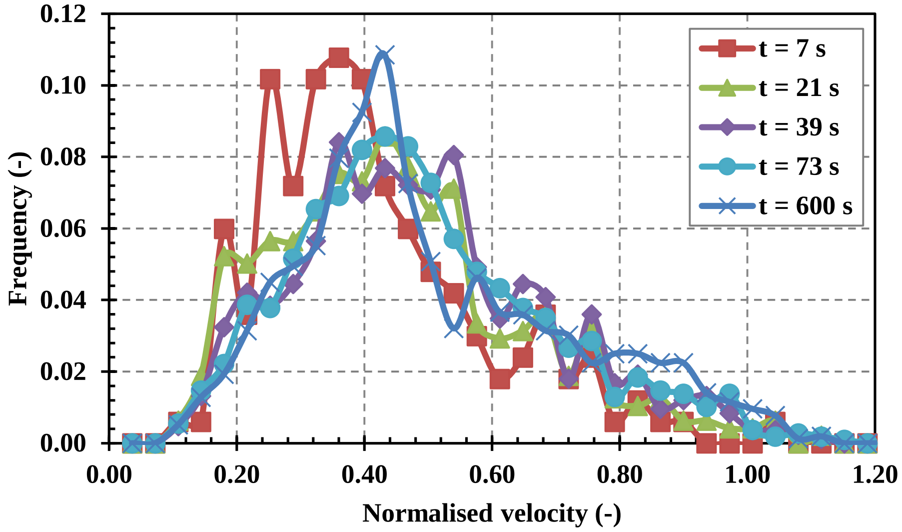

Figure 5: Tracer normalised velocity distribution at different simulations time: 7, 21, 39, 73 and 600 s

As it can be seen in Figure 5, the normalised tracer velocity distribution develops with time. If the velocity distribution does not change after some simulation time, it can be concluded that at that time the velocity distribution is developed and therefore there is no need to carry on the simulations (or in experiments carrying out the PEPT experiments). This can be seen in Figure 6, where the normalised velocity distribution of the tracer does not change much after about 251 seconds of simulation time.

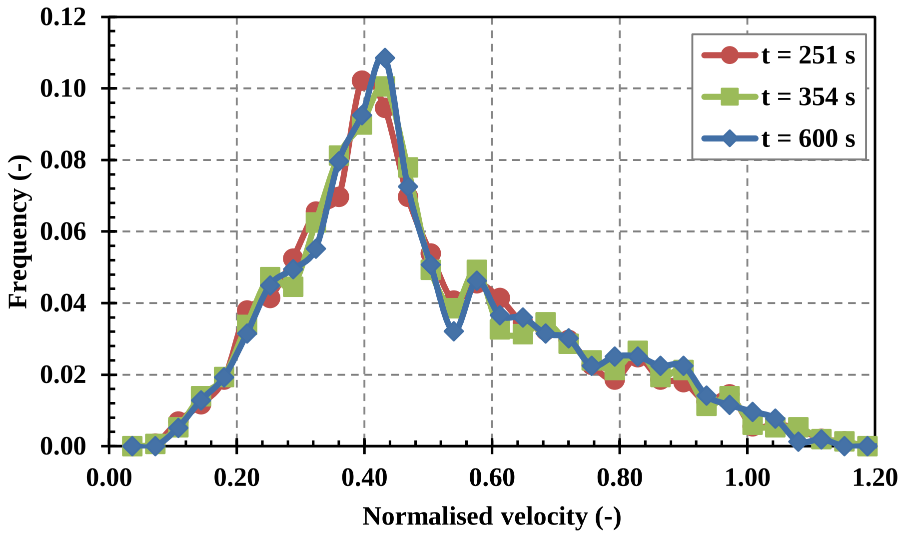

Figure 6: Tracer normalised velocity distribution at different simulations time: 251, 354 and 600 s

In order to investigate the effects of multiple tracers in the velocity distribution, five particles were tracked in the simulations. These five particles were selected randomly at different positions inside the mixer at the end of the simulation (i.e. at t = 600 s), then post processing started from initial time (0 s) for these particles. Figure 7 shows the normalised tracer velocity distribution using 1-5 tracers at the end of simulation (i.e. t = 600 s). For the multiple tracer cases, the normalised velocity is calculated by taking the average value of the normalised velocity of the tracers in each bin. It must be noted that the sampling rate can affect the distributions however since all the distribution are based on the same sampling rate (every 0.01 seconds), the comparative conclusions are valid.

