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Non-deterministic Analysis of A Liquid Polymeric-film Drying Process*

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Abstract

In this study we employed the Monte Carlo/Latin Hypercube sampling technique to generate input parameters for a liquid polymeric-film drying model with prescribed uncertainty distributions. The one-dimensional drying model employed in this study was that developed by Cairncross et al.[1] We found that the non-deterministic analysis with Monte Carlo/ Latin Hypercube sampling provides a useful tool for characterizing the two responses (residual solvent volume and the maximum solvent partial vapor pressure) of a liquid polymeric-film drying process. More precisely, we found that the non-deterministic analysis via Monte Carlo/Latin Hypercube sampling not only provides estimates of statistical variations of the response variables but also yields more realistic estimates of mean values, which can differ significantly from those calculated using deterministic simulation. For input-parameter uncertainties in the range from two to ten percent of their respective means, variations of response variables were found to be comparable to the mean values.

Introduction

In recent years advances in computer hardware and numerical analysis have made it possible to model, theoretically, many complex engineering processes such as liquid polymeric-film drying; and systematic 'numerical experiments' can be carried out on a computer for the purpose of process design and optimization before any testing is conducted on an actual apparatus. These process simulations are often done in a deterministic fashion, i.e., process conditions and physical properties involved are usually taken to be precisely known. In real-world processes, however, some levels of uncertainties are always present. At issue is how to characterize the responses of processes such as liquid polymeric-film drying given uncertainties in both process conditions and physical properties.

After being freshly coated onto a substrate support, a liquid polymeric coating is usually solidified by hot-air convection drying. This is an important manufacturing process for producing imaging/information-recording products such as photographic and xerographic films, and video and audio tapes. The heat and mass transfer involved in such a drying process can be predicted via numerical analysis as demonstrated by Cairncross et al.[1] However, uncertainties abound in both physical properties and process conditions such as solvent-diffusion coefficient, heat and mass transfer coefficients, and oven temperature. Two relevant response variables that are of practical interest are the residual solvent volume and the maximum solvent partial vapor pressure. The former determines the extent of dryness of the coated film after drying and the latter controls bubble formation in the coated film. To prevent the coated film from sticking on the conveying roll surfaces, the residual solvent volume must be below a certain level when the dried film exits the oven. Also, the maximum solvent partial vapor pressure must be less than the oven ambient pressure (normally 1 atm) in order to avoid bubble formation, which can give rise to various coating defects.

In the present study we employed the one-dimensional computer model developed by Cairncross[2] in computing the two response variables of residual solvent volume at the oven exit and maximum solvent partial vapor pressure inside the oven. In this model, there are twelve parameters associated with estimation of the binary mutual *diffusion coefficient*. In addition, there are another nine input parameters associated with physical/transport properties (e.g., *heat and mass transfer coefficients*) and process conditions (e.g., *oven temperature*). In all, there are 21 input parameters required for computing the two response variables chosen in this study. In the present study, only the following three of the 21 input parameters were assigned uncertainty distributions (i.e.vary statistically within prescribed bounds): the *pre-exponential factor* of the diffusion coefficient (D_{01}), the *ratio of solvent and polymer jumping units* (ξ), and the *oven temperature* (T^{∞}). The first two are key parameters in estimating the diffusion coefficient. Effects of uncertainties of the above three input parameters on the two response variables were examined using non-deterministic analysis via Monte Carlo/Latin Hypercube sampling.

The Deterministic Drying Model

Details of the deterministic one-dimensional drying model have been documented elsewhere[1,2]. Briefly, the heat and mass transfer are described by transient one-dimensional convection-diffusion equations of energy and mass conservations. Because the liquid film is thin, lateral variations in composition, temperature and film thickness are

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calculated with 10,000 runs using LHS) using LHS whereas more than 2,000 runs are required to achieve the same level of convergence using simple sampling. For the mean value of the maximum solvent partial vapor pressure, only 20 runs are needed to approximate its converged value to within 1% using LHS whereas more than 300 runs are required using simple sampling. For the standard deviation of residual solvent volume, it takes about 400 runs to obtain the 99% convergence (i.e., reduce the error to within 1%) using LHS whereas more than 2,000 runs are necessary using simple sampling. For the standard deviation of the maximum solvent partial vapor pressure, the required number of runs to reduce the estimate error to within 1% are about 700 and more than 4,000, respectively for using LHS and simple sampling.

