CHAPTER IV

SIMULATION PROCEDURE

In modeling natural phenomena, two distinctive approaches are available; deterministic and stochastic. Deterministic models are those in which each variable and parameter can be assigned a definite number, or a series of definite numbers, for any given set of conditions. On the other hand, for stochastic or random models, uncertainty is inherent. The variables or parameters used to describe the structure of the elements (and the constraints) may not be precisely known. The former approach is less demanding computationally than the latter and could more frequently be solved analytically.

To represent random variables, a source of randomness is required. A random number generator and its appropriate use play significant roles in any simulation experiments involving a stochastic system. The random number generator in the present work is the subroutine in SPSS program and the proper initial random seed numbers are obtained from Beyer, W. H. (1976).

This chapter presents the preparation of input parameters required in running of the ISCST3 model as well as the methodology of Monte-Carlo simulation.

4.1 Preparation of Inputs and Parameters for the ISCST3 Model

Two basic types of data files are needed to run the ISCST3 model. They are (i) the runstream setup file and (ii) the hourly meteorological data file. The runstream setup file contains the selected modeling options, as well as source locations and parameter data, receptor locations, meteorological data file specifications, and output options. The hourly meteorological data file generally consists of the average wind speed, wind direction, ambient temperature, Pasquill-Gifford stability class, and mixing height. This section describes random input parameters preparations, which employed the well-established statistical package, SPSS, for probability density function analysis, as well as for random variables generation.

4.1.1 Meteorological Inputs

4.1.1.1 Wind Speed and Direction

To generate suitable wind speed and direction with uncertainty, firstly, both hourly average wind speed and wind direction data collected over the past 6 years (January 1995 - December 2000) at the local monitoring station of PCD in Saraburi Province were obtained. Secondly, the past wind speed and direction data at the same hours of the days were analyzed month by month to obtain the mean values of the wind speed and direction at each hour of the days in the month of interest. In addition, the probability distribution subroutine in SPSS program was used to find out a most suitable probability density function (PDF) for the wind speed and wind direction, respectively. Eventually, 50 independent sets of random hourly wind speed and direction for a whole year were generated according to those PDF with the use of the SPSS random generator subroutine.

4.1.1.2 Ambient Temperature

As in 4.1.1.1, past hourly ambient temperature records collected for the years 1995 - 2000 were obtained from PCD. Again the same statistical approach as in 4.1.1.1 was used to generate 50 independent annual sets of random hourly ambient temperature data for use in each Monte-Carlo simulation.

4.1.1.3 Mixing Height

To estimate hourly mixing height data from records collected at 3-hour intervals, this study applied the simple linear interpolation technique to historical synoptic mixing height records obtained from TMD for year 1993 – 2000 at the measuring stations in Bangkok. As in 4.1.1.1, the same statistical approach was used to generate 50 independent annual sets of random hourly mixing height records were generated for each Monte-Carlo simulation.

4.1.1.4 Atmospheric Stability Class

Atmospheric stability class was estimated by considering the wind speed at approximately ten meters above the ground in conjunction with the incoming solar radiation (insolation) in the day time or cloud cover at nighttime. To estimate the solar insolation based on the Pasquill-Gifford stability classification described in Chapter 3, three categories of solar insolation; strong, moderate, or slight insolation which directly depends on the angle of insolation (α), were adopted. The angle of insolation can be calculated by

$$\sin\alpha = \sin\phi \sin K_d + \cos\phi \cos K_d \cos H_A \tag{4.1}$$

with

$$H_A = \left(\frac{\pi}{12}\right)(\tau - E_m) - \lambda \tag{4.2}$$

$$E_m = 12.0 + 0.12357 \sin(D) - 0.004289 \cos(D)$$
$$+ 0.153809 \sin(2D) + 0.060783 \cos(2D) \tag{4.3}$$

$$D = (d-1)\left(\frac{360}{365.242}\right)\left(\frac{\pi}{180}\right) \tag{4.4}$$

$$K_d = \sin^{-1}\left[0.39784989 \sin\left(\frac{\pi\,\sigma_A}{180}\right)\right] \tag{4.5}$$

$$\sigma_A = 279.9348 + D\left(\frac{180}{\pi}\right) + 1.914827 \sin(D) \tag{4.6}$$

where:

ϕ is the latitude (radians) of the location

λ is the longitude (radians) of the location

d is the Julian day

τ is the time of day (hours GMT)

The information on the latitude and longitude of Saraburi Province as well as an example of calculation for estimating the solar insolation angle is shown in Appendix A.

