CHAPTER 5

VALIDATION OF COMPONENT MODELS

After suitable component models to use in the fertilizer granulation process have been adopted, a computer code in the FORTRAN 77 language is next written for the process. Subsequently, validation of each component model must be made to ensure its suitability and ability to predict the existing data. In this thesis, the simulation results of each component model will first be compared to published experimental data and plant data.

5.1 Validation of drum granulator model

The population balance model for drum granulation of materials with broad size distribution of Adetayo (1993) is adopted for this work. The computer model is written in FORTRAN 77.

Adetayo (1993) makes numerous comparisons of his simulation results with his laboratory-scale experimental data. The data available for 3 fertilizers are as follows :

Ammonium sulfate (AS) at 4% , 6% and 8% moisture content.
Mono-ammonium phosphate (MAP) at 3%, 4%, and 5% moisture content.
Di-ammonium phosphate (DAP) at 2% , 4% and 5% moisture content.

Data were collected at 3 granulation times : 5, 15 and 25 minutes. All fertilizer were granulated starting from the same standard initial size distribution (20% < 1.0 mm., in Table 5.1). He also compared his simulation results with lab-scale experimental data for DAP, granulated from two other initial size distributions containing progressively more fine particles (30% < 1.0 mm. and 50% < 1.0 mm.).

Adetayo's model (1993) gives a reasonably good fit to the full granule size distribution for the complete range of data. The estimated parameters, k_1 and k_2, for each fertilizer type are given in table 5.2.

He reports that, for experiments in which an equilibrium size distribution is quickly reached, the best estimate of k_2 is statistically not significantly different from 0, i.e. the second stage of granulation does not occur. His simulations clearly match well the narrowing of the size distribution as granulation proceeds.

Adetayo also investigates the characteristics of the two kernel types in order to see the effect of the type of kernel on the shape of the predicted granule size distribution curve. Fig 5.1 shows the two size distributions, each obtained with the same median particle size produced by solving the population balance with only one of the two kernels. All simulations start with the same initial granule size distribution. Obviously, the single zero-order kernel (Eq. (3.22)) produces a much narrower size distribution than the first-order kernel (Eq. (3.23)). With the zero-order kernel, fine particles in the initial size distribution rapidly disappear with little change to the coarse end of the size distribution. In contrast, the single first-order kernel broadens the initial size distribution and fails to remove completely the fine particles even after a significant extent of granulation.

5.1.1 Comparison of the present simulation results with Adetayo's experimental data

None of the single kernels as presented above (shown in figure 5.1) could, on its own, correctly predicts the shape of the granule size distribution for the full range of data. The single zero-order kernel (Eq.(3.22)) does not predict the subsequent broadening of the granule size distribution at higher moisture contents and longer granulation times for MAP and DAP.

Table 5.1 Coalescence rate constant for AS,MAP and DAP

Moisture Content	Solution phase ratio, y	S_{sat}	S_{crit}	k_1 (min^{-1})	k_2 (mm^{-3} min^{-}	Particle Density (kg/m^3)	t_1 (min)
Ammoniumsulphate (AS)							
4%	0.106	0.20578	>0.36	2.85	0.0002	170	1.7
6%	0.165	0.28159	>0.36	3.90	0.0013	170	1.7
8%	0.228	0.34657	>0.36	4.80	0.0006	170	1.7
Mono-ammonium phosphate (MAP)							
4%	0.090	0.13178	0.2	1.70	-0.0016	160	2.0
5%	0.115	0.17829	0.2	2.30	-0.0060	160	2.0
6%	0.135	0.23256	0.2	3.00	0.0120	160	2.0
Di-ammonium phosphate (DAP)							
2%	0.045	0.073	0.13	1.38	0.0043	150	2.0
4%	0.092	0.150	0.13	3.39	0.0033	150	2.0
6%	0.144	0.235	0.13	5.98	0.0006	150	2.0

The first-order kernel (Eq.(3.23)) fails to predict the total removal of the fine particles from the initial size distribution. Adetayo's experimental data do support a two-stage granulation mechanism. In Figure 5.1, the final experimental granule size distribution is compared to simulations with two single kernels and the two-stage kernel.

Only the two-stage kernel can predict the correct shape of the granule size distribution. Thus the two-stage kernel has been adopted for granulator drum modeling to predict the granulated fertilizer particle size distribution.

The evaluation of the present simulation results against Adetayo's experimental cumulative granule size distribution (symbols) is shown in Figures 5.2 to 5.10. As expected, the present model gives a reasonably good fit to the full granule size distribution for the complete range of data because it is essentially based on Adetayo's model..

Appendix II shows the 9 different sets of experimental data for AS, MAP, DAP granules Adetayo used for comparison to his simulated results.

5.1.2 Sensitivity analysis of the present drum granulator model

For the present drum granulator model, a study on the model sensitivity to perturbations made to its kernel parameters is next made.

More specifically, the sensitivity study is carried out by changing either k_1 or k_2. As shown in Figure 5.11 the granulator model is found to be quite insensitive to a variation in k_2 (with $k_1 = 0$ and $t_1 = 0$). There is insignificant difference between the cumulative mass fractions of the granulated stream with $k_2 = 0.00516$, $k_2 = 0.0043$ or $k_2 = 0.00344$ for DAP fertilizer at moisture 4% data.

In the case of increasing k_1 value by 20%,the particle size distribution of DAP at 4% moisture content narrows when compared to the normal case of $k_1$value. Upon decreasing k_1 value by 20%, the granule size distribution compared to the normal case is broadened.

5.2 Validation of the screen model

The screening unit is comprised of a product screen underneath and an oversize screen above it. For the “product screen” , the product granule size distribution was taken as the ‘oversize stream’. The input to the ‘product screen’ is taken as the difference between the mass of particles entering the screening unit as feed and that exiting the unit as oversize. In other words, the input to the product screen is the undersize stream of the oversize screen.

5.2.1 Comparison of the present simulation results with published plant data

The present screen model which is written in FORTRAN 77 is validated against data obtained from the industrial screen of a fertilizer company (Lister, 1989). The different sets of data for one grade of fertilizer granules have been used by Lister for the parameter estimation.

For all sets of data, the estimated parameters are not significantly different from each other. Lister recommends $m_o = 30$ and $m_p = 400$ be taken as the model parameters for the oversize and the product screen, respectively.

As expected, good agreement is observed between the prediction of the present model and the observed cumulative mass fraction of the oversize and the product streams, as shown in Figure 5.12.

5.2.2 Sensitivity analysis of the present screen model

A sensitivity study of the present screen model is made by varying either of the two parameters, m_o and m_p. As reported by Adetayo, the screen model is found to be quite insensitive to variations in m_p. Though not shown here, there is no significant difference in the cumulative mass fraction of the product stream when $m_p = 400$ and $m_p = 100$.

As shown in Figure 5.13, the present sensitivity study confirms that the predicted oversize granule size distribution is significantly affected by changes made to m_o. For example, increasing m_o to 80 from the normal case (30) reduces the amount of minus 4 mm. size particles from approximately 20 to 10%. The decrease in m_o however results in a big reduction in the classification efficiency of the oversize screen with approximately 40% of minus 4 mm. size particles being carried away in the oversize stream.

5.3 Validation of the present crusher model

5.3.1 Comparison of the present simulation results with published plant data

The present crusher model is validated against data collected from an operating granulation plant (Lister, 1989). The problem is to find N_s, N_b and N_c

which give good agreement between the observed and predicted cumulative mass fraction of particles in the ith size interval exiting the crusher as crushed oversize.

Observation of the data sets reveals that granules bigger than 8 mm. are present in the crusher product. For the selection function, Lister recommends d^s_{upp} = 16.0 mm. and d^s_{low} = 0.25 mm. whereas d^c_{upp} = 4 mm. and d^c_{low} = 2 mm. for the classification function.

Results from the estimation of the parameters of the crusher model by Adetayo (1993) reveal that N_c is not significantly different from zero, indicating that negligible classification occurs in the crusher. Thus it may be assumed here that $N_c = 0$. The estimation of the parameters N_s and N_b using DAP fertilizer data (Lister, 1989) gives $N_s = 7.0$ and $N_b = 0.165$. For other grades of fertilizer, re-estimation of the model parameters should be carried out on new data sets.

5.3.2 Sensitivity analysis of the present crusher model

A sensitivity study on the present crusher model is carried out by changing one of the parameters of interest while keeping the rest constant.