In short, for the mean value estimate, LHS outperforms simple sampling by more than an order of magnitude. For the standard-deviation estimate, the LHS results in run-number reduction by a factor of five or more when compared with the simple sampling. For response calculations that require intensive CPU time, reduction in the number of runs needed to achieve the desired level of convergence translates into huge savings in computational costs.

It is informative to compare predictions of the two response variables computed from deterministic simulations with that determined from nondeterministic analysis. Using the respective mean values as input to the deterministic model, the residual solvent volume (per unit area of drying surface) was calculated to be 120.85 *µm* and the maximum solvent partial pressure to be 1.0197 *atm*. With the distribution functions and degrees of scattering for the three input parameters chosen here, the nondeterministic model (with LHS) yielded an estimate of 658.73 *µm* as the expected or mean value for the residual solvent volume and the corresponding standard deviation of 825.22 *µm*; for the maximum solvent partial vapor pressure, the estimates were 1.0523 *atm* and 0.2705 *atm*, respectively for the mean value and the standard deviation. In short, the mean value of maximum solvent partial vapor pressure estimated from nondeterministic analysis differs from that calculated from the deterministic model by a mere 3.1% but the corresponding standard deviation was found to be quite significant (24.4% of the mean value). As for the residual solvent volume, the mean value estimated from the nondeterministic model is 5.45 times of that calculated from the deterministic model; moreover, the estimated standard deviation is actually greater than the mean value. This implies that the chosen degrees of scattering for the three input parameters are too high (particularly for the oven temperature) and the estimates are not reliable. In other words, the standard deviations for the three input parameters need to be smaller in order to obtain realistic estimates for the residual solvent volume. In practice, to obtain lower degrees of scattering of the input-parameter data certainly demands better measurement techniques and more precise instruments. In any case, as demonstrated here, nondeterministic analysis provides a useful tool for determining the statistical variations of response variables in manufacturing processes like liquid polymeric-film drying.

Effect of Uncertainty-distribution-function Types

To generate input parameters using either simple sampling or LHS, we must specify the types of uncertainty distributions. It is certainly ideal if we have complete descriptions of the uncertainty distributions (e.g., via proper measurements). But more often than not, only very limited information regarding the uncertainty distributions is known. In this case, how an analyst chooses an uncertainty distribution becomes a very relevant question. If only the lower and upper bounds of a distribution are known, one may want to start with the *uniform* distribution. If the mean or expected value is also available, one can use the *maximum entropy* (i.e. a truncated exponential) distribution. When both mean value and standard deviation are known, one can certainly employ the *normal distribution*, which provides a more complete description over either the uniform or maximum entropy distribution.

To examine effects of distribution types on statistics of response variables, we computed predictions of mean value and standard deviation for the residual solvent volume and the maximum solvent partial vapor pressure, using *uniform*, *maximum entropy*, and *bounded normal distributions* with various standard deviations, respectively. The results are plotted in Figures 3 & 4. In all cases, three input parameters, the pre-exponential factor (D_{01}), the ratio of solvent and polymer jumping units (ξ), and the oven temperature (T^{∞}), were varied statistically and assigned the same type of distribution function. Here, the lower bound for D_{01} was set to $4.338\text{x}10^{-8}$ m^2/s and the upper bound to $5.302\text{x}10^{-8}$ m^2/s; for ξ, the lower bound was 0.765 and the upper bound 0.935; T^{∞} has a lower bound of 114 °C and an upper bound of 118 °C. For the maximum entropy distribution, mean values of $4.82\text{x}10^{-8}$ m^2/s, 0.85 and 116 °C were specified, respectively for D_{01}, ξ, and T^{∞}; and the lower and upper bounds were set identically as that for the case of uniform distribution. In the case of bounded normal distribution, the lower and upper bounds and the mean value were the same as that for the case of maximum entropy distribution; four different sets of standard deviations were specified: in the basecase set, standard deviations for D_{01}, ξ, and T^{∞} were set to $0.241\text{x}10^{-8}$ m^2/s, 0.0425 and 1.16 °C, respectively; in the second set, each standard deviation was doubled, e.g. D_{01} now has a standard deviation of $0.482\text{x}10^{-8}$ m^2/s; in the third set, each standard deviation was tripled, e.g. D_{01} now has a standard deviation of $0.723\text{x}10^{-8}$ m^2/s; in the fourth set, each standard deviation was quadrupled, e.g. D_{01} now has a standard deviation of $0.964\text{x}10^{-8}$ m^2/s.