For cloud cover data, the past 20-year cloudiness data collected from January 1981 to December 2000 was obtained from TMD. The missing hourly data of synoptic cloud cover was produced by linear interpolation technique. As in 4.1.1.1, the same statistical approach was used to generate 50 independent annual sets of cloudiness data, from which corresponding sets of atmospheric stability class were predicted by using the criteria shown in Table 3.1.

Each set of uncorrelated random hourly meteorological data such as the wind speed, wind direction, mixing height, cloudiness and ambient temperature were then auto-correlated using the exponential smoothing technique. One of the three values of the weighting parameter (α), 0.25, 0.5, and 0.75 was used to create the auto-correlated random hourly meteorological data from the above uncorrelated data sets and Equations (4.7) and (4.8)

$$F_{t+1} = \alpha X_t + (1-\alpha) F_t \quad ; t = 1,2,3,\ldots N \tag{4.7}$$

with

$$F_t = \alpha X_{t-1} + (1-\alpha) F_{t-1} \tag{4.8}$$

where:

X_t = data at time t ; t = 1,2,3,...N

α = weighting parameter

F_{t+1} = predicted data at time $t+1$

The most appropriate value of the weighting parameter was next determined by comparing the mean hourly values of the past meteorological data with the corresponding mean values calculated from 100 independent annual sets of each random hourly meteorological input generated according to its PDF.

4.1.2 Source Inventory

Strictly speaking, quarry, stockpiles, and stone crushing activity represent low-level or ground-level releases without plume rise, and should be considered as an area source. The ISCST3 code accepts only rectangular areas as area source and their angles of orientation must be specified relative to the north-south orientation. In this study, there were nearly 50 stone-processing plants in action but there were only limited information of each plant. Only the nominal production capacity is known, not to mention the precise plant layout or the actual hourly capacity. Consequently, the present study had no better alternative than to simplify the source inventory by adopting the point source option for each stone processing plant while modifying the physical stack parameters to be as consistent as possible with the source reality. The equivalent stack parameters are described in section 4.1.2.2.

4.1.2.1 Coordinate System of the Sources

The topography of the area where the stone-processing plants were situated was not flat terrain. Therefore, each of the 48 stone-crushing plant in the study area must be considered as an elevated point source. The actual coordinate and elevated height of each source were obtained from the survey data shown on the topographical map of Royal Thai Survey Department. Based on the average population density, which was less than 750 people/km^2, the interest area may be considered as rural area (U.S. EPA, 1995).

4.1.2.2 Equivalent Stack Parameters

The basic parameters required for a single point source in the ISCST3 model are (i) stack inside diameter, (ii) exit gas velocity, (iii) emission rate, (iv) effective stack height,(v) stack coordinates, and (vi) exit gas temperature.

Figures 4.1 (a) and (b) illustrate the dimensions of one of the surveyed stone-processing lines (Meechumna, P., et al., 1999) where the primary crushing process is highlighted. The approximate dimensions of its floor area were 16.5 m x 8.0 m. Therefore, the rectangular area housing the primary crusher was 132 m^2. In this study, the equivalent stack height or release height was assumed to be about 10 meter above the ground, or about a half of typical height of the primary crushing facility (20 m). In fact, the heights of the various stockpiles, where the final stone products are dumped and stored, temporarily were about 10 meter. As for the equivalent stack inside diameter, it was estimated from the floor area of the primary crushing facility. It was further assumed that the main characteristics of all 48 stone-processing plants in this study area may be represented by some average values. Based on this assumption, the equivalent stack inside diameter of 12.96 meter was estimated.

As for the equivalent exit gas temperature, it was assumed to be the same as the ambient temperature because no plume rise existed during the crushing process. According to the survey data of Meechumna, P., et al. (1999), the exit velocity of fugitive dust from the primary jaw crusher, which was taken as the equivalent gas exit velocity of a point source, is 0.1 m/s. Table 4.1 shows a summary of the equivalent stack parameters used in the present study for the typical stone-processing plant.