1. Changing N_s

A reduction in N_s results in poor crushing as the size distribution of the granules exiting the crusher has a significant proportion of large granules. In fact the average diameter of the granules exiting the crusher is significantly increased, as shown in Fig. 5.15.

2. Changing N_b

Figure 5.15 also shows that a reduction in N_b from 0.165 to 0.1 results in the generation of a significant amount of fines. To simulate a highly efficient crusher with at least 90% of its product being smaller than 4mm., various combinations of N_s and N_b are unsuccessful. Even reducing d_{upp}^{s} from 16 to 4 mm. does not give the desired efficiency. This is due to the fact that without the classification function, particles pass through the breakage zone of the crusher only once. Particles larger than 4 mm. in diameter are produced as a result of the breakage of even larger particles. These particles then come out with the product stream.

3. Changes to the Classification Function

The efficiency of the crusher can be improved by the introduction of a separate classifier, increasing the intensity of crushing or by using new sets of hammers in the crusher. The breakage function is not expected to be significantly affected as long as the same type of crusher is used. However, a significant effect on the overall selection function is expected. To simulate this effect on the selection function, a classifier is introduced into the model. It is assumed that due to the presence of the classifier, particles greater than 4 mm. cannot exit the crusher. These granules are assumed to be returned back to the breakage zone to undergo further breakage. This phenomenon is simulated with $d_{upp}^{c} = 4$ mm. and, $N_c = 1$ (linear dependency of the classifier on size difference).

Figure 5.15 shows that a big improvement of the crusher performance is achieved without a significant production of fines. This crusher model is flexible enough to account for different crusher types.

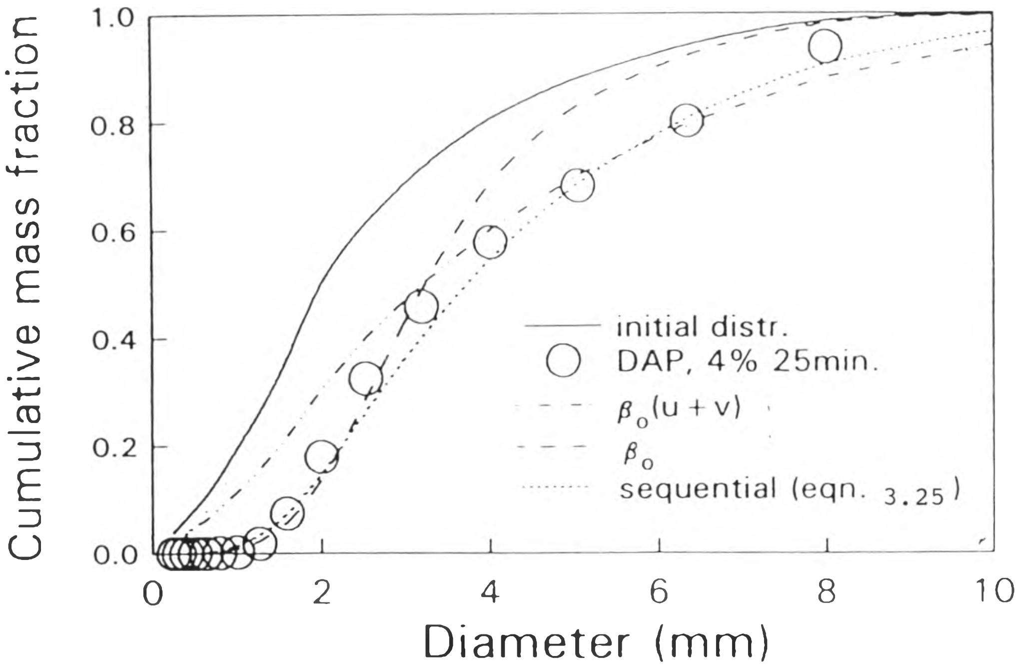

Figure 5.1 : Comparison of the predicted cumulative mass fraction with experimental data for type I initial size distribution of DAP with 4% moisture content granulated for 25 minutes

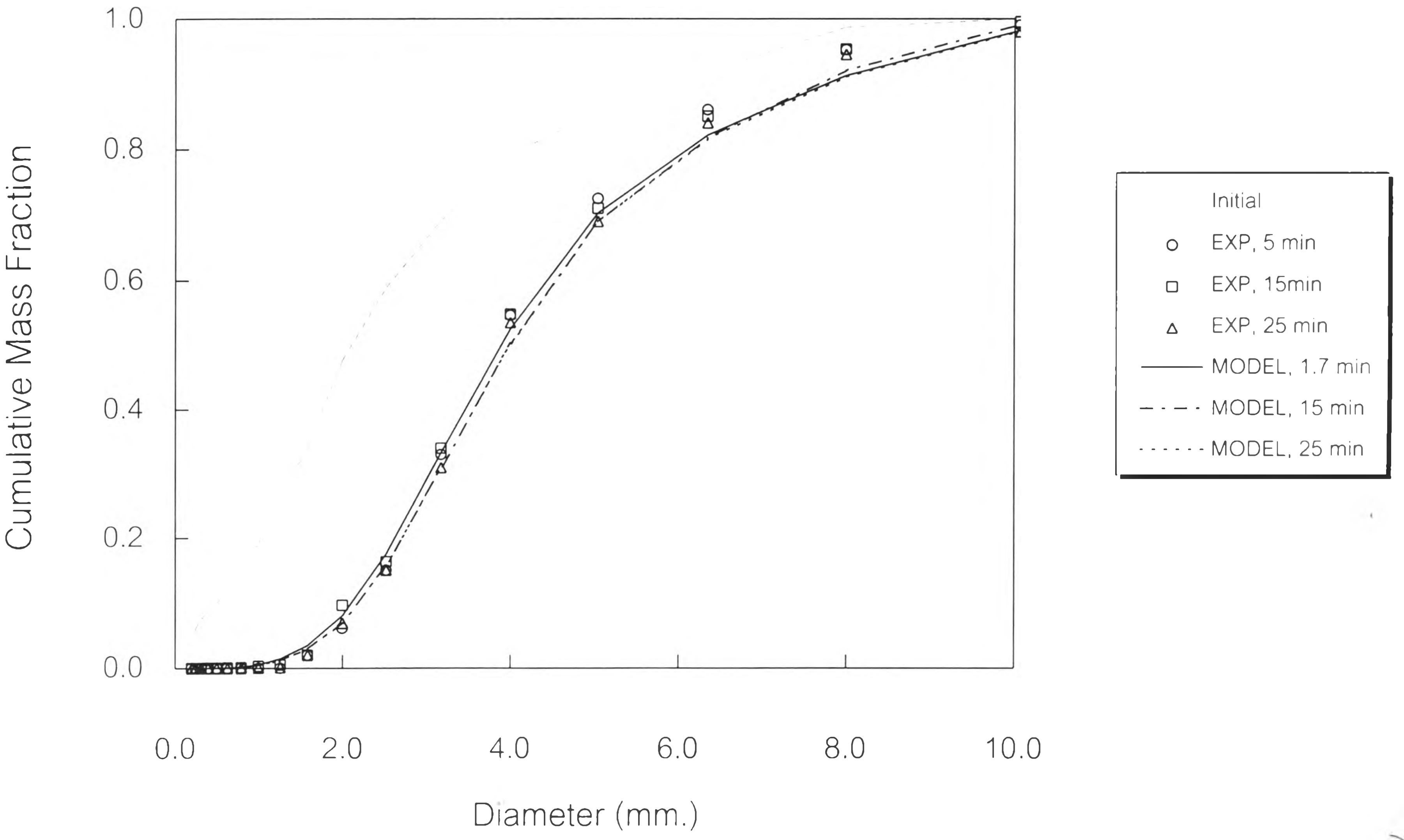

Figure 5.4 Simulation result VS experimental data (Adetayo,1993) for AS at 8% moisture content

