# The Minimum Control Area Characterizing Hydrodynamic Macro Properties Dispersion Systems

**Haoran Zhang, Xiaohan Yan, Huixia Feng, and Yongtu Liang**

**Abstract** Studies on various dispersion systems have been developed with their widespread in engineering production, consisting of numerical simulation and experimental means. Experimental methods focus on hydrodynamic macro properties while simulation methods can be employed for interparticle interaction that closely relates with the non-Newtonian behaviors of dispersions. In this paper, a theoretical study method of the minimum control area (MCA) for dispersion systems was first proposed from the meso-scale perspective. It is a smallest infinitesimal extracted from a uniformly distributed dispersion system, which can characterize hydrodynamic macro properties of the system. The MCA method considers the interparticle interaction and is characterized by micro infinity and macro infinitesimal. It is representative through ensuring the key factor, involving the number and size distribution of dispersed particles in this area, conforms to the real dispersion system. We anticipated this method can be combined with computer technique to improve the study accuracy for the hydrodynamic macro properties of dispersion systems in the future.

**Keywords** Dispersion · Minimum control area (MCA) · Hydrodynamic macro property · Non-Newtonian behavior · Particle number and size distribution

## Nomenclature

| | |
|---|---|
| $i$ | A class of dispersed particles with the same size $i$ |
| $S_{\mathrm{a\ min}}$ | The minimum control area (MCA) |
| $p_i$ | The probability whether the dispersed particles of a size $i$ will be divided |

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S. N. Atluri and I. Vušanović (eds.), *Computational and Experimental Simulations in Engineering*, Mechanisms and Machine Science 98,
https://doi.org/10.1007/978-3-030-67090-0_6

$R_i$ The radius of dispersed particles of the same size $i$
$V$ The dispersion sample volume
$h$ The height from the cutting position to the center of a dispersed particle
$\overline{S}_i$ The average cut profile of dispersed particles of a size $i$
$S_i$ The cut profile of dispersed particles of a size $i$
$k_i$ The cut numbers of dispersed particles of a size $i$
$n_i$ The total dispersed particles of a size $i$ in the sample dispersion
$P_i$ The binomial distribution of the possibility that dispersed particles of a size $i$ can be cut
$k_i$ The number of dispersed particles of a size i displayed in the MCA
$\phi$ The dispersed particle volume fraction of the sample dispersion
$C_i$ The number of dispersed particles of a size $i$ per volume of dispersed particles in the dispersion, which can be known from experiments
$M$ The size number of all the dispersed particles
$\gamma$ The derived dispersed particle volume fraction in $S_{\mathrm{a\,min}}$
$e$ The variance between $\gamma$ and $\phi$
$b$ The parameter valued as $1/e$

# 1 Introduction

Dispersion system is a kind of multi-medium fluid where dispersed medium distributes in the other immiscible continuous medium in the form of particles, which consists of solid-liquid, liquid-liquid, and gas-liquid systems. It is ubiquitous but also important in a variety of industries ranging from food, cosmetic, pharmaceutical, oil and mine, which produce an appreciable fraction of dispersed substances to be disposed. Thus, the prediction and analysis on hydrodynamic macro properties of dispersion systems is of considerable significance for stable and effective production.

There is much research on experimental methods for hydrodynamic macro properties of dispersion systems [1–3, 41]. In the view of large amounts of literatures [4–7], the volume fraction and size distribution of dispersed-phase have been claimed to the most important factor governing the non-Newtonian hydrodynamic macro properties. Recently, many scholars devoted themselves to experimenting on dispersions with different physical structures of interphases and analyzing the results from the micro perspective, in order to construct a relationship between the macro experimental phenomenon with the basic micro mechanism [8, 9]. However, it is of great difficulty to extent to micro-scale study merely relying on experimental means, and thereby some numerical simulation methods are necessary [10–14].

