CHAPTER I

INTRODUCTION

At present, compounded material is one of the fastest growing and increasingly important classes of engineering material in use. It is widely used in such fields as engineering plastics, fine ceramics, foods, medicines and so on. All plastic processors use compounding as one of the preferred methods of upgrading the properties of existing products. Typically, additives are selected to improve the properties of plastic (matrix), such as mechanical, thermal, electrical, optical, chemical and so on. Since generally a small amount of each additive is used, its uniform distribution in the matrix is crucial.

One way of investigating the dispersion of additives is to use computer simulation. A number of idealized mixing patterns (perfect random mixture and ordered mixture) are simulated using Monte-Carlo technique.

Traditionally the dispersion state of one or more additives is often evaluated qualitatively or semi-quantitatively by experiences or by visual and/or microscopic inspection. Occasionally statistical quantities indicative of the degree of mixing were used to evaluate the degree of homogeneity of the distribution of additives in the material. More powerful quantitative indices for evaluating the dispersion state are indispensable to the characterization and development of compounded material.

The fractal analysis method is a novel quantitative analytical method that uses the concept of fractal geometry to characterize a mixture or a system of complex morphology using the so-called fractal dimension. Several kinds of quantities have been used in the determination of the fractal dimension, such as area-based fractal dimension and count-based fractal dimension.

In addition to the area-based fractal dimension, Terashita et.al. (1993) proposed the use of the coordination number to evaluate the dispersion state of an ordered mixture.

Conventional methods [experience or statistical methods] to evaluate the dispersion state of additives provide only at the mesoscale (semi-macroscale) information. However, since the fractal analysis can and the coordination number does yield information down to the microscale level, they should provide quantitative indices that can differentiate whether the resulting mixture is simply a perfectly random mixture ,an ordered mixture or both, as well as distinguish between the effect of particle size and sample population size (additive concentration) on these quantitative indices.

1.1 Objectives of present study

In the present study, Monte-Carlo technique is used to simulate the idealized dispersion states of single and binary additives. Next several quantitative indices (area-based fractal dimension, count-based fractal dimension, degree of mixedness and coordination number) are used to evaluate the dispersion state of these additives. The main objectives of the present work are as follows :

1.1.1 To study and propose suitable quantitative indices for evaluating the degree of dispersion of single and binary additives in a matrix material and for differentiating between perfectly random mixture and ordered mixture and their combination.

1.1.2 To verify the usefulness of the proposed quantitative indices based computer simulations.

1.2 Scope of this study

1.2.1 Development of computer programs to simulate idealized mixtures of single and binary additives. The idealized dispersion states can be of uniform random type or normal random type. The idealized mixing patterns can be perfectly random or perfectly ordered or somewhere in between.

1.2.2 Application of various quantitative indices to the evaluation of the dispersion state and the mixing pattern.

1.2.3 Studying the effect of sample population size (additive concentration)on each of the quantitative indices.

1.2.4 Studying the effect of particle size on each of the quantitative indices.

1.2.5 Studying the effect of adhesion probability of particles B on particles A on each of the quantitative indices.

1.2.6 Comparing the pros and cons of each the quantitative indices.

1.2.7 Discussion and conclusion.