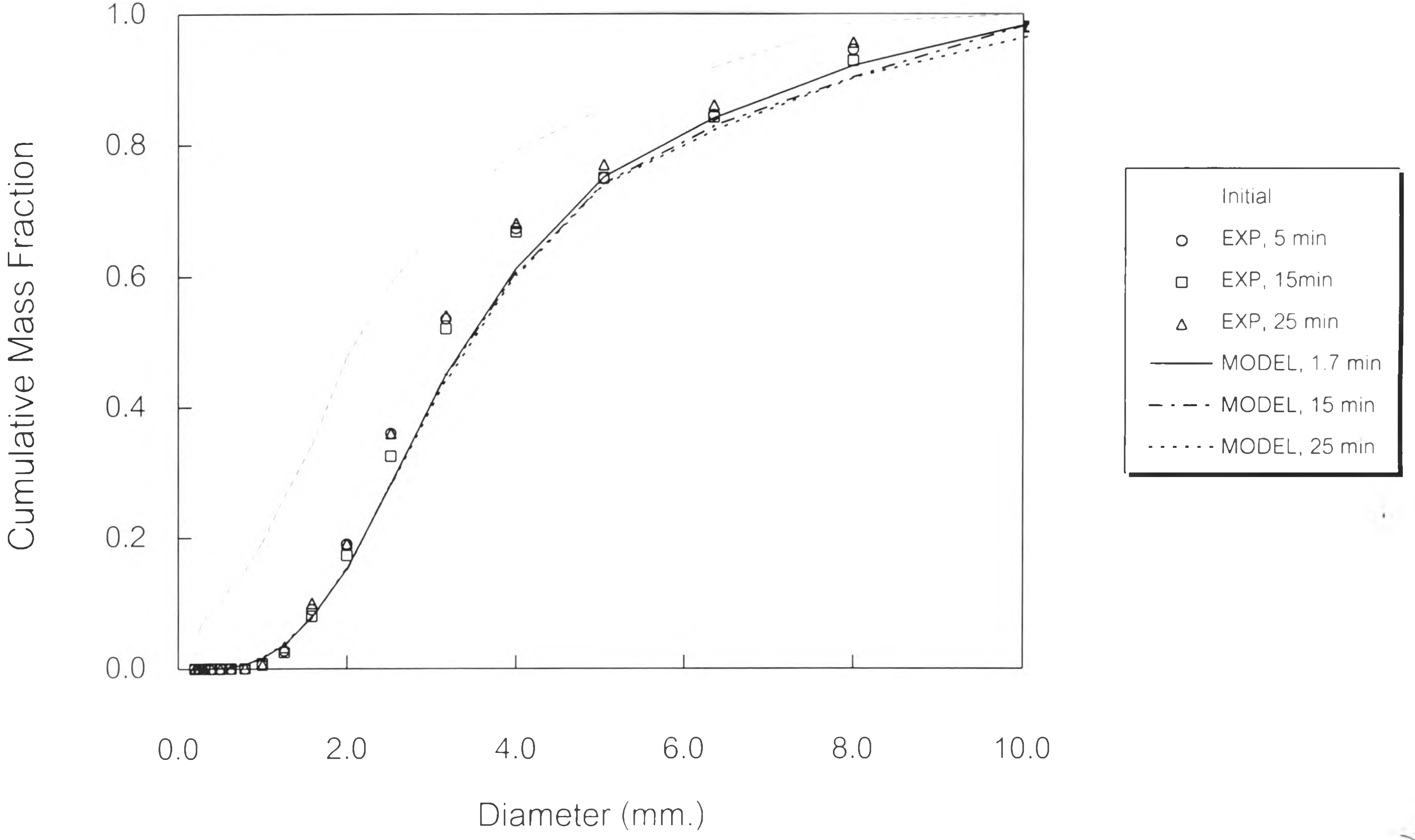

Figure 5.3 Simulation result VS experimental data (Adetayo,1993) for AS at 6% moisture content

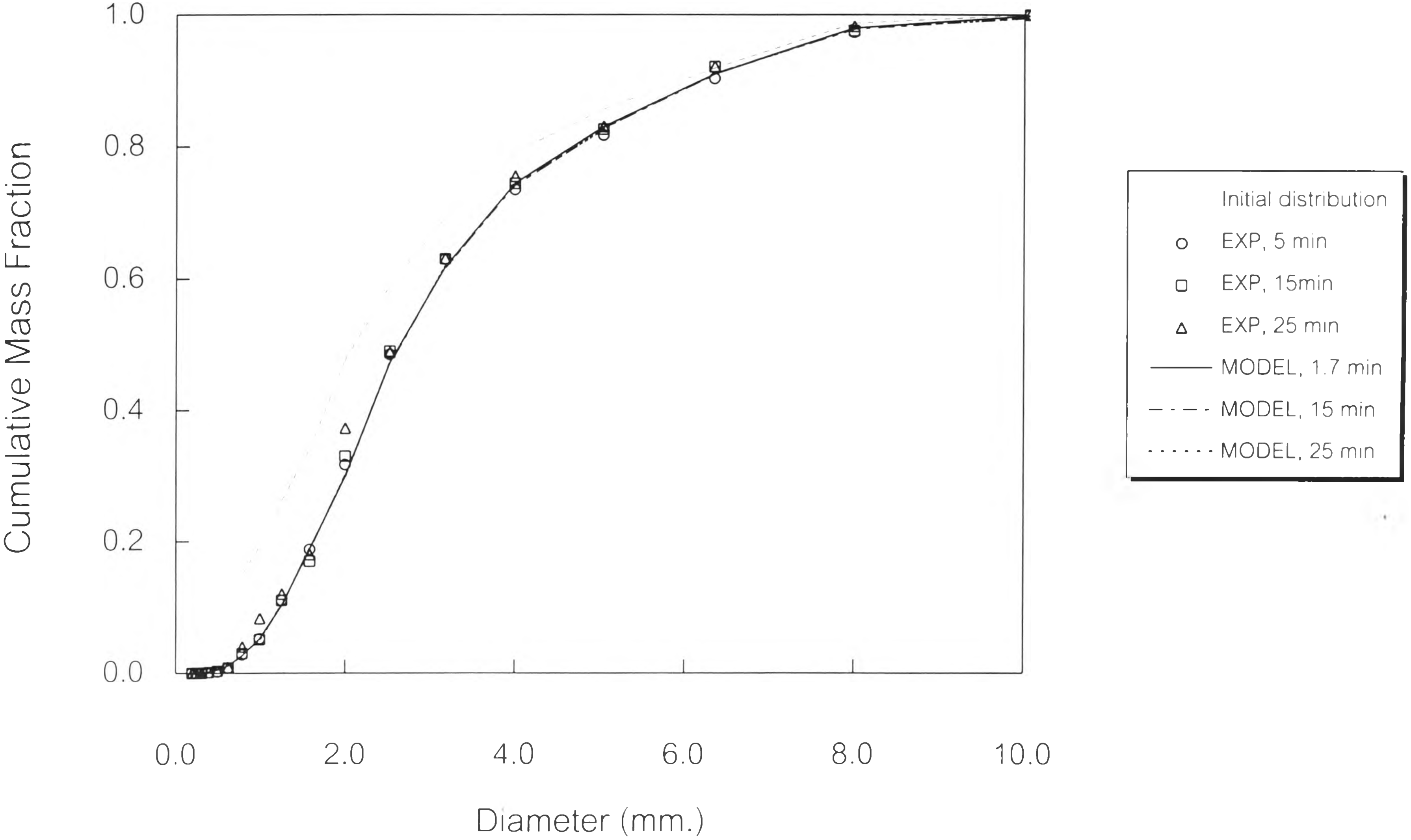

Figure 5.2 Simulation results VS experimental data (Adetayo,1993) for AS at 4% moisture content