The multi-particle interaction in dispersions is a hot issue since it is a complex process associating with diverse certain forces such as buoyancy force, drag force, gravity [15–17] and uncertain forces such as Brownian force [18], and special physical features of dispersed and continuous phases [19]. To cope with it, the direct numerical simulation (DNS) [20] can be utilized to model steady or turbulent flow fields, and the Lagrangian tracking means are required to model the dispersed particle movement. This DNS method facilitates the study and analysis on basic physical behaviors of dynamics systems. Carrier fluid and particle characteristics are obtained simultaneously. Later, the exchanges between the traditional numerical methods and the discrete element method (DEM) have been put forward [21]. The coupled the Lattice-Boltzmann numerical simulation and DEM, and the coupled DNS and DEM were developed and became popular in terms of a relatively higher simulation efficiency [22]. And there is an improved approach combining the DEM with the computational fluid dynamics (CFD) [23, 24]. DEM is used to model discrete particles while CFD is used to model the continuous phases based on the N-S equation, which can play an important role in the explicitly particle-particle, particle-wall, as well as particle-liquid collisions.

Most of the simulation methods coupled with the particle-discrete ideas are employed for single or several particles or dilute dispersions and can be well implemented, whereas larger amounts of dispersed particles need to be involved when considering a real condition. These methods mainly focus on the theoretical mechanism research but relatively ignore the connection between theory and reality. Further improvements need to be made by considering the movement of more dispersed particles. The micro-scale interaction should be displayed through macro visible phenomena. Although there are other computational simulation methods such as CFD, not only considering the micro interaction among dispersed particles but also focusing on macro fluid flow in dispersions [25–27], the simplification and artificial experience decrease the simulation accuracy [28] and the micro mechanism cannot be comprehensively taken into consideration.

From this point, we put forward a study method of the minimum control area (MCA) on the meso scale. It is proved to be the smallest study unit that can characterize the hydrodynamic macro property of a whole dispersion system, taking the number and size distribution of dispersed particles into account. This MCA allows micro study methods to be applied to the more accurate exploration of macro properties, since the study object scale and computational load can be considerably shrunk.

The present paper is organized as follows. The details of the methodology used are presented in Sect. 2. The derivation of the MCA analytical expression is performed in Sect. 3. The discussion for the application development and value of the MCA method is presented in Sect. 4.

## 2 Methodology Description

With respect to a homogenous dispersion system as a sample, it can be infinitely large to be studied but unrealistic, so there is a way to try to obtain a proper volume on behalf of the whole system. If half of the dispersion sample is taken, its property can be ensured to represent the whole system. And if half of the half dispersion is determined, it may be representative as well. While if we continue to divide the dispersion by half for each time, there must be an infinitely small divided volume failing to represent the whole dispersion, since the dispersed particles containing in the infinite small volume is so locally distributed leading to a distortion from the real system. In this sense, there must be a lower limit volume representative of the hydrodynamic macro properties of the whole dispersion.

To further simplify the volume concept for universal application, the three-dimensional volume can be converted into a two-dimensional area by means of cutting the volume in any direction, and the obtained infinitely small profile of the volume is defined as the MCA. Figure 1 displays this conversion procedure. And as seen in the Fig. 1(b) and (c), it is possible that the sphere particles can be cut at any position, thus, they can be regarded as circular profiles of different diameters in the MCA.

The hydrodynamic macro properties of dispersions are mostly subjected to the hydrodynamic interaction among dispersed particles [15–17], which is mainly associated with two factors: the particle number and size distribution. The particle number determines the frequency of particles' colliding and flocculating, while the particle size distribution determines the strength and effect of colliding and flocculating [29–31]. Based on this, the MCA is representative since it ensures the two factors of this area almost accord with those of the whole dispersion. According to Li et al. [32–34], the MCA can be regarded on the meso scale that can be perceived as a study perspective between micro and macro scales. If a study area is larger than the MCA, it belongs to a macro problem, leading to computational cost and the micro mechanism difficult to be involved; while a study area is smaller than the MCA, it belongs to a micro problem, leading to the theoretical mechanism study focusing on single or several particles and failing to characterize the whole systems.

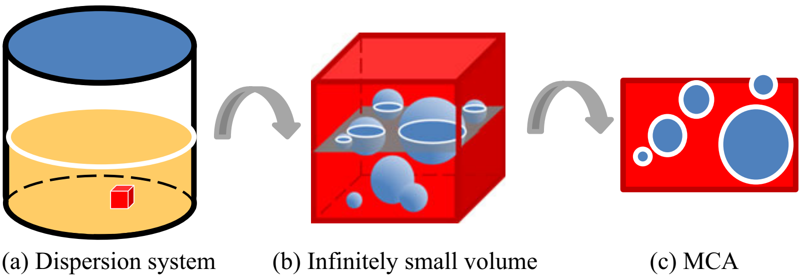


**Fig. 1** Conversion procedure for MCA

The meso scale has both the macro and micro characters; in other words, the micro mechanism such as multiple interactions among dispersed particles can be extended into a macro scale and illustrated by macro-study means.

