STUDY ON THE EFFECT PARTICLE SIZE DISTRIBUTION AND BLAINE FINENESS ON THE HYDRATION OF CEMENT

Shiju Joseph (1) (2), Shashank Bishnoi (2)

(1) Building Materials and Building Technology Division, Department of Civil Engineering, KU Leuven, Belgium
(2) Dept. of Civil Engineering, Indian Institute of Technology Delhi, India

Abstract

While Blaine’s fineness has been traditionally used to measure the fineness of cements, laser diffractometry is being increasingly used to measure its particle size distribution. These measurements are often used to understand and model the hydration of cement, strength development, etc. Although laser diffractometry results are usually directly used in these studies, the particle sizes are often truncated to control computational costs. Results from Blaine’s fineness are often converted to discrete particle size distributions using various equations involving the mode diameter and range of particle sizes. Both techniques, thus, require assumptions that may affect the final results and inferences from models. Numerical simulations are used in this article to study the effect of various assumptions made while using fineness and particle size distribution on hydration kinetics and development of microstructure. The results from this study shows that significant reduction in computational effort is possible without compromising the accuracy on truncation of the particle size distribution used in modelling.

1. INTRODUCTION

Blaine fineness and laser diffractometry are the common techniques that are used to characterize the fineness of cement. While Blaine fineness could provide the specific surface area, laser diffractometry is able to provide the particle size distribution. Surface area not only depends on the particle sizes but also the shape of independent particles and hence it cannot be accurately captured or modelled using laser diffractometry.

One of the common ways to model cement fineness is by assuming that the ranges of particle sizes which are provided by the laser diffractometry are spheres. But this kind of an assumption will not be able to capture the surface area of cement which has an impact on the kinetics of hydration. Moreover, the particle size distribution (PSD) has to be truncated at some point due to computational limitations. This is because, when the minimum diameter is very less the number of particles generated will be very high. This would need higher memory capacity to store the PSD and needs more processing power to calculate the reactions involved with them. Upon truncation, the specific surface area decreases again as most of the surface area is provided by the finer particles.
To negotiate with the Blaine surface area, what is done generally is to modify the particle size distributions by making it finer so that the computed surface area is equal to or around the surface area measured using BET or Blaine’s air permeability test. Alternatively fines of the lowest particle size generated could be added more to get the required surface area, keeping the total mass constant.

Another way and the easiest way to generate a particle size distribution is using the Blaine surface area and the Rosin Rammler (RR) function. By iterating the spread of the equation and mode diameter, PSD of any surface area could be generated within the range determined by the lowest particle size. Over here also the RR function must be truncated at some point for the same reason mentioned above.

The aim of this paper is to study the effect of truncation on particle size distribution and effect of different particle size distribution having the same fineness. The question that we intend to answer with this paper is weather one must go with the particle size distribution and not care about the fineness or will it be appropriate to model just using Blaine surface area. Another question this paper intends to answer is at what diameter the particle size distributions could be truncated so that there is a balance between the computational effort and the accuracy of the model.

The effect of particle size distribution on the cement hydration was studied and modelled by many researchers [1] [2]. But the effect of truncation on the degree of hydration and the effect of specific surface area has not been studied.

In this paper different particle size distributions are generated and is been simulated on the microstructural modelling platform µic [3]. Avarami-diffusion kinetics [4] and reaction thickness mechanism [5] are used for simulation of degree of hydration.

2. SIMULATIONS

Ten different particle size distributions (PSD) are used for this study. The first 5 PSD (Sim01-Sim05) are having a uniform Blaine surface area of around 4500cm²/g (Figure 1). And 6 PSDs are of the same particle size distribution which are truncated at different diameters(Sim02, Sim06 - Sim10). Rossin rammler equation with a slight modification was used for the simulation of particle size distributions. Different trials have been done to achieve the same Blaine surface area. The details of the PSDs used are summarized in Table 1.

\[ f = 1.0 - \exp\left(-0.913 \left(\frac{d}{d_m}\right)^{w_d}\right) \]

Where, f is the fraction of powder below a certain diameter d and d_m is the mean diameter or commonly known as d_60 and w_d is the width of the function which spread the PSD. This equation is modified with a coefficient to make sure that the d_60 of the simulated PSD coincides with d_m.

Simulations have been done for two different rate controlling mechanisms which are diffusion controlled. The most commonly used diffusion controlled kinetics is the Avarami-diffusion mechanism and the reaction thickness method.
Table 1: Simulation details of different particle size distributions used