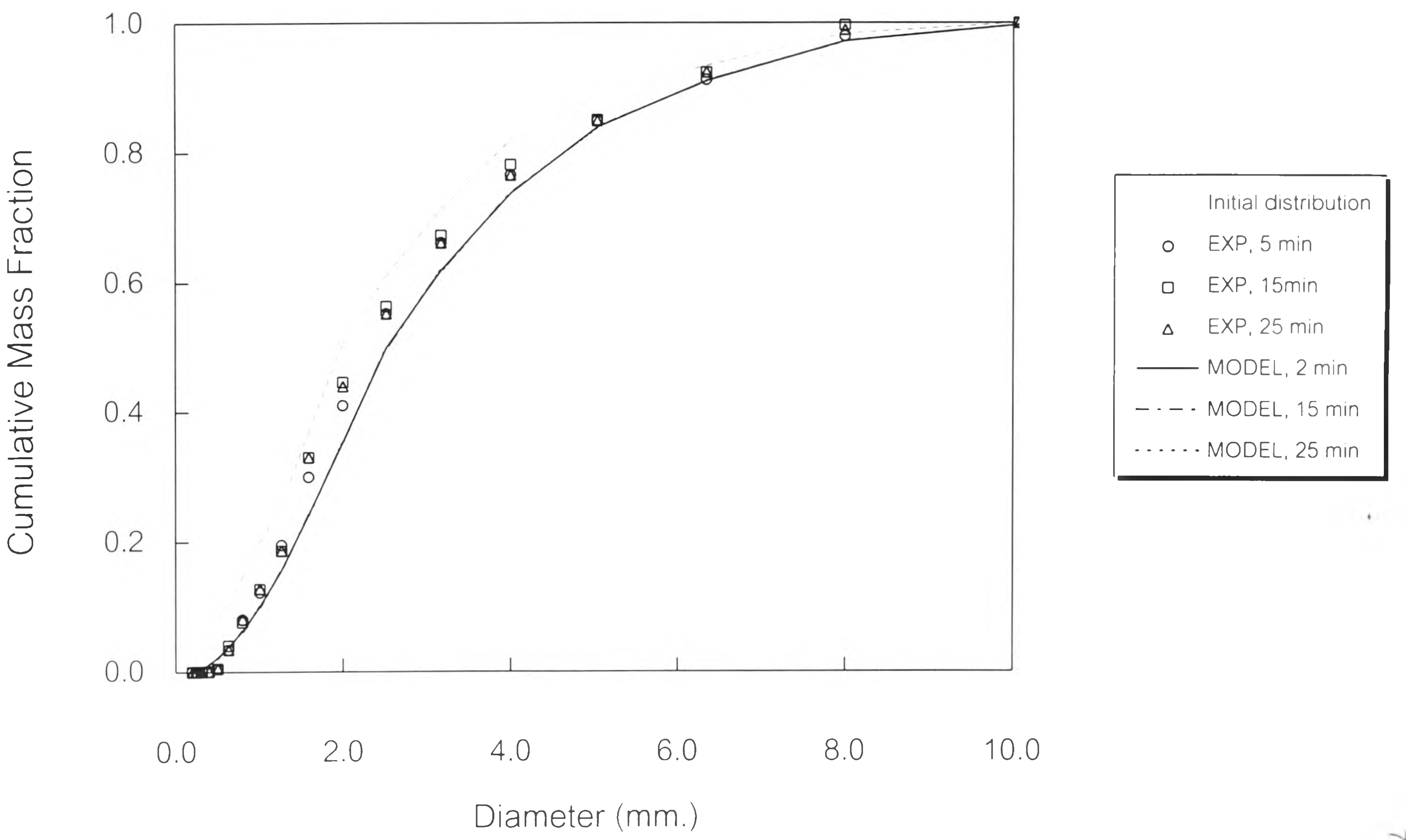

Figure 5.5 Simulation result VS experimental data (Adetayo,1993) for MAP at 4% moisture content

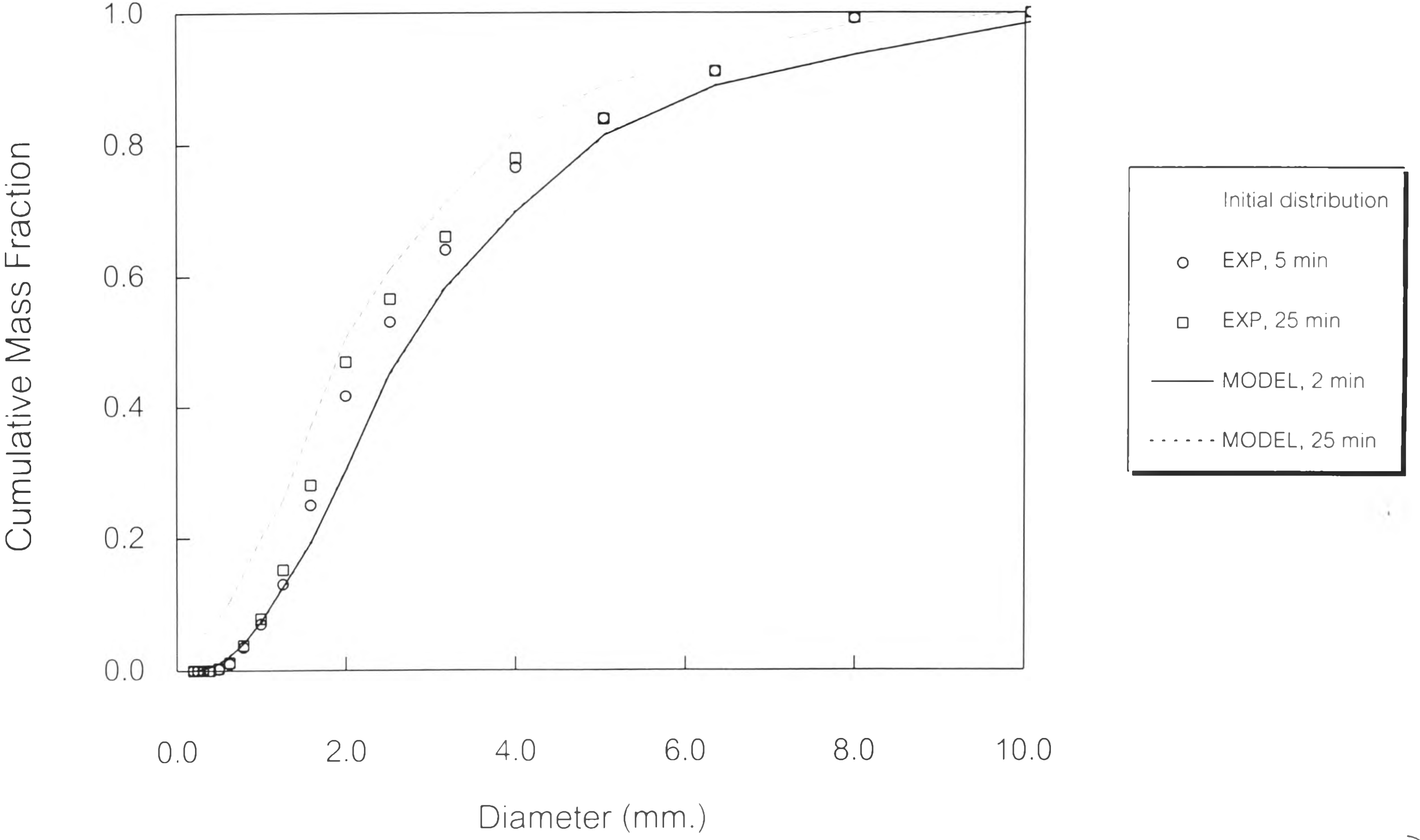

Figure 5.6 Simulation result VS experimental data (Adetayo,1993) for MAP at 5% moisture content