# 3 Methodology Derivation

The MCA analytical equation was derived based on probability theories from the particle-scale perspective. And the derivation principle accords with the particle volume content and distribution of the extracted study object agreeable with the original dispersion system. Firstly, some assumptions are given:

- The dispersion should be regarded as a homogenous system.
- The dispersed particles should be treated as rigid spheres with no deformation.
- With specified sample dispersions and environment conditions, the hydrodynamic interaction among particles is only subjected to the number and size distribution of dispersed particles in the MCA.

## *3.1 MCA*

The conversion from three-dimension to two-dimension can be regarded as the volume being cross-cut to get its profile. Whereas it is inevitable that some of the dispersed particles in the volume will be divided into two halves possibly of different sizes with each one. And the probability that the dispersed particles of a size $i$ will be divided is given by the following:

$$p_i = \frac{2S_{amin}R_i}{V} \tag{1}$$

where: $2S_{\mathrm{a\,min}}R_i$ represents a cube that will be cut in a dispersion sample. $2R_i$ is the height and $S_{\mathrm{a\,min}}$ is the base of the cube. Suppose that some dispersed particles of size $i$ are cut at a distance $h$ to the particle center, then the particle spheres are transformed into profiles and yield:

$$S_i = \pi(R_i^2 - h^2) \tag{2}$$

And the probability that this size of dispersed particles will be cut to be profiles is expressed by:

$$\mathrm{p}(S_i) = \frac{1}{2R_i} \tag{3}$$

The profiles of one size of particles are different with one another since the cut positions (i.e. $h$) are different. But we can obtain the average profiles of one size of dispersed particles regardless of cutting position by combining Eqs. (2) and (3), shown as below:

$$\overline{S_i} = \int_{-R_i}^{R_i} S_i \frac{1}{p(S_i)} dh = \frac{2\pi R_i^3 - \frac{2}{3}\pi R_i^3}{2R_i} = \frac{2}{3}\pi R_i^2 \quad (4)$$

If the dispersed particles of size $i$ fall in the range of the MCA, $S_{\mathrm{a\ min}}$, the probability will be $p_i$, shown as Eq. (1); otherwise it will be $1 - p_i$, which can be described by a binomial distribution. Suppose that the cut number of one size of dispersed particles is $k_i$ and the total dispersed particle number of the whole dispersion is $n_i$. Then the binomial distribution can be established as:

$$P_i(k_i) = C_{n_i}^{k_i} p_i^{k_i} (1 - p_i)^{n_i - k_i} \quad (5)$$

which can also be denoted by the expression:

$$k_i \sim \mathrm{B}(n_i, p_i) \quad (6)$$

When the sample dispersion is characterized by higher concentration, the total dispersed particle number $n_i$ will tend to be infinitely large, contributing to the binomial distribution converging towards a normal distribution, namely:

$$k_i \sim \mathrm{N}(n_i p_i, n_i p_i (1 - p_i)) \quad (7)$$

The number of total dispersed particles $n_i$ in the sample dispersion can be expressed as:

$$n_i = \mathrm{V}\emptyset C_i \quad (8)$$

And there is another equation defining $C_i$ as:

$$\frac{4}{3}\pi \sum_{i}^{M} C_i R_i^3 = 1 \quad (9)$$

where: $\frac{4}{3}\pi C_i R_i^3$ can be interpreted as the ratio of the total particle volume of a size $i$ to a volume of dispersed particles of the whole sample, $V_{\mathrm{s}}$, and summing up it can carry out the ratio of total particle volume of all sizes to $V_{\mathrm{s}}$, which equals to 1.