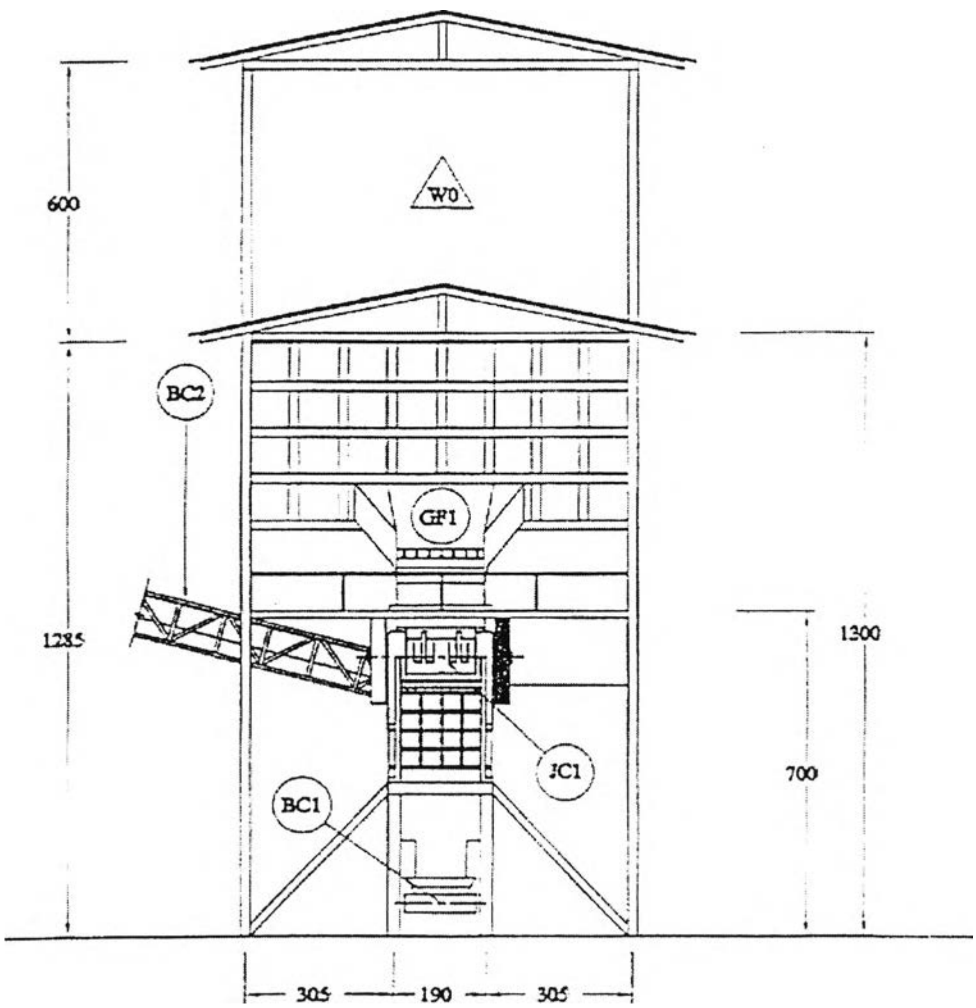

Figure 4.1 (a) The front view of the primary crushing facility of an actual stone processing plant