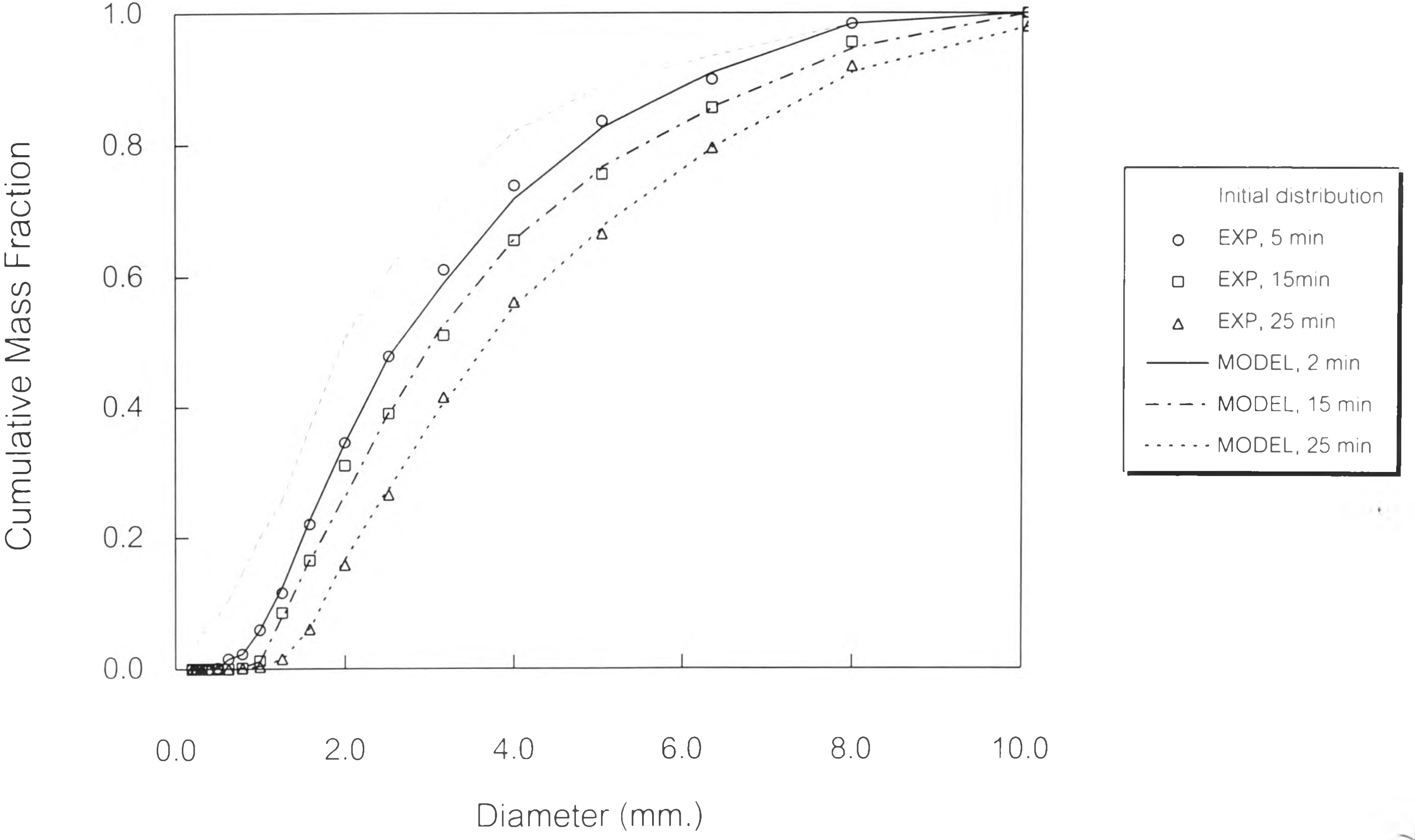

Figure 5.7 Simulation result VS experimental data (Adetayo,1993) for MAP at 6% moisture content

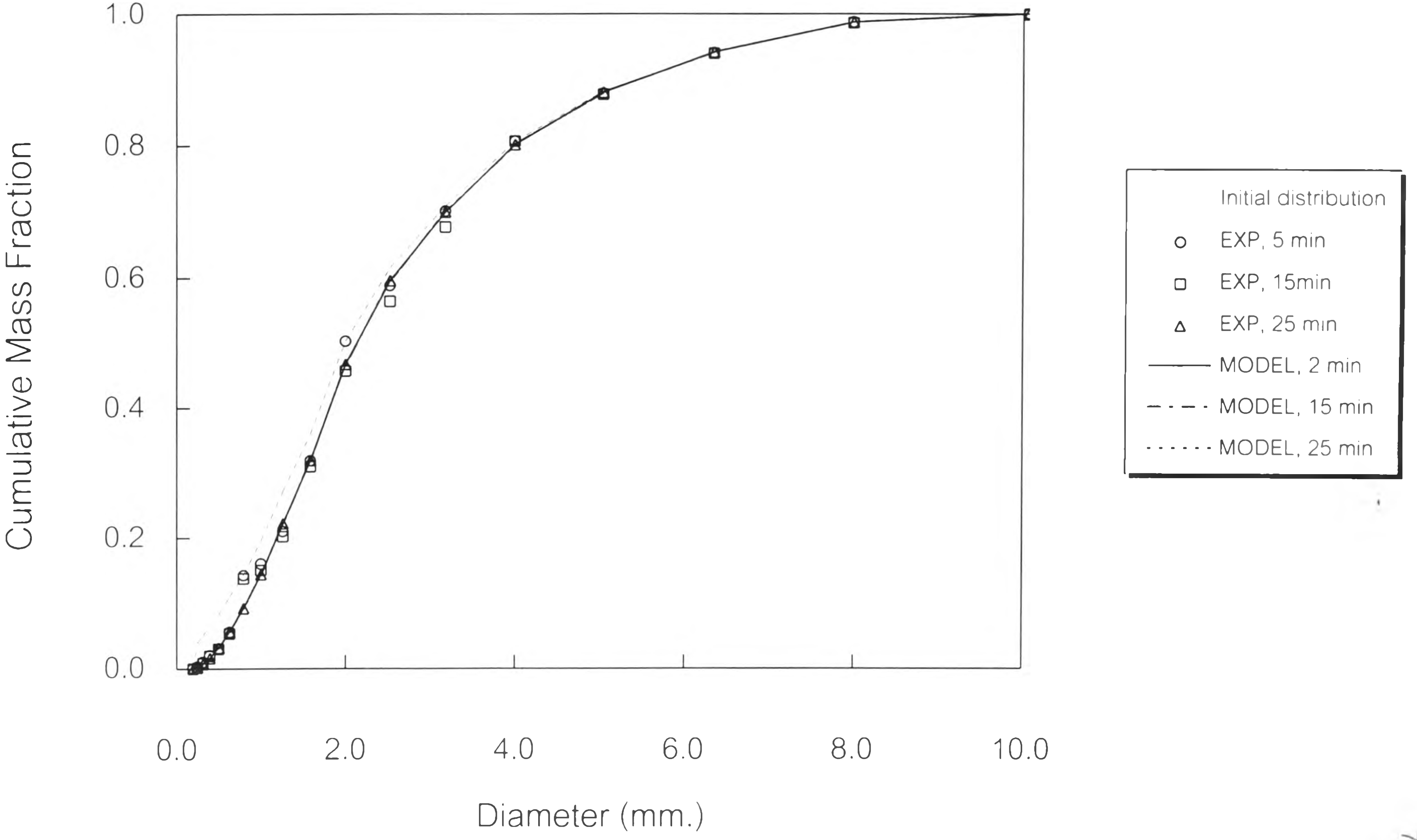

Figure 5.8 Simulation result VS experimental data (Adetayo,1993) for DAP at 2% moisture content