As shown in Figures 3 & 4, statistics of the two response variables calculated using the *uniform* and *maximum entropy* distributions are very close, to within five significant figures (it should be pointed that both the uniform and maximum entropy distribution functions yield spurious estimates, i.e., spikes, at run numbers of 300 and 4000, respectively; what causes this is not clear to the authors at this point). The bounded normal distribution with small standard deviations yields statistics close to that predicted with both the uniform and maximum entropy distributions. As the input data become more scattered (i.e. the standard deviation varies but the mean value is kept the same), however, discrepancies rise rapidly. In Figure 5, the mean values of residual solvent volume and maximum solvent partial pressure estimated from the <u>nondeterministic</u> model with different input distribution functions are further compared with that calculated from the <u>deterministic</u> model. For residual solvent volume, estimates obtained using the uniform and maximum entropy distribution functions are very close, and they differ only slightly from that using the bounded normal distribution function with small standard deviations. But the discrepancy rises rapidly as input data become more scattered. The same is true for maximum solvent partial vapor pressure though the effects are much smaller.

In short, with the small uncertainties as specified here for the three input parameters, the effect on the predicted residual solvent volume is significant but the effect on the maximum solvent partial vapor pressure is small. For the residual solvent volume, its calculated standard deviation is nearly 30% of its predicted mean value. For the maximum solvent partial vapor pressure, its standard deviation was estimated to be more than 3%.

Again, it should be noted that the uncertainty levels chosen in this sub-section are less than that specified in the previous sub-section on the effects of number of observations; moreover, <u>unbounded</u> normal and lognormal distributions were used in that previous sub-section whereas <u>bounded</u> distribution functions were employed in this sub-section.

Summary and Conclusions

It was demonstrated in the present study that the nondeterministic analysis with Monte Carlo/Latin Hypercube sampling provides a useful tool for characterizing the two responses (residual solvent volume and the maximum solvent partial vapor pressure) of a liquid polymeric-film drying process subject to uncertainties in the three input parameters: pre-exponential factor of the diffusivity, the ratio of solvent and polymer jumping units, and the oven temperature. By employing the Latin Hypercube Sampling technique, we were able to reduce the number of observations or runs required to achieve the same level of convergence for the response variables by as much as an order of magnitude when compared with using simple sampling. Also, the uncertainty-distribution types were shown to affect variations of response variables, which implies that accurate characterization of uncertainty distributions of the input parameters are necessary in obtaining objective assessment of the statistical variations of response variables of the liquid polymeric-film drying process. We found that the non-deterministic analysis via Monte Carlo/Latin Hypercube sampling not only provides estimates of statistical variations of the response variables but also yields more realistic estimates of mean values, which can differ significantly from that calculated using deterministic simulation. For input-parameter uncertainties in the range from two to ten percent of their respective means, variations of response variables were found to be comparable to the mean values.

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Table 1. Input Parameters in the Base Case

D_{01}	4.82×10^{-8}	m^2/s
ξ	0.82	
χ	0.393	
E/R	0	^oK
$V^0{}_1$	1.154×10^{-3}	m^3/kg
$V^0{}_2$	0.970×10^{-3}	m^3/kg
$V^*{}_1$	0.917×10^{-3}	m^3/kg
$V^*{}_2$	0.728×10^{-3}	m^3/kg
K_{11}/γ	1.45×10^{-6}	$m^3/kg/^oK$
$K_{12} - T_{g1}$	-86.32	^oK
K_{12}/γ	0.433×10^{-6}	$m^3/kg/^oK$
$K_{22} - T_{g2}$	-258.2	^oK
T^{∞}	116	^oC
C_p	1254	$J/kg/^oC$
ΔH_v	8.8×10^4	J/kg
κ	0.326	$kg\ m/s^3/^oK$
$P^0{}_v$	0	atm
h_{BS}	3.96×10^5	$kg/s^3/^oK$
h_{FS}	3.96×10^5	$kg/s^3/^oK$
k_G	0.132	m/s
h_0	250	μm
t	30	s

Note: the first 12 parameters are associated with estimation of diffusion coefficient. C_p is heat capacity, ΔH_v heat of vaporization, κ thermal conductivity, $P^0{}_v$ oven ambient partial vapor pressure, h_{BS} heat transfer coefficient at the substrate surface, h_{FS} heat transfer coefficient at the drying surface, k_G mass transfer coefficient, h_0 initial wet liquid polymeric-film thickness, and t drying time. In the present study, the three input parameters that were varied statistically within prescribed bounds are: pre-exponential factor, D_{01}; the ratio of solvent and polymer jumping units, ξ; and oven temperature, T^{∞}.