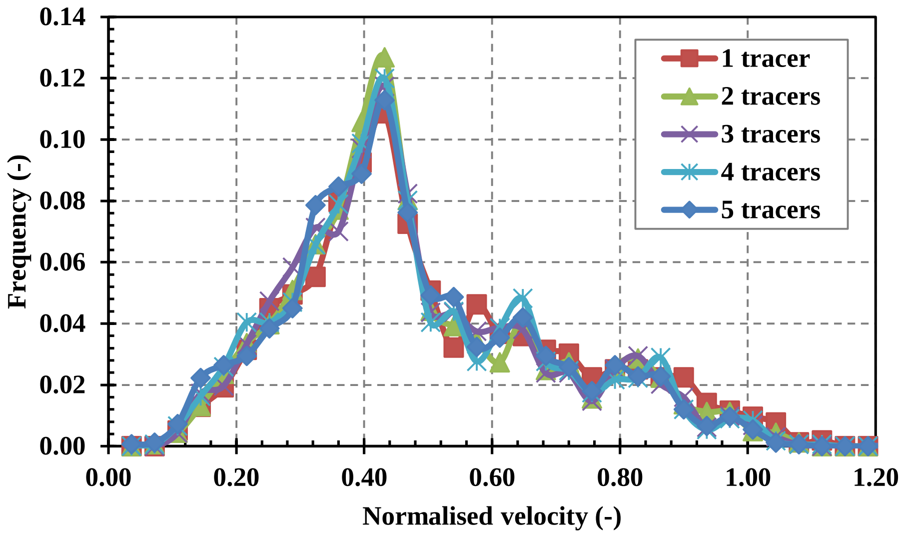

Figure 7: Normalised tracer velocity distribution using 1-5 tracers at t = 600 s

As it can be seen, increasing the number of tracers in this paddle mixer system does not influence the velocity distribution. In addition, for the system studied in this work it has been observed that increasing the number of tracers does not significantly shorten the time required to achieve a representative and time independent data. Furthermore for experimental PEPT the data acquisition and analysis could be more complex and time consuming. Therefore, one conclude that the use of multiple tracers in PEPT measurements does not provide improvements in the velocity distribution results and hence little benefit in this respect could be achieved. Figure 8 compares the normalised velocity distributions obtained from the experimental PEPT, one tracer particle in DEM and all the population of particles in DEM. The data on all particles has not been analysed in bins and rather data on each particle was time averaged and their distribution was plotted. The aim was to compare if PEPT results are representative of entire system in terms of entire particle population velocity distribution.

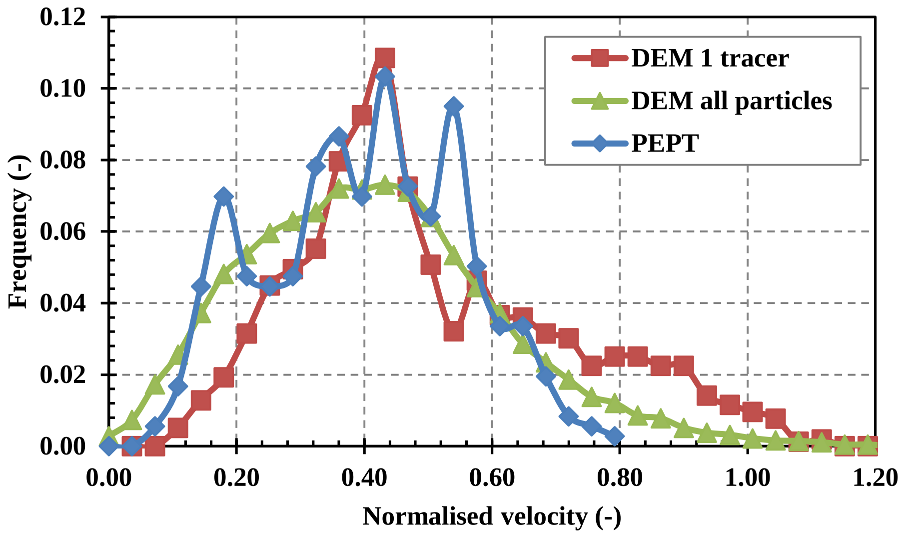

Figure 8: Comparison of normalised velocity distributions obtained from the experimental PEPT, 1 tracer particle in DEM and all the population of particles in DEM.