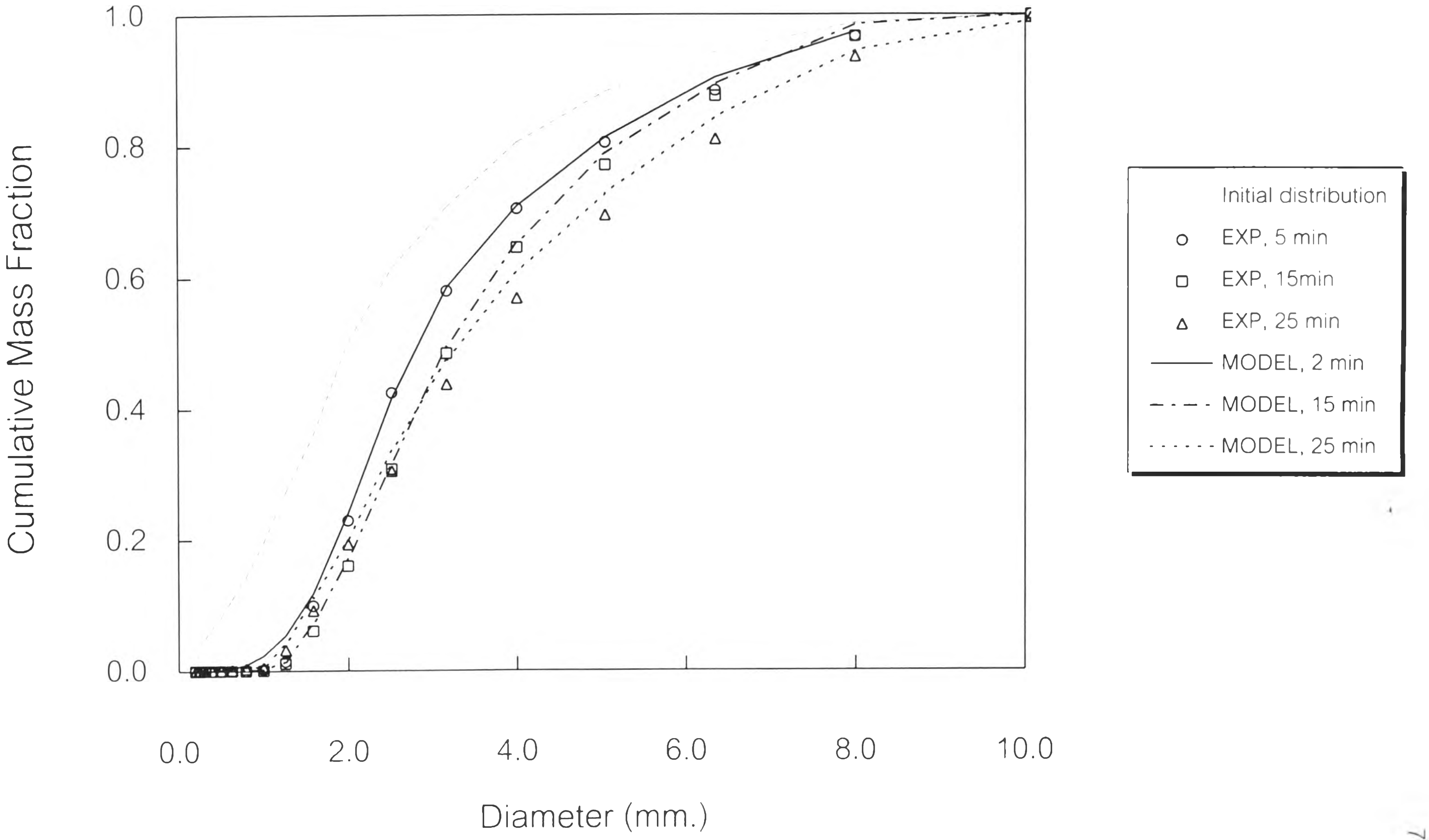

Figure 5.9 Simulation result VS experimental data (Adetayo,1993) for DAP at 4% moisture content

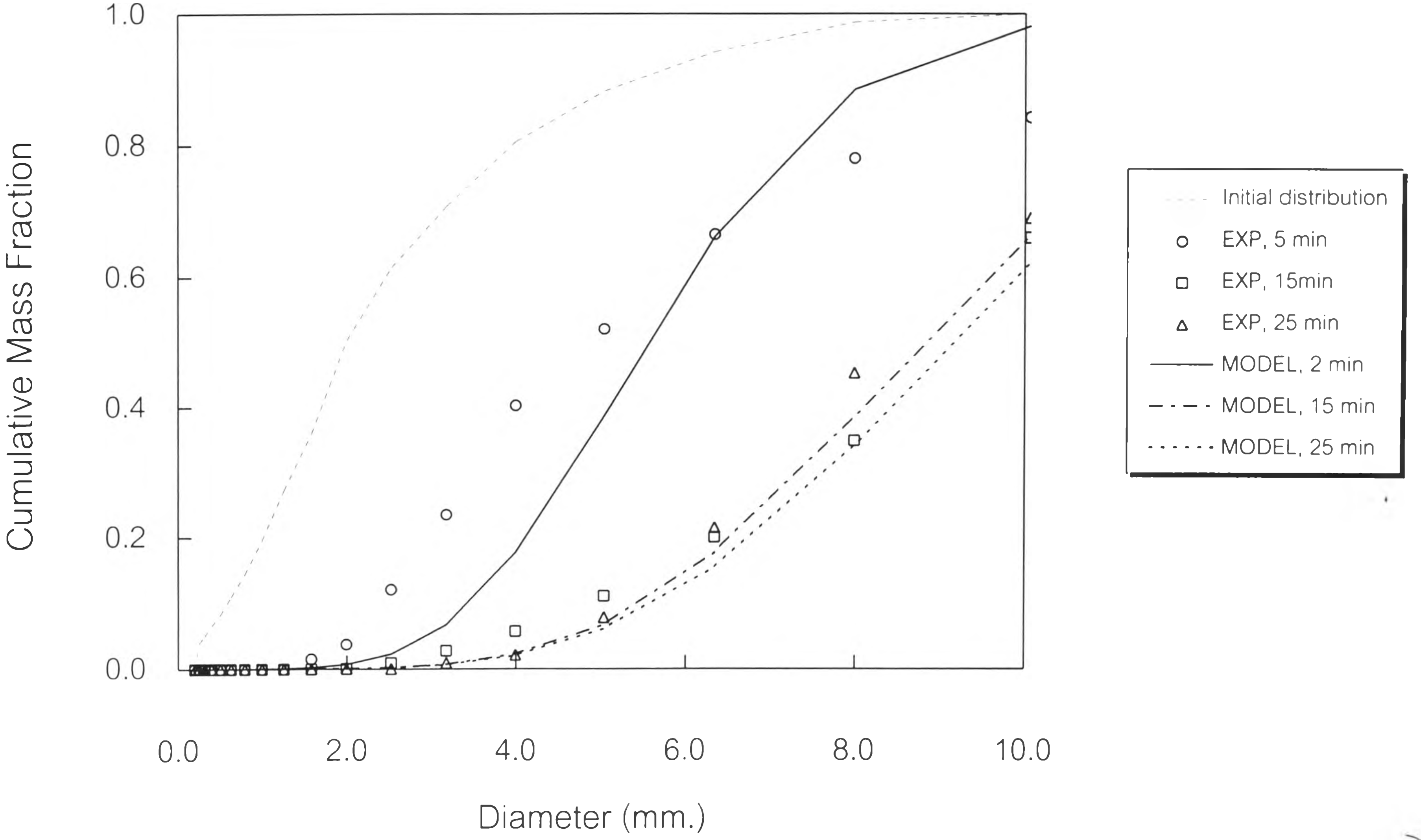

Figure 5.10 Simulation result VS experimental data (Adetayo,1993) for DAP at 6% moisture content

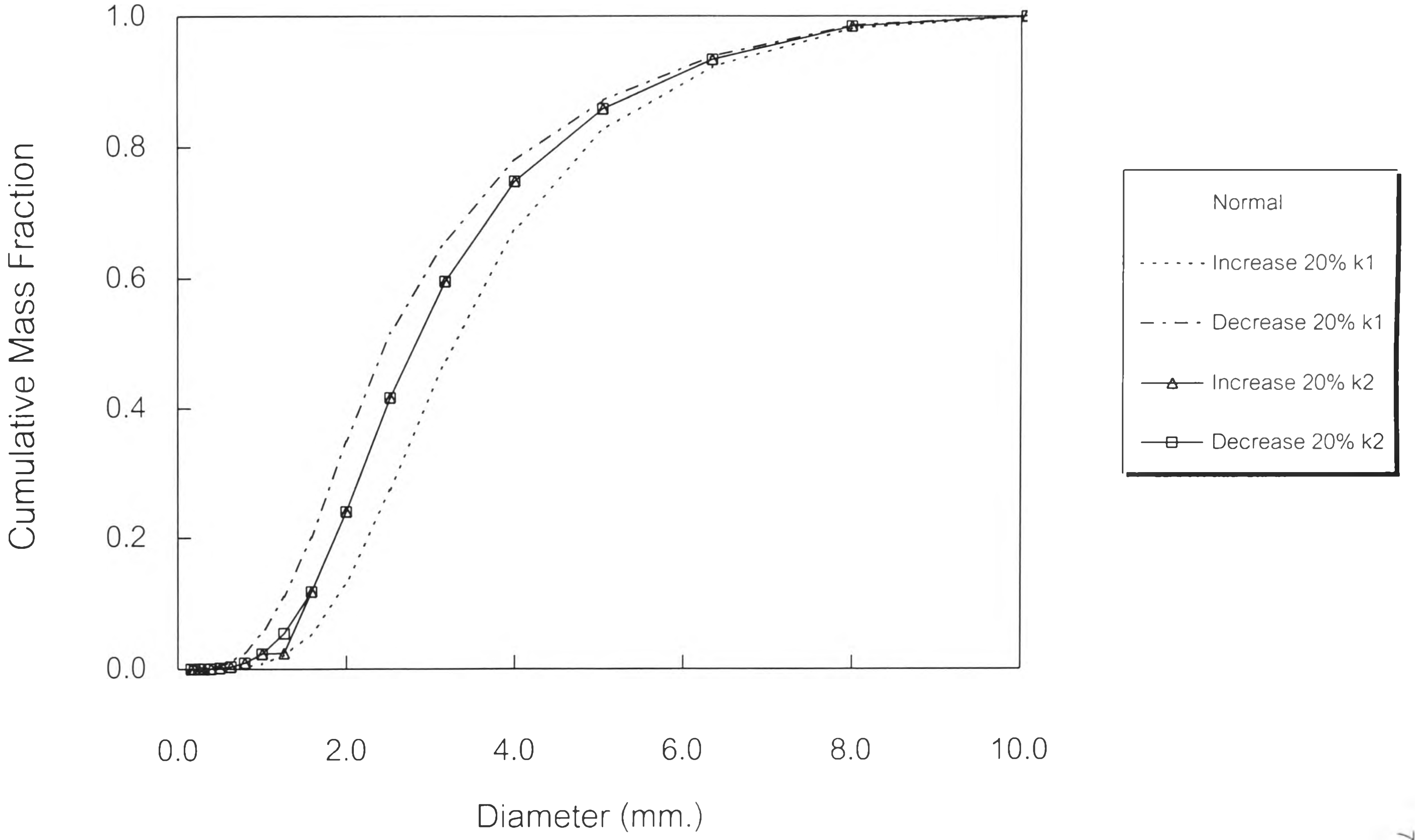

Figure 5.11 Sensitivity analysis of granulaion drum model.