And next is to deal with Eq. (7). First of all, multiplying Eq. (7) by the mean profile $\overline{S_i}$ obtained from Eq. (4) yields:

$$\frac{2}{3}\pi R_i^2 k_i \sim N(\frac{2}{3}\pi R_i^2 n_i p_i, \frac{4}{9}\pi^2 R_i^4 n_i p_i(1-p_i)) \quad (10)$$

And sum up Eq. (10) to include all sizes of dispersed particles:

$$\sum_i^M \frac{2}{3}\pi R_i^2 k_i \sim N(\sum_i^M \frac{4}{3}\pi R_i^2 n_i p_i, \sum_i^M \frac{4}{9}\pi^2 R_i^4 n_i p_i(1-p_i)) \quad (11)$$

Then combining Eq. (11) with Eqs. (1) and (8) yields:

$$\sum_i^M \frac{2}{3}\pi R_i^2 k_i \sim N(\sum_i^M \frac{4}{3}\pi R_i^3 \emptyset C_i S_{amin}, \sum_i^M \frac{8}{9}\pi^2 R_i^5 \emptyset C_i S_{amin}(1-p_i)) \quad (12)$$

Since the MCA is particle-scale and infinitely small, the probability $p_i$ can be perceived as infinitely small as well. On the contrary, the probability of $(1-p_i)$ will approach to 1, then Eq. (12) can be simplified:

$$\sum_i^M \frac{2}{3}\pi R_i^2 k_i \sim N(\sum_i^M \frac{4}{3}\pi R_i^3 \emptyset C_i S_{amin}, \sum_i^M \frac{8}{9}\pi^2 R_i^5 \emptyset C_i S_{amin}) \quad (13)$$

Equation (13) divided by $S_{\text{amin}}$ yields:

$$\gamma = \frac{\sum_i^M \frac{2}{3}\pi R_i^2 k_i}{S_{amin}} \sim N(\sum_i^M \frac{4}{3}\pi R_i^3 \emptyset C_i, \frac{\sum_i^M \frac{8}{9}\pi^2 R_i^5 n_i \emptyset C_i}{S_{amin}}) \quad (14)$$

According to Eq. (9), the mean value $\sum_i^M \frac{4}{3}\pi R_i^3 \phi C_i$ equals to $\phi$ constantly. And incorporating Eq. (9) with Eq. (14) yields:

$$\gamma \sim N(\emptyset, \frac{\sum_i^M \frac{8}{9}\pi^2 R_i^5 n_i \emptyset C_i}{S_{amin}}) \quad (15)$$

It is known that the $\gamma$ in Eq. (15) represents the volume fraction of dispersed particles of $S_{\text{amin}}$ that we have derived, which illustrates $\gamma$ keeps the same physical significance with $\phi$. From the equation, the mean value of the derived fraction $\gamma$ equals to the volume fraction $\phi$ of dispersed particles of the whole dispersion that can be measured by experiments. Since it is expected that the volume fraction of $S_{\text{amin}}$ should conform to the dispersion, a specified minimum error $\sqrt{e}$ is given here:

$$\frac{\sum_i^M \frac{8}{9}\pi^2 R_i^5 n_i \emptyset C_i}{S_{amin}} = e \quad (16)$$

And $S_{\text{amin}}$ can be given by:

$$S_{amin}\frac{\sum_{i}^{M}\frac{8}{9}\pi^{2}R_{i}^{5}n_{i}\emptyset C_{i}}{e}) \tag{17}$$

It is the variance to indicate how much the difference is between $\gamma$ and $\phi$. And $S_{\text{amin}}$ is obtained from Eq. (17), where all the parameters including $R_i$, $n_i$, $\phi$, $C_i$, and $M$ can be known from experimenting on the sample dispersion.

## 3.2 Particle Number in MCA

As shown in Fig. 1(c), there are dispersed particles of different sizes in the MCA, which are especially important in the MCA similarity with the original dispersion. Under the premise of a known MCA equation, we can continue to carry out the analytical equation of the particle numbers of different sizes.

Set $b = \frac{1}{e}$, and incorporating it and Eq. (4) into Eq. (17) yields:

$$S_{amin} = b\frac{8}{9}\pi^{2}\emptyset\sum_{i}^{M}R_{i}^{5}n_{i}C_{i} = b\frac{2}{3}\pi\emptyset\sum_{i}^{M}R_{i}^{2} = b\emptyset\sum_{i}^{M}\bar{\mathrm{S}}_{i} \tag{18}$$

According to Eq. (7), summing up $k_i$ yields the normal distribution for total particle number that are transformed to profiles, as below:

$$\sum_{i}^{M}k_{i}\sim \mathrm{N}(\sum_{i}^{M}n_{i}p_{i},\sum_{i}^{M}n_{i}p_{i}(1-p_{i})) \tag{19}$$