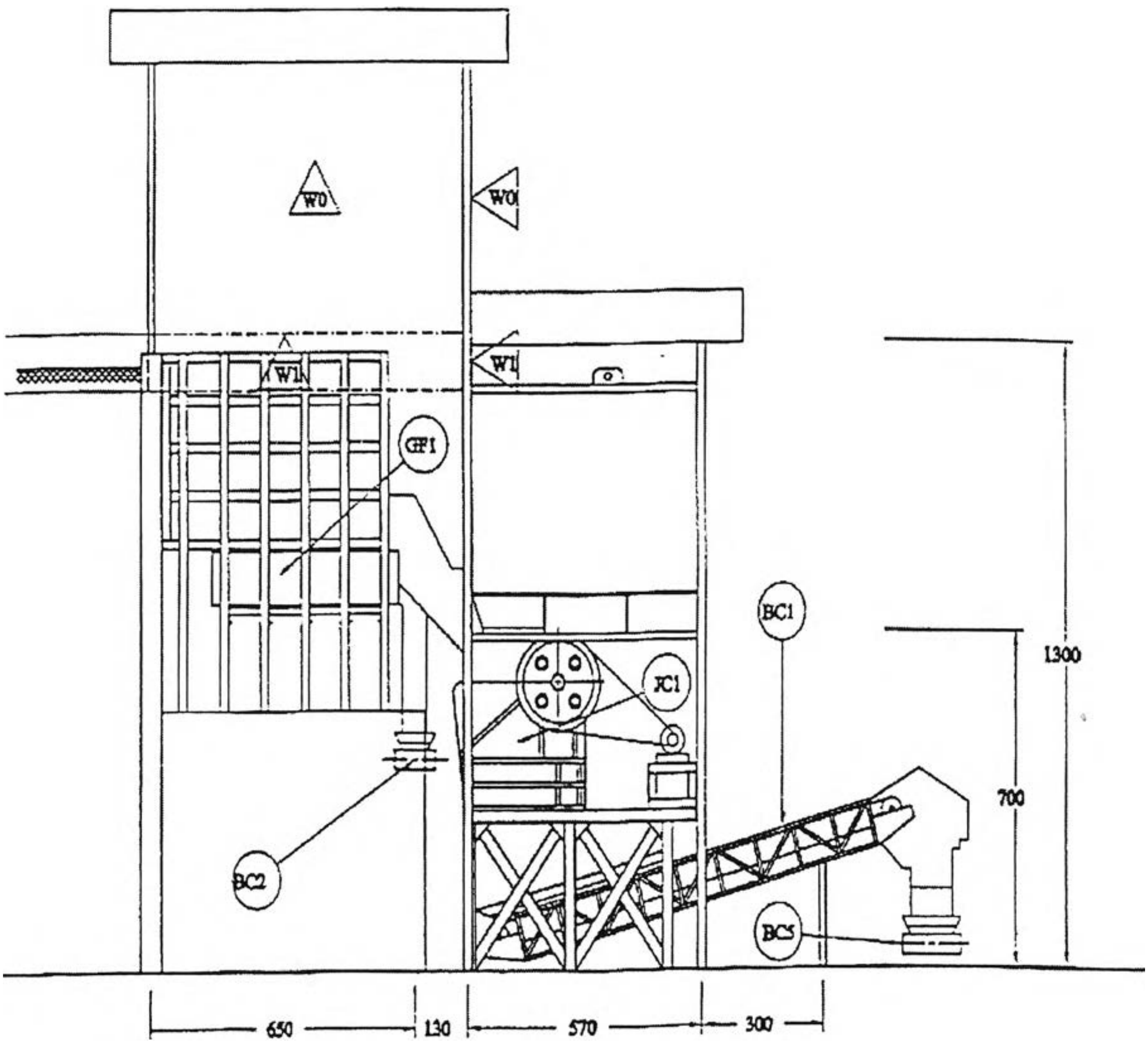

Figure 4.1 (b) The side view of the primary crushing facility of an actual stone processing plant

Table 4.1 Summary of the equivalent stack parameters for a typical stone-processing plant

Equivalent Stack Height (m)	10
Equivalent Stack Diameter (m)	12.96
Equivalent Exit Velocity (m /s)	0.1
Equivalent Exit Temperature (K)	303

4.1.2.3 Emission Rate of Fugitive Dust

Because of lack of reliable data and actual measurements, the emission rate of each type of source was estimated by using the available Emission Factor. The various emission factors for PM_{10} used in this work were taken from the U.S. EPA AP-42 document. As displayed in Table 4.2, the emission factors for PM_{10} were used for the case without any dust control system. An example of the calculation of the emission rate of a typical stone-processing plant in the study area is shown in Appendix B.

Table 4.2 Uncontrolled emission factor for stone processing operations (kg dust generated per ton of processing capacity) (U.S. EPA, 1992)

Sources	PM_{10} (kg/ton)
Truck Unloading	0.00008
Primary Crushing	0.00017
Secondary Crushing	0.00045
Tertiary Crushing	0.0012
Screening	0.0076
Fine Screening	0.036
Conveyor Transfer	0.00072
Truck Loading	0.00005

Note : There are approximately 10 conveyor transfer points in a typical stone processing plant

4.1.3 Coordinates of Receptor Locations

Similar to the coordinate system used to represent the source locations, the actual coordinates and elevated height of each receptor were obtained from the survey data shown on the map of Royal Thai Survey Department. As for the receptor locations, the present study used the Cartesian grid-receptor network option in ISCST3 with a total of 265 grid receptors as well as 5 discrete receptors that represent the 5 monitoring stations. The receptor heights were chosen to be 2 meters above the ground level.