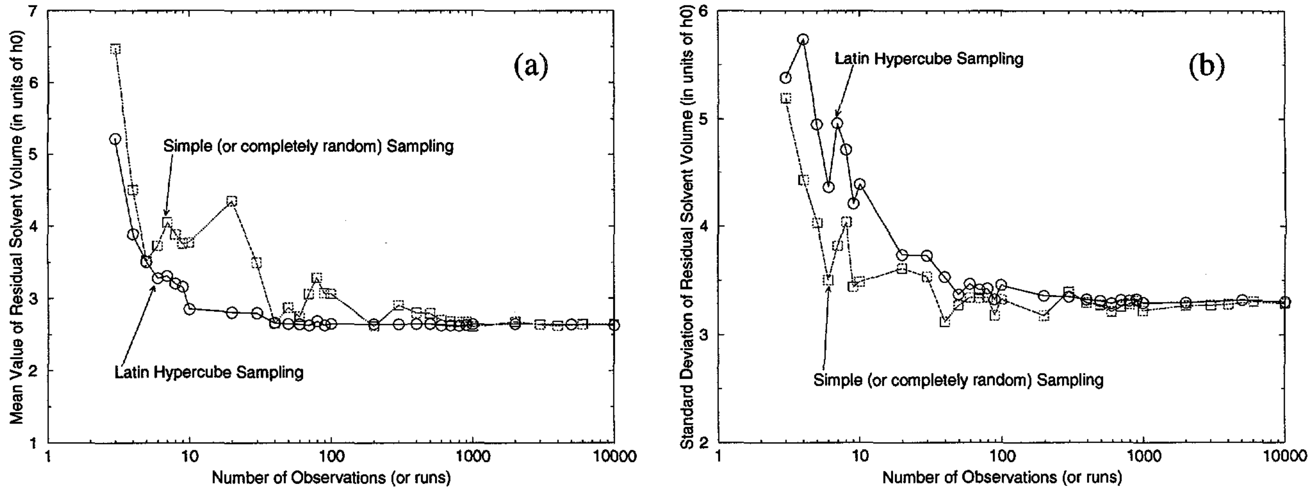

Figure 1. Effect of number of observations on convergence of predicted residual solvent volume (with unbounded lognormal distribution): (a) mean value; (b) standard deviation.

