

Modelling nucleation in wet granulation

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Abstract

Nucleation is the first stage in any granulation process where binder liquid first comes into contact with the powder. This paper investigates the nucleation process where binder liquid is added to a fine powder with a spray nozzle. The dimensionless spray flux approach of Hapgood et al. (Powder Technol. 141 (2004) 20) is extended to account for nonuniform spray patterns and allow for overlap of nuclei granules rather than spray drops. A dimensionless nuclei distribution function which describes the effects of the design and operating parameters of the nucleation process (binder spray characteristics, the nucleation area ratio between droplets and nuclei and the powder bed velocity) on the fractional surface area coverage of nuclei on a moving powder bed is developed. From this starting point, a Monte Carlo nucleation model that simulates full nuclei size distributions as a function of the design and operating parameters that were implemented in the dimensionless nuclei distribution function is developed. The nucleation model was then used to investigate the effects of the design and operating parameters on the formed nuclei size distributions and to correlate these effects to changes of the dimensionless nuclei distribution function. Model simulations also showed that it is possible to predict nuclei size distributions beyond the drop controlled nucleation regime in Hapgood's nucleation regime map. Qualitative comparison of model simulations and experimental nucleation data showed similar shapes of the nuclei size distributions. In its current form, the nucleation model can replace the nucleation term in one-dimensional population balance models describing wet granulation processes. Implementation of more sophisticated nucleation kinetics can make the model applicable to multi-dimensional population balance models.

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1. Introduction

Agglomeration is the formation of aggregates from powder feed material (Ennis and Litster, 1997). Agglomeration using a binder liquid and some form of agitation is referred to as wet granulation. Wet granulation can be divided in three major phenomena occurring simultaneously in a granulator (Iveson et al., 2001): nucleation and binder distribution, consolidation and growth, and attrition and breakage. Nucleation and binder distribution generally occur at the start of a granulation process (batch granulation) or near the powder feed inlet of a granulator (continuous

granulation). Only in the last few years, the effects of nucleation on the final product properties have been recognized. Therefore there is only limited research relating to binder liquid addition, nucleation and binder liquid distribution. Rankell et al. (1964) investigated the relationship between the rate of binder liquid addition and the effect of the powder bed velocity perpendicular to the binder liquid spray on the average granule size (see Fig. 1). The main findings were a linear relation between the spray rate and average granule size and a decrease in granule size with increasing powder bed velocity. Tardos et al. (1997) found a similar effect for the powder bed velocity, but also observed a narrowing particle size distribution with increasing spray surface area and powder bed velocity. Schaafsma et al. (1999) investigated the effect of drop size and spray rate on the granule size. They found that there was a direct relationship between the droplet size and the granule size in the early growth phase of

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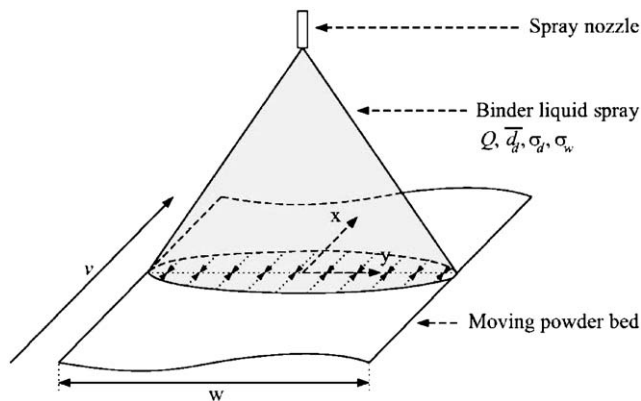


Fig. 1. Schematic representation of the spray zone when adding binder liquid to a moving powder bed with a flat fan spray nozzle.

granulation. Litster et al. (2002) have derived a dimensionless spray flux that is a measure for the density of droplets landing on a powder bed surface. The dimensionless spray flux is used as a tool to predict the controlling mechanism of the nucleation process. Hapgood et al. (2004) extended this work using a Monte Carlo model to predict the extent of drop overlap in the spray zone and therefore the proportion of drops that produce single nuclei. This model compared favorably with experimental data from nucleation experiments. However, the model stopped short of predicting the full nuclei size distribution leaving the spray zone. Hapgood and coworkers also developed a nucleation regime map that predicts the controlling nucleation mechanism as a function of the dimensionless spray flux and a dimensionless drop penetration time (Hapgood et al., 2003). The dimensionless drop penetration time is defined as the quotient of the penetration time of spray drops in the powder bed and the circulation time of the powder to return to the spray zone.