4.1.4 Deposition Parameters

As mentioned in the previous chapter, the ISCST code has a dry deposition algorithm and a wet deposition algorithm. The selected dry deposition algorithm requires additional meteorological data, such as the Monin-Obukhov length, surface roughness and friction velocity. In addition, the characteristics of the particulate matter such as mass mean diameter, mass fraction, and density, are required.

4.1.4.1 Fugitive Dust Characteristics

The PM_{10} characteristics required in running the selected option were size distribution and true density. The size distribution was obtained using a cascade impactor to measure the size distribution around some dust generating points such as over the primary crusher and the fine sifter. Table 4.3 shows an example of the size distribution of fugitive dust generated in a stone processing plant in Nah Pra Laan area, which was reported by Meechumna, P., et al. (1999) and used in the present simulation. The typical density of stone dust was 2600 kg/m^3.

Table 4.3 Mass fraction versus mass mean diameter of particles used in the simulation.

Size Range (μm)	Mean Diameter (μm)	Mass Fraction
< 0.43	0.43	0.00437
0.43 – 0.65	0.54	0.00044
0.65 – 1.1	0.88	0.00429
1.1 – 2.1	1.60	0.00216
2.1 – 3.3	2.70	0.00521
3.3 – 4.7	4.00	0.0167
4.7 – 7.0	5.85	0.0436
7.0 – 11.0	9.00	0.05152
> 11.0	11.00	0.87171

4.1.4.2 Surface Roughness

Based on the type of land use in the study area as described in Table 3.2, Chapter 3, it was reasonable to assume that the study area corresponds to the suburban area. Therefore, this study used a surface roughness (z_o) value equal to 60 centimeter.

4.1.4.3 Monin-Obukhov Length

The Monin-Obukhov length (L) is a parameter that characterizes the atmospheric stability of the surface layer and was calculated from suitable ground-level measurements. Golder (1972) proposed an semiempirical relation between L, Turner stability class and surface roughness length (z_o) as shown in Figure 4.2. The figure was used to estimate the value of L required to run the selected option of dry deposition.