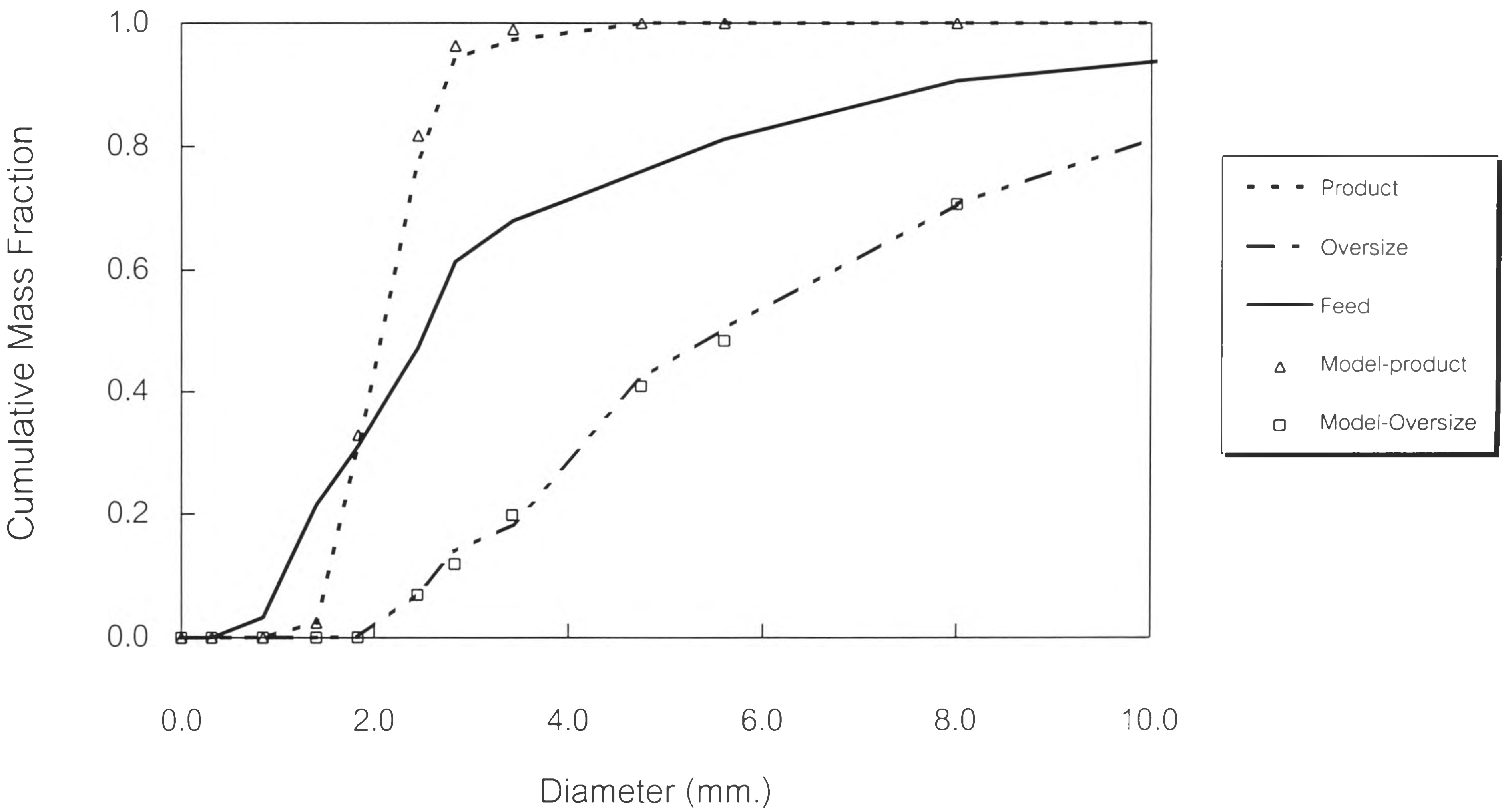

Figure 5.12 Comparision of the predicted and observed cumulative mass fraction for the screen.

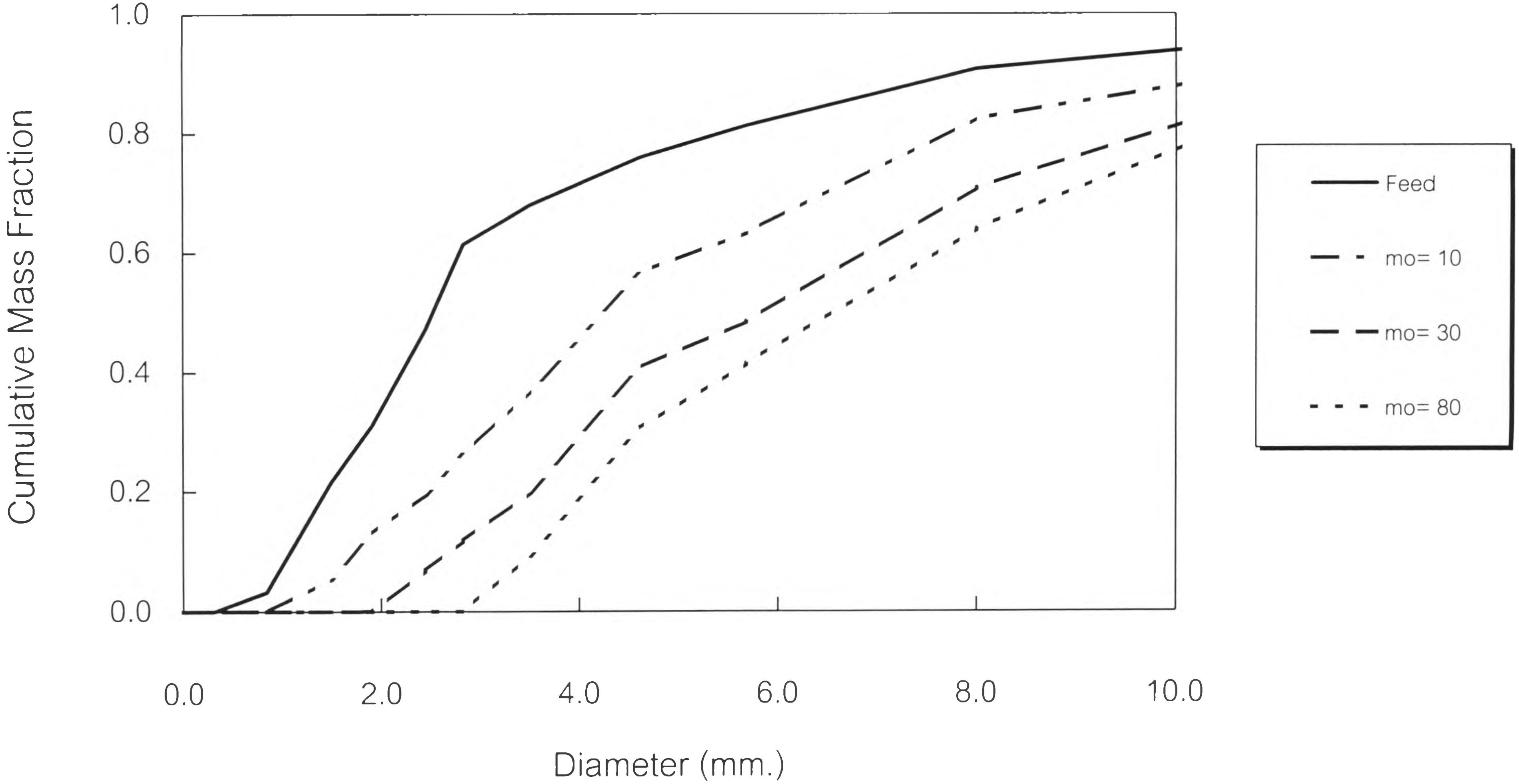

Figure 5.13 Sensitivity analysis of the screen model.