In modelling granulation processes, population balances are a very commonly used tool (Adetayo and Ennis, 1997; Hounslow et al., 1998; Kapur and Fuerstenau, 1969; Liu and Litster, 1998, 2000). Traditionally, population balances were one dimensional. These population balances described particle size changes but did not include information such as particle porosity and particle moisture content. More recently population balance models have been extended to multiple dimensions (Iveson, 1999; Vermury et al., 1997; Biggs and Hounslow, 2001; Verkoeijen et al., 2002; Wauters, 2001; Xiong and Pratsinis, 1993). Multi-dimensional population balance models include additional particle properties such as porosity and moisture content. However, the focus of the model has always been on granulation mechanisms such as consolidation, layering and growth. The representation of the nucleation process in population balances describing granulation processes is poor. Generally nucleation is modelled by adding nuclei of a specific size at a constant rate to the process where the rate constant is used as a fitting parameter. Further, the porosity and moisture content of the nuclei are assumed to be equal for all nuclei.

Nucleation and binder distribution studies demonstrate that binder liquid addition and powder bed flow have a strong influence on the resulting nuclei size distribution. However, no attempt has been made to quantitatively predict the nuclei size distribution based on the properties of the binder liquid spray, binder liquid addition method and powder bed flow properties. This paper uses the theoretical developments of Hapgood and coworkers to develop a physically based nucleation model to predict the initial nuclei size distribution from binder liquid addition with a spray nozzle onto a moving powder bed with primary particles smaller than the spray droplets.

2. Theory

2.1. Dimensionless spray flux

In many granulation processes, the binder liquid is sprayed with a nozzle onto a moving powder bed surface as shown in Fig. 1. The footprint of the spray is defined as the spray zone. Due to the agitation within a granulator, there is a continuous flux of powder through the spray zone. When the binder liquid droplets come into contact with the powder bed surface, they penetrate into the bed and form nuclei.

Hapgood et al. (2003) developed a nucleation regime map (Fig. 2) that describes the mechanisms that control the formation of nuclei in terms of a dimensionless drop penetration time (τ_p) and a dimensionless spray flux (ψ_a). At low spray fluxes and short penetration times, the density of drops on the powder surface will be low and the drops will penetrate into the bed and form nuclei quickly. It is assumed that

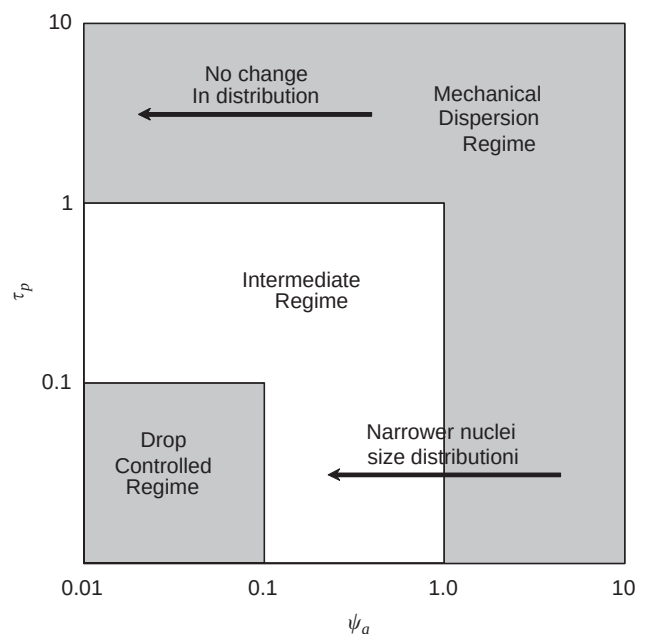


Fig. 2. Nucleation regime map by Hapgood et al. (2003).

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