CHAPTER 4

SIMULATION TECHNIQUE

4.1 Data Manipulation and Analysis

4.1.1 Measuring the particle size

Particle size data are essential for this work. Expressing the size of a single particle is not a simple task when the particle is not exactly spherical. The various methods of expressing particle size depend upon the type of measuring devices used.

Randolph and Larson (1988) define the particle size as the linear dimension that best characterizes the state of subdivision of the material within the context of the typical shape of the particles. Due to many different possible structures a particle might be subjected to , different methods of size characterization such as volume equivalent size, projected area size, sieve size, etc. are available. Unless otherwise stated, the sieve diameter has been used throughout Adetayo's work as well as the present work.

4.1.2 Relationship between number, volume and mass of particles

Adetayo (1993) assumes that the product granule density is essentially independent of its size, and states that this is a reasonable assumption for a well-packed granule.

The mass of particles in size interval i (M_i) is given by

$$(M_i) = N_i \rho_g k_v d_i^{-3} \quad (4.1)$$

where k_v = volume shape factor compared to the spherical particle,

ρ_g = granule density (g/cm^3)

N_i = number of particles in the ith interval

$\overline{d_i}$ = average diameter of particles in the ith interval

For a geometric discretization system

$$\overline{d_i} = \left(\frac{6\overline{v_i}}{\pi}\right)^{1/3} \quad (4.2)$$

where

$$\overline{v_i} = \sqrt{v_i . v_{i-1}} \quad (4.3)$$

v_i = volume of single granule volume

$\overline{v_i}$ = average volume of single granule between interval

The volume of particles in the i^{th} interval V_i for the spherical particles as assumed above is given by

$$V_i \;=\; \frac{\pi}{6} N_i \overline{d}_i^3 = \overline{v_i} N_i \qquad (4.4)$$

4.1.3 Presentation of the size distribution data

Particle size distribution can be expressed on a mass, volume or number basis. In fertilizer granulation practice, the key quality criterion is the mass of granules within the required size interval. Hence in this thesis, cumulative particle mass distribution will be utilized hereafter.

Figure 4.1 Illustrates the common methods of presenting a particle size distribution.

4.1.4 Measure of liquid content (% moisture)

The volume of water, Vw ,required to build up xw% of moisture for a feed is determined from the following equation.

$$V_w \;=\; \frac{x_w G}{\left(100 - x_w\right)\rho_w} \qquad (4.5)$$

where G = mass of dry granule (g)

ρ_w = water density , ($1 g/cm^3$)

thus we can calculate the water volume required. For example we want 4% moisture for a feed of 10g. fertilizer. Then

$$V_w = \frac{4x10}{(100-4)\,1} = 0.4167\ cm^3 \qquad (4.6)$$

The above volume of liquid phase is present during granulation.

The solution phase ratio (y) is the ratio of the volume of the solution to that of the solid in the granule.

$$y = \frac{x_w^{'}(1+s)\rho_f}{\left(1-x_w^{'}s\right)\rho_l} \qquad (4.7)$$

where $x_w^{'}$ = weight ratio of water to dry granule

s = solubility of fertilizer salt in water (g/g water)

ρ_f = fertilizer salt density (g/cm^3)

ρ_l = fertilizer solution density (g/cm^3)

The above equation is derived, as follows. Consider a unit weight of solid fertilizer. Let W be the weight of water per unit weight of solid fertilizer. $x_w^{'}$ be the ratio by weight of the water to that of the solid fertilizer and s be the solubility of the fertilizer salt in water. Then

The volume of fertilizer solution $V_l = \dfrac{x_w^{'}(1+S)}{\rho_l}$

The volume of undissolved Fertilizer $V_p = \dfrac{(1-x_w^{'}s)}{\rho_f}$

The solution phase ratio y is given by

$$y = \frac{V_l}{V_\rho} = \frac{x_w^{'}(1+s)\rho_f}{\left(1+x_w^{'}\right)} x\,100 \qquad (4.8)$$

The mass fraction of water is

$$x_w = \left(\frac{x_w^{'}}{\left(1+x_w^{'}\right)}\right) x\,100 \qquad (4.9)$$

or

$$x_w^{'} = \frac{x_w}{100-x_\omega} \qquad (4.10)$$

Bulk porosity is given by

$$p = 1-\left(\frac{\rho_b}{\rho_g}\right) \qquad (4.11)$$

For a granule of porosity p, the solution phase ratio y is related to its fractional saturation S_{sat} (Adetayo et. Al 1993) as follows

$$S_{sat} = \frac{y(1-p)}{p} \qquad (4.12)$$

In the case of NPK fertilizer 16-16-8 of urea base grade

$$\rho_b = 0.90 \quad g/ml$$

$$\rho_g = 1.65 \quad g/cm^3$$

Then

$$p = 1 - \left(\frac{0.90}{1.65}\right) = 0.46$$

For grade 16-16-8 with 1.5% moisture content at granulating condition, then

$$\rho_f = 1.829 \quad g/cm^3$$
$$\rho_l = 1.22 \quad g/cm^3$$

s = 0.64 (g solid/ g water)

$$x_w = \frac{1.5}{100 - 1.5}$$

y = 0.378

Then s_{sat} = 0.444

4.2 Modeling Technique

4.2.1 Granulation Drum Modeling of Drum Granulator

The population balance modeling technique is found to be the most suitable for use in modeling the granulation process, as explained in chapter 3. The Hounslow sectional mid-point model is simple and accurate enough for use in modeling the fertilizer granulation process.

The population balance equation (3.21) is to be solved with the coalescence kernel containing parameters k_1 and k_2. In the present model, the particle size distribution in the drum is approximated as 24 size intervals. The top size of the first interval is 0.157 mm. The size range between each interval is determined by multiplying the bottom size with the factor 1.26 to get the top size of that interval.

The interval size limits are as follows : 0.157, 0.198, 0.25, 0.314, 0.396, 0.499, 0.628, 0.792, 0.998, 1.257, 1.584, 1.996, 2.516, 3.170, 3.994, 5.033, 6.341, 7.990, 10.068, 12.686, 15.984, 20.140, 25.377 and 31.975 (mm).

Thus the population balance equation (3.21) for the drum granulator is a set of 22 ordinary differential equations (ODE's) which are integrated simultaneously using the 4^{th} - order Runge-Kutta method for the desired residence time up to 25 minutes.

4.2.2 Modeling of Screen

The 24 size intervals are also utilized in the pseudo-steady screen model, the interval limits being the same as those of the drum granulator model. The probability that a particle in the ith size interval will not pass through the screen is given by equation (3.2). The screen model is coded as one subroutine, which can represent both the oversize screen and product screen by selecting the parameters for the particular screen. Obviously the simulation results of the probability Y_{di} for the granules in the interval whose diameters lie between $d_{i-1} < h_s$ and $d_i > h_s$ will be between 0 and 1.

4.2.3 Modeling of Crusher

The oversize output from the oversize screen is sent to the crusher in order to produce that the crushed particles smaller than 4 mm. For the crusher the same 24 size intervals as those of the drum granulator model are also used.