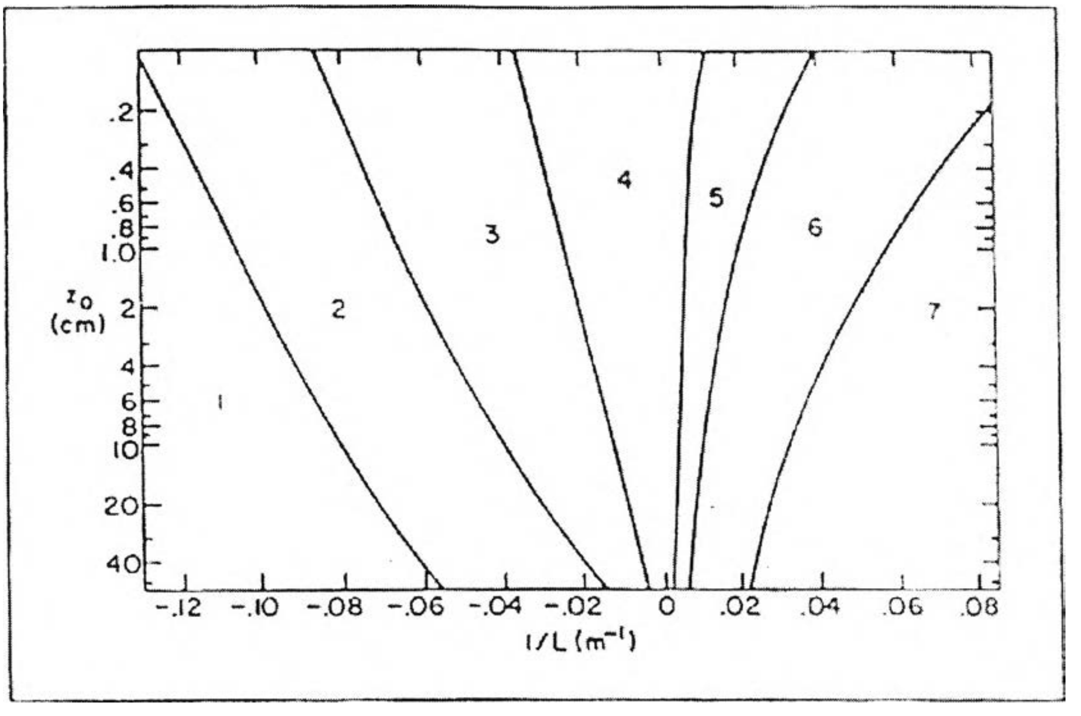

Figure 4.2 Semiempirical relation between L, Turner stability class, and z_o

4.1.4.4 Friction Velocity

The friction velocity (u_*) which is caused by objects standing on the ground surface can be calculated under different atmospheric stability classifications as follows (Schnelle, K. B., Jr., and Dey, P. R. (1999)):

$$u_* = \frac{k_a \bar{u}}{\ln\left(\frac{z}{z_o}\right) - \psi_m\left(\frac{z}{L}\right)} \tag{4.9}$$

Stable Condition

$$\psi_m = -5\left(\frac{z}{L}\right) \tag{4.10}$$

Unstable Condition

$$\psi_m = 2\ln\left[\frac{1+x}{2}\right] + \ln\left[\frac{1+x^2}{2}\right] - 2\arctan(x) + \frac{\pi}{2} \tag{4.11}$$

with $$x = \left(1 - 16\frac{z}{L}\right)^{1/4}$$

Neutral Condition

$$u_* = \frac{k_a \bar{u}}{\ln\left(\frac{z}{z_o}\right)} \tag{4.12}$$

where:

u_* = friction velocity (m/s)

k_a = von Karman constant (= 0.40)

$\bar{u}$ = mean wind speed measured at height z (m)

z_o = surface roughness length (m)

L = Monin-Obukhov length (m)

ψ_m = Monin-Obukhov similarity function for normalized velocity

4.2 Methodology of Monte-Carlo Simulation

Monte Carlo simulations are carried out for different meteorological conditions or emission rates with uncertainty in order to elucidate the stochastic nature of the PM_{10} concentration. The suitable value of the weighting parameter is described in section 4.2.1.4. A compromise of 50 Monte-Carlo simulations of each case study is adopted.

A Monte-Carlo simulation essentially consists of solving a set of model equations repetitively over the same time period (one year in this study) but with appropriate different instantaneous values for the random inputs and/or random parameters, so that data for sample statistics, such as means, standard deviations and frequency distributions, of any of the outputs of interest can be collected and analyzed.

Tanthapanichakoon (1978) briefly described the general procedure for a Monte-Carlo simulation as follows:

1) Develop a realistic mathematical model for the actual process
2) Determine the stochastic nature of the process inputs and/or parameters. If past time records for the inputs are available, their expected values, standard deviations, statistical correlations, and types of distributions may be postulated and tested by the use of null hypotheses. Furthermore, if corresponding records for the outputs are available, the stochastic nature of the process parameters may be inferred by the use of appropriate parameter estimation technique.
3) If possible, carry out a sensitivity analysis to determine the relative significance of each input and parameter. This will help save time and energy because it tells the investigator which inputs and/or parameters

need not to be treated as random variables and how much effort should be expended to study the stochastic nature of a particular random input or parameter.

4) Determine what initial conditions to use. Depending on the objective of an investigation, the initial values might remain fixed throughout the whole Monte-Carlo simulation, or be allowed to change randomly according to some probabilistic law.
5) Generate appropriate values to represent the value of the random inputs and/or parameters at time t.
6) With the appropriate value for each random input or parameter, solve the model equations for one time step, using a suitable numerical technique. For certain random parameters, their value might remain constant during one entire time record.
7) Record the values of those outputs of interest at predetermined sampling times.
8) Repeat Steps (4) through (7) to generate enough time records so that the desired sample size be attained.
9) Compute sample statistics of interest, such as means, variances and frequency distributions, from the values recorded in Step (6). These statistics will serve as estimates of the ensemble statistics at a particular sampling time.
10) Finally, hypotheses concerning the stochastic nature of the output can be postulated and tested by the use of appropriate statistical tests.

In the present investigation, the random inputs of interest were: wind speed, wind direction, ambient temperature, mixing height, and cloudiness. No random parameters were involved, however.