<table>
<thead>
<tr>
<th>PSD ID</th>
<th>Blaine (cm²/g)</th>
<th>No of Particles</th>
<th>Mean Diameter (µm)</th>
<th>Width</th>
<th>Min diameter (µm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sim01</td>
<td>4505.7</td>
<td>4093174</td>
<td>36</td>
<td>1.45</td>
<td>0.1</td>
</tr>
<tr>
<td>Sim02</td>
<td>4499.1</td>
<td>3289420</td>
<td>25</td>
<td>0.95</td>
<td>0.1</td>
</tr>
<tr>
<td>Sim03</td>
<td>4503.7</td>
<td>2729820</td>
<td>18</td>
<td>1.075</td>
<td>0.1</td>
</tr>
<tr>
<td>Sim04</td>
<td>4502.3</td>
<td>4399962</td>
<td>44</td>
<td>0.975</td>
<td>0.1</td>
</tr>
<tr>
<td>Sim05</td>
<td>4505.6</td>
<td>1928108</td>
<td>13</td>
<td>1.1</td>
<td>0.1</td>
</tr>
<tr>
<td>Sim06</td>
<td>3883.3</td>
<td>822071</td>
<td>25</td>
<td>0.95</td>
<td>0.2</td>
</tr>
<tr>
<td>Sim07</td>
<td>3182.6</td>
<td>143451</td>
<td>25</td>
<td>0.95</td>
<td>0.5</td>
</tr>
<tr>
<td>Sim08</td>
<td>2549.3</td>
<td>28946</td>
<td>25</td>
<td>0.95</td>
<td>1</td>
</tr>
<tr>
<td>Sim09</td>
<td>2112.7</td>
<td>8213</td>
<td>25</td>
<td>0.95</td>
<td>2</td>
</tr>
<tr>
<td>Sim10</td>
<td>1486.1</td>
<td>1188</td>
<td>25</td>
<td>0.95</td>
<td>5</td>
</tr>
</tbody>
</table>

Figure 1: Particle Size Distributions of different PSD ID

2.1. Avarami - diffusion mechanism

Avarami kinetics [6] which was originally used for nucleation of particles freely in the space is commonly used for a diffusion controlled mechanism. It is used along with a diffusion model. The Avarami part can predict the acceleration and deceleration part in a
common heat of hydration curve (Stage 3 and Stage 4) and the diffusion model can predict the final stages (Stage 4 and Stage 5).

Figure 2 shows the absolute deviation of the degree of hydration of Sim01-Sim04 with respect to Sim05. The deviation cannot be called as error as the correct values are unknown. Figure 3 shows the independent deviations from Sim02, which is truncated at lowest diameter of 0.1µm for PSDs Sim06-Sim10.

Figure 2: Absolute deviation in the degree of hydration of different PSDs of same Blaine surface area with PSD of Sim05 (Avarami-diffusion Mechanism)

Figure 3: Absolute deviation from the degree of hydration which are truncated at different minimum diameters (Compared to Sim02, Avarami-diffusion mechanism)
2.2. Reaction thickness kinetics

Reaction thickness kinetics is another way for representing the diffusion mechanism. Figure 4 shows its deviation from one of the PSD (Sim05) with others of the same Blaine surface area. Figure 5 shows its deviation in degree of hydration of Sim06-Sim10 from Sim02.

Figure 4: Absolute deviation in the degree of hydration of different PSDs of same Blaine surface area with PSD of Sim05 (Reaction thickness Mechanism)

Figure 5: Absolute deviation from the degree of hydration which are truncated at different minimum diameters (Compared to Sim02, Reaction thickness mechanism)
3. DISCUSSIONS

There are mainly two schools of thought on the hydration kinetics of alite and cement. One being the nucleation and growth controlled kinetics and other being the diffusion controlled kinetics. A diffusion controlled mechanism is easy to model and capture compared to a nucleation and growth kind of model. Different models were proposed for nucleation and growth kinetics over the years to capture the different experimental evidences [4] [7] [8] [9] [10] [11].

If it is a diffusion controlled mechanism, it is evident from the simulation results that the surface area does not play any role and all it matters is the particle size distribution. And it can also be noted that there is no significant deviation of degree of hydration upon truncation of particle size distribution. When PSDs are truncated on higher diameters, the computational effort needed is very minimal. It could mean that simulations can be done on a normal personal computer with no significant loss of accuracy.

From Figure 3 and Figure 5 it can be seen that truncation up to 2µm does not significantly deviate from a minimum particle size diameter of 0.1µm. And even for truncation at higher diameters, it would be taken care in the later ages. Say if a simulation is done for predicting the degree of hydration at 28 days or so, a higher truncation diameter will hardly have any effect on the same and a different particle size distribution with the same fineness could deviate a lot.

It can also be seen that even though the Blaine fineness are the same for PSDs Sim01-Sim05, the degrees of hydration varies quite a lot. It must be noted that identical parameters was used for the kinetics for all the simulations. So it would be wiser to use results from laser diffractometry and generate the particles without taking into account for the Blaine surface area.

In the case it is a nucleation and growth kinetics which is more increasingly getting its popularity the scenario would be slight different. In such a system the initial surface area and the instantaneous surface area plays a role in the hydration kinetics. But in that case also the instantaneous surface area will depend on the particle size distribution along with the initial surface area.

When computational efforts are considered the truncation would be of great advantage for the same. Figure 6 shows how the computational effort is affected when the number of particles are changed for a microstructural model.

Computational efforts would be much more if a multi-scale modelling is to be performed. Multi-scale modelling are more used for either predicting the strength of concrete block or predicting the heat of hydration in a mass concrete. For those purposes particles have to simulated n number of times where n is the number of nodes in the macro scale for a particular time step. It would be of greater advantage for using a PSD which is truncated at a higher particle diameter for those purposes. It could drastically cut the computational cost associated with it.
4. CONCLUSION

Different particle size distributions with same Blaine fineness and particle size distributions which are truncated at different minimum diameters are simulated. It was found that Blaine surface area does not have any effect on dissolution mechanisms and truncation will not significantly change the results from modelling a hydration. Significant reduction in computational effort is possible with truncation of a particle size distribution without adversely changing the result.

REFERENCES