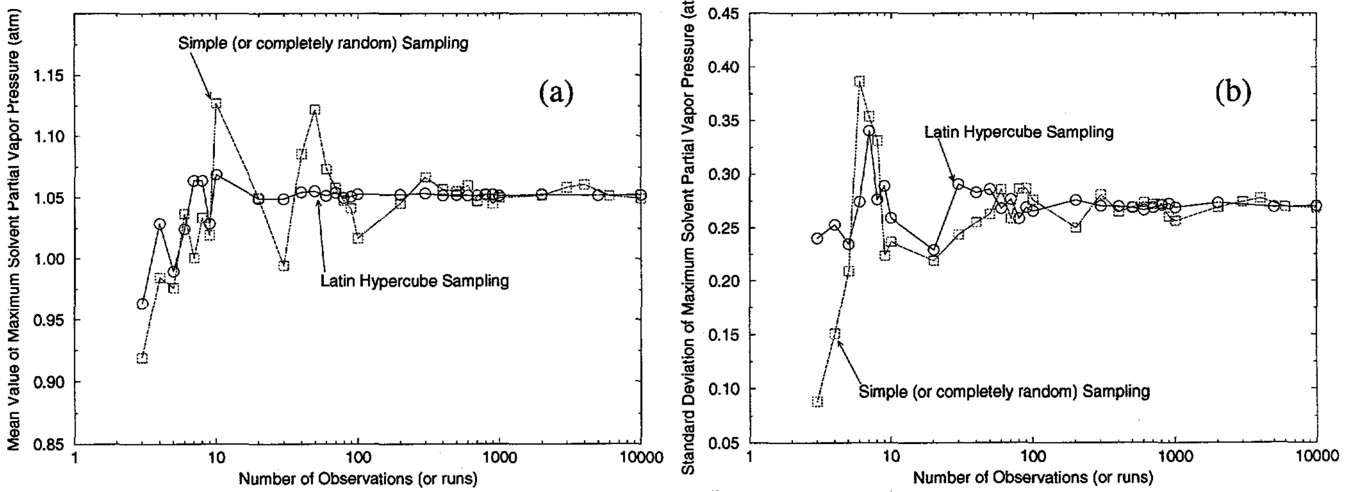

Figure 2. Effect of number of observations on convergence of predicted maximum solvent partial vapor pressure (with unbounded lognormal distribution): (a) mean value; (b) standard deviation.

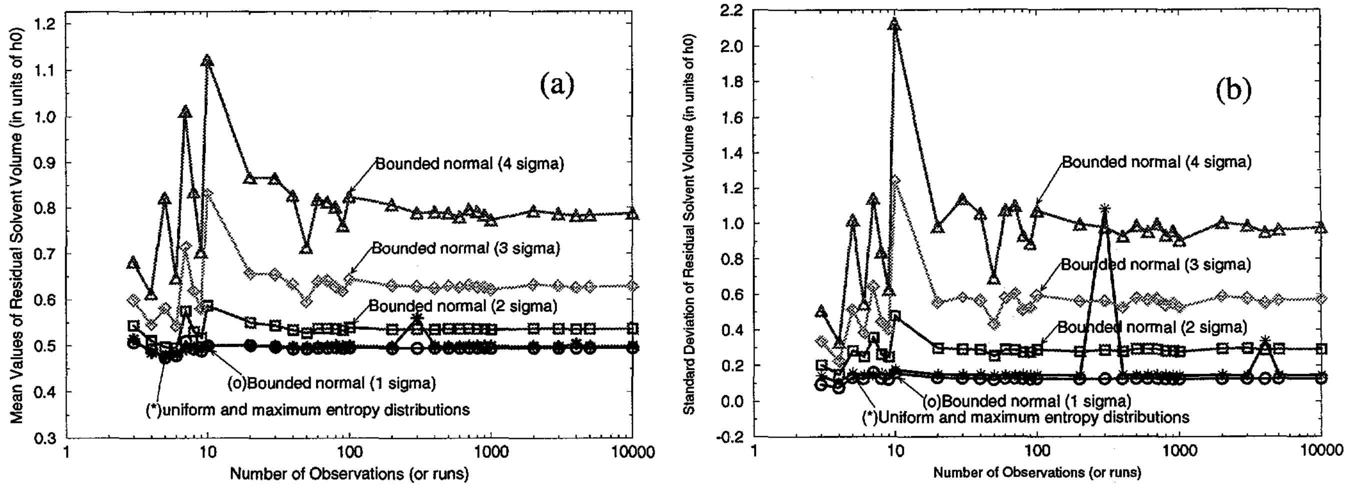

Figure 3. Effect of distribution types and specifications on convergence of predicted residual solvent volume: (a) mean value; (b) standard deviation. (Here, sigma denotes the standard deviation in the three input parameters chosen to vary).