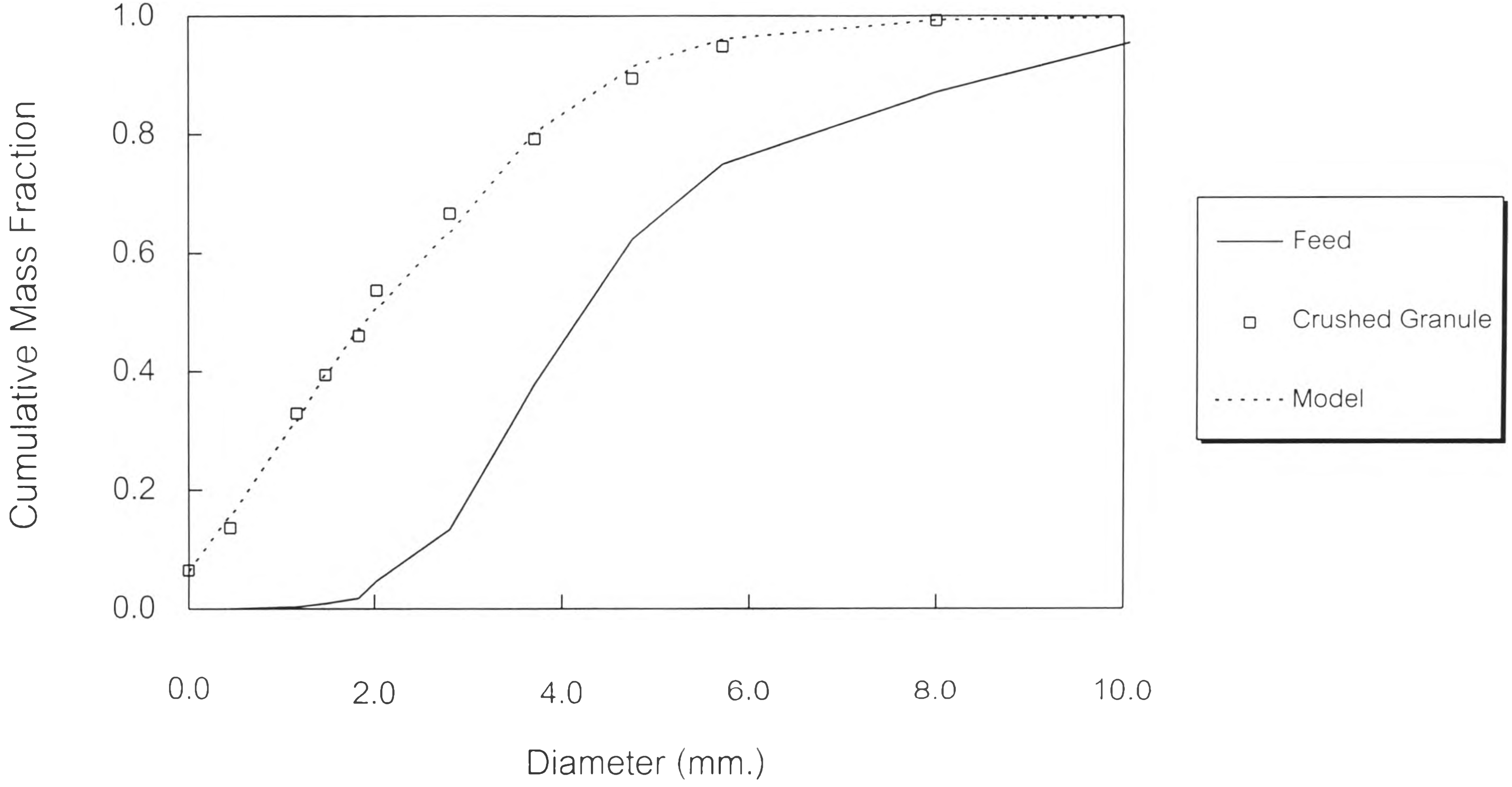

Figure 5.14 Comparison of the simulated and plant crushed granule data by Lister(1989).

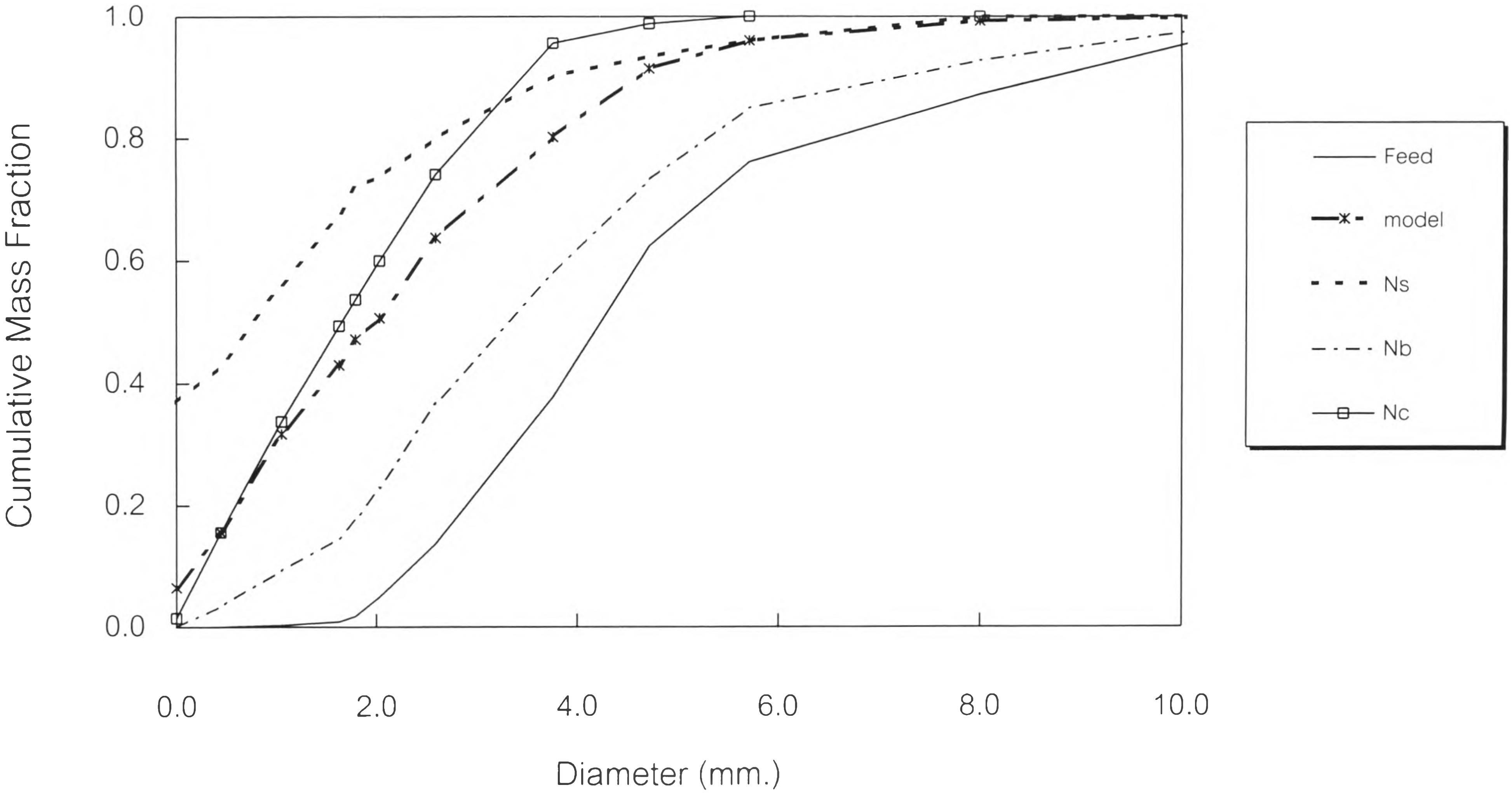

Figure 5.15 Sensitivity analysis of crusher model performance