Sum up the multiplication of Eqs. (1) and (8):

$$\sum_{i}^{M}n_{i}p_{i} = \sum_{i}^{M}2S_{amin}\emptyset R_{i}C_{i} \tag{20}$$

$$\sum_{i}^{M}n_{i}p_{i}(1-p_{i}) = \sum_{i}^{M}2S_{amin}\emptyset R_{i}C_{i}(1-\frac{2S_{amin}R_{i}}{V_{T}}) \tag{21}$$

Then coupling Eq. (19) with Eqs. (20) and (21) yields:

$$\sum_{i}^{M}k_{i}\sim N\left[\sum_{i}^{M}2S_{amin}\emptyset R_{i}C_{i},\sum_{i}^{M}2S_{amin}\emptyset R_{i}C_{i}(1-\frac{2S_{amin}R_{i}}{V_{T}})\right] \tag{22}$$

As seen from Eq. (22), it indicates that $\sum_{i}^{M} k_i$, the total particle number that is cut, should fluctuate around the mean value $\sum_{i}^{M} 2S_{\mathrm{a\,min}}\phi R_i C_i$ with the variance of $\sum_{i}^{M} 2S_{\mathrm{a\,min}}\phi R_i C_i\left(1-\frac{2S_{\mathrm{a\,min}}R_i}{V_{\mathrm{T}}}\right)$. While the value of $1-\frac{2S_{\mathrm{a\,min}}R_i}{V_{\mathrm{T}}}$ approaches to 1, thus $k_i$ can be calculated by the following equation:

$$\sum_{i}^{M} k_i \approx \sum_{i}^{M} 2S_{amin}\emptyset R_i C_i \tag{23}$$

The parameter, $k_i$ is perceived as a key factor deciding the MCA similarity and exerting great influence on the hydrodynamic macro properties of dispersion, as a result of both the total particle number and size distribution involved.

## 4 Conclusion Remarks

To our knowledge, considerable investigations on hydrodynamic macro properties of dispersion systems have been done, which drives a lot of research directions such as the rheology and viscosity prediction [35–37], the relevant numerical simulation methods [12, 38], the interparticle micro mechanism [15, 39], etc. In the future, the MCA method proposed in this paper aims to be applied to these study areas by coupling with computational simulation methods such as computational fluid dynamics (CFD), molecular dynamic (MD) simulation, dissipative particle dynamic (DPD) simulation, etc. For example, when modelling a dispersion system, the basic data for numerical simulation, especially the MCA size is required. On the one hand, the simulation should conform to the real condition; on the other, the calculation time is better to be shortened as much as possible. Thus, the MCA is able to work out a minimum dispersion area consisting of the smallest number and a real size distribution of dispersed particles. It cannot only improve the simulation efficiency but also increase the implementation value of the simulation, in virtue of the macro properties of the modelled dispersion satisfactory with real conditions.

Furthermore, there is a key factor $k_i$ illustrating the number and the size distribution of dispersed particles in the MCA, which have tremendous impact on hydrodynamic macro properties of dispersions [40, 41]. For example, it is essential that the dispersion rheology is mainly dominated by the interparticle interaction that is closely related to $k_i$ for the interaction possibility and effect are determined by the particle number and size distribution respectively. With more concentrated dispersions (i.e. larger value of $k_i$), there is more intense interaction highlighting the rheological behaviors. Hence, studies on dispersion rheology have paid much attention to the influence of dispersed particle concentration and size distribution.

From this point, the key factor $k_i$, worked out by the MCA method, will be another novel study idea provided for theoretical analysis, which is able to be combined with experiments and contribute to more reliable hydrodynamic property prediction for non-Newtonian dispersion systems.

**Acknowledgements** Haoran Zhang and all the co-authors would like to greatly acknowledge the National Natural Science Foundation of China (grant number 51474228) for financial supports and the Beijing Key Laboratory of Urban oil and Gas Distribution Technology, China University of Petroleum-Beijing for technical supports.

**Author Contributions** Haoran Zhang wrote the initial paper, Xiaohan Yan and Huixia Feng checked grammar and drew. Yongtu Liang provided the overall idea of the article and revised the paper. All authors contributed to the final manuscript.

**Additional Information** Competing interests: The authors declare no competing financial interests.

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