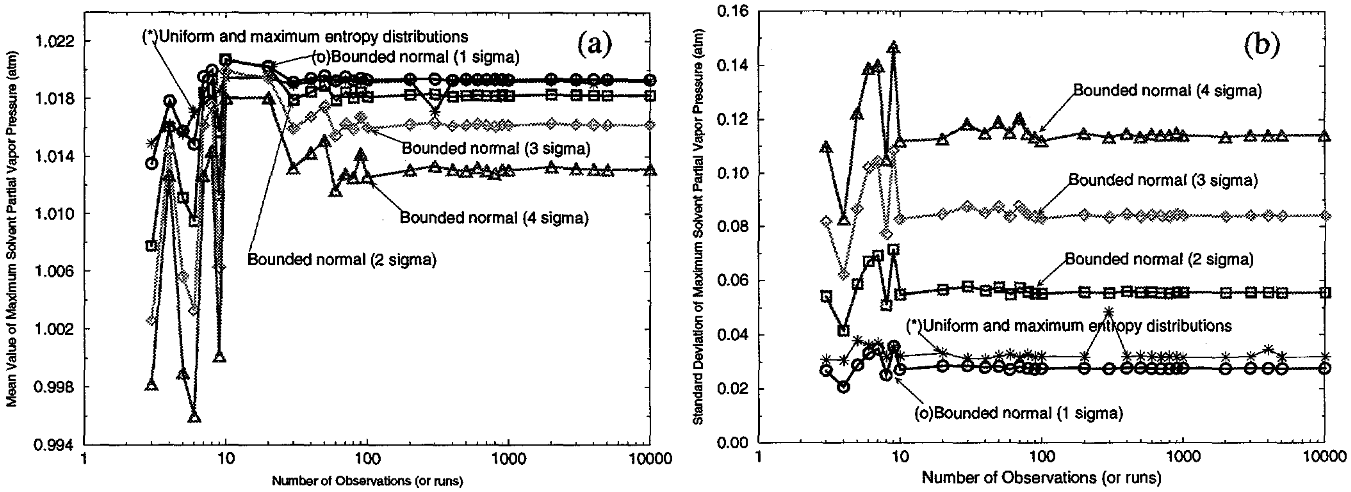

Figure 4. Effect of distribution types and specifications on convergence of predicted maximum solvent partial vapor pressure: (a) mean value; (b) standard deviation. (Here, sigma denotes the standard deviation in the three input parameters chosen to vary).

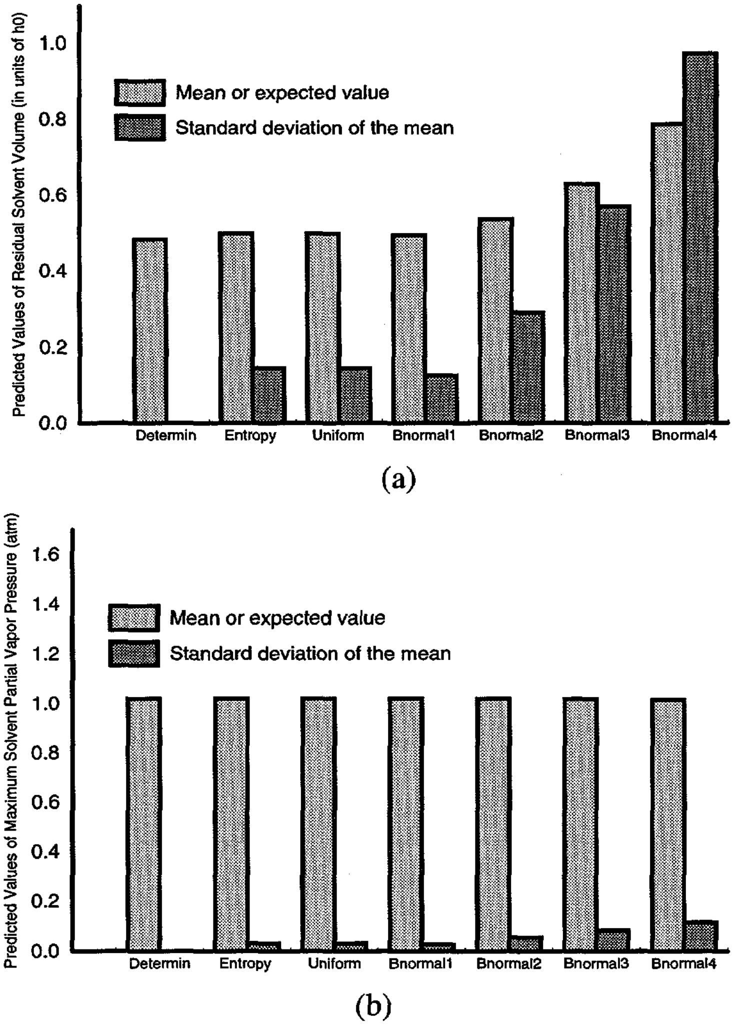

Figure 5. Effect of distribution types and specifications on predicted response variable values at 10,000 observations or runs. (a) residual solvent volume; (b) maximum solvent partial vapor pressure. (Here, Bnormal1 denotes bounded normal distribution with 1 standard deviation in input parameters, Bnormal2 with 2 standard deviation, Bnormal3 with 3 standard deviations, etc.)