The figure shows although the peak frequencies of the velocity distribution for PEPT and DEM with one tracer are very similar, there are discrepancies over the width of the distribution and the frequencies of tracer with higher velocities. DEM tracer predicts a wider velocity distribution compared to PEPT. For normalised velocity of 0.7 and higher, the frequency distribution of DEM tracer is significantly higher than PEPT. One reason for this observation could be the differences in particle shape and size distribution for DEM and the experiment. Furthermore, the velocity for all particles in DEM shows a smooth distribution with a peak frequency of the velocity distribution lower than PEPT and DEM tracer. The velocity distribution data for the population of particles in DEM are based on a large number of particles (60,000 in this case), while for PEPT and DEM tracers it is based on time-averaged velocity distribution of a single tracer. Therefore the scatter and fluctuations in PEPT and DEM one tracer data, relative to DEM population, is expected. Potential explanations for the difference in the peak of the distribution could be attributed to the aforementioned particle size discrepancies and/or the sampling method: PEPT and DEM tracer analyses are based on data from only one particle within a discretised domain, i.e. the bins, while the DEM results consider the velocity profiles of the whole population of particles. Furthermore, in contrast to the DEM with one tracer data and PEPT, it can be seen that the data for all particles show that about 0.3% of particles are stagnant at any instance. When tracking a single tracer in DEM or PEPT, it may not be possible to detect zero velocity at any time. This could have implications for diagnosing stagnant regions where some particles in the mixer have no motion. This is a short coming of single tracer data which could not be representing all particles, particularly those which are stagnant. This requires further attention in future work.

5. Conclusions

The DEM results indicate that for the investigated paddle mixer, it takes 251 seconds for one tracer to travel adequately in all the dynamic space of the system. The tracer velocity fluctuates around the average value obtained for all the particles in the system suggesting the average tracer velocity could be representative of the average particle velocity in the system. Increasing the number of tracers in the paddle mixer system does not influence the average velocity distribution. The data of PEPT with one tracer with those of DEM with one tracer provide a good agreement; however for normalised velocity of 0.7 and higher, the frequency distribution of DEM tracer was found to be higher than PEPT. One reason for this observation could be the differences in particle shape and size distribution for DEM and the experiment. The velocity for all particles in DEM shows a smooth distribution with a peak frequency of the velocity distribution lower than PEPT and DEM tracer. The velocity distribution data for the population of particles in DEM are based on a large number of particles which reduce the scatter and fluctuations. Potential explanations for the difference in the peak of the distribution could be attributed to the particle size differences and the sampling method: PEPT and DEM tracer analyses are based on data from only one particle within a discretised domain, while the DEM results consider the velocity profiles of the whole population of particles. When tracking a single tracer in DEM or PEPT, particle having zero velocity may not be detected, while the data for all particles shows that about 0.3% of particles are stationary.

References

[1] G.R. Chandratilleke, A.B. Yu, J. Bridgwater, K. Shinohara, A particle-scale index in the quantification of mixing of particles, AIChE Journal 58 (2012) 1099-1118.

[2] B.F.C. Laurent, J. Bridgwater, Motion in a particle bed agitated by a single blade, AIChE Journal 46 (2000) 1723–1734.

[3] B.H. Ng, C.C. Kwan, Y.L. Ding, M. Ghadiri, Z.F. Fan, Solids motion in a conical frustum-shaped high shear mixer granulator, Chemical Engineering Science 62 (3) (2007) 756–765.

[4] D.J. Parker, C.J. Broadbent, P. Fowles, M.R. Hawkesworth, P. McNeil, Positron emission particle tracking—a technique for studying flow within engineering equipment, Nuclear Instruments and Methods in Physics Research A326 (1993) 592-607

[5] A. Hassanpour, H. Tan, A. Bayly, P. Gopalkrishnan, B. Ng, M. Ghadiri, Analysis of particle motion in a paddle mixer using Discrete Element Method (DEM), Powder Technology, 206 (2011) 189-194.

[6] Z. Yang, D.J. Parker, P.J. Fryer, S. Bakalis, X. Fan, Multiple-particle tracking—an improvement for positron particle tracking, Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment, 564 (2006) 332-338

[7] P.A. Cundall, O.D.L. Strack, A discrete numerical model for granular assemblies, Geotechnique, 29 (1979) 47–65

[8] H.P. Zhu, Z.Y. Zhou, R.Y. Yang, A.B. Yu, Discrete particle simulation of particulate systems: theoretical developments, Chemical Engineering Science, 62 (2007) 3378–3396

[9] H. Hertz, Über die Berührung fester elastischer Körper, Journal für die reine und angewandte Mathematik, 92 (1882) 156–171

[10] A. Hassanpour, C.C. Kwan, B.H. Ng, N. Rahmanian, Y.L. Ding, S.J. Antony, X.D. Jia, M. Ghadiri, Effect of granulation scale-up on the strength of granules, Powder Technology, 189 (2009) 304–312