A Comparison of the Reliability Analysis Methods in Stream Water Quality Modeling

강물의 수질오염 Modeling에 사용되는 신뢰도 분석방법에 대한 비교연구

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적 요

공학분야에 널리 사용되고 있는 신뢰도 분석방법중에서 Monte Carlo simulation (MC), Mean-value First-Order Second-Moment Method(MFOSM), and Advanced First-Order Second-Moment(AFOSM) method들을 강물의 오염물질 농도와 수질기준치사이의 신뢰도 분석에 적용하였다. 미환경보건국에서 개발 보급한 QUAL2E를 이용하여 New Jersey에 위치한 Passaic강의 수질예측에서 4가지 주요인자(용존산소, 생물학적 산소요구량, 암모니아 그리고 조류)들이 정해진 수질기준치를 유지 할 수 있는 확률을 세가지 방법에 의해 추정한 후에 상호 비교하였다.

MC방법에 의해 2,000회 simulation시켜서 그 결과가 시스템의 추계학적 성질을 잘 반영한 것으로 판단하여 비교기준으로 삼고 MFOSM과 AFOSM에 의해 추정한 결과와 비교하였다. MFOSM의 결과보다는 AFOSM의 결과가 전체적으로 MC의 결과에 더 근접하였으며, 이유는 AFOSM의 계산방법이 MFOSM의 선형근사로 인한 오차를 줄일 수 있었기 때문인 것으로 판단된다. MC방법의 결과와 다른방법들의 결과사이의 차이가 입력변수들이 평균값에서 멀어질 때 많았는데 이는 MC의 경우 입력변수들이 일정범위를 벗어나서 비현실적인 상황이면 model이 정지하는데, 다른 방법들은 simulation에 의한 것이 아니고 수학적인 계산에 의해서 신뢰도가 추정되기 때문에 이러한 상황이 반영될 수 없기 때문이다. 강물의 수질을 취급하는 공학적인 측면에서 보면, 이중에 가장 간편한 MFOSM이 많은 simulation이 필요한 MC나 계산방법이 상대적으로 복잡한 AFOSM에 비해 오차가 크지 않아서 이들을 대신하여 사용될 수 있다고 판단된다.

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키워드 : Reliability, Water Quality Modeling, Monte Carlo Simulation, First Order Reliability Analysis, BOD(Biochemical Oxygen), DO(Dissolved Oxygen) Ammonia, Chlorophyll

I. Introduction

Reliability can be defined as the probabilistic measure of whether a system meets certain performance standards. Reliability problems for engineering systems may be cast essentially as a problem of Load versus Resistance. In case of reliability of a structure, the concern is insuring that the strength of the structure(resistance) is sufficient to withstand the applied load (load). For a projection part of water quality modeling, the predicted constituent concentrations(load) should meet the water quality standards (resistance) set by regulatory agencies. In reality, the determinations of an available resistance and maximum load are not simple. Because engineering information is invariably incomplete and future conditions can only be estimated, estimation and prediction are necessary for these processes, and uncertainties are unavoidable. In light of such uncertainties, the reliability may be stated only in terms of probability[1].

Reliability analysis for the system of interest is necessary to evaluate the system performance. Many approaches have been used to investigate the uncertainty and the resulting reliability of the system. Among them are Monte Carlo (MC) simulation and First-Order Reliability Analysis (FORA) methods. MC method represents most the stochastic properties of the system, involves generation of random numbers and requires over 1,000 simulations in general. Kothandaraman and Ewing[2] applied MC technique to determine the Dissolved Oxygen (DO) response of stream modeled with the Streeter-Phelps[3] equation. Scavia et al. [4] examined the difference between the tes of variance from MC and FORA methods for a lake eutrophication model. Warwick and Cale [5] used MC method to investigate the effect of input parameter uncertainty on model output uncertainty for a one dimensional, steady state, uniform flow equation. Warwick and Cale[6] used MC method to quantify the the model output uncertainty caused by input parameter measurement error for the Streeter-Phelps equation.

FORA involves first-order approximation of Taylor series expansion and has two methods depending on the point of expansion, mean-value first-order second-moment method (MFOSM) and advanced first-order second-mement (AFOSM) method where the Taylor series is expanded with respect to the mean of the variables and the failure point, respectively. Burges and Lettenmaier[7] applied MFOSM method to estimate the uncertainty due to uncertain parameters for the Streeter-Phelps equation, and checked the accuracy of the result by MC method. Chaddertion et al.[8] used MFOSM method to determine the relative contributions to uncertainty ind DO prediction for the Streeter-Phelps equation. Tung and Hathhorn[9] used MFOSM method to estimate the statistical moments of the DO deficit for the Streeter-Phelps equation and verified them using MC method. Melching and Anmangandla[10] used AFOSM method on the Streeter-Phelps equation to estimate the probability distribution of critical DO deficit, and the result demonstrated that it provides a close approximation to that of MC simulation.

The objective of this study is to apply these reliability analysis methods to the stream water quality modeling using QUAE2E model and compare the results each other.

II. Theories

Risk is defined as the probability of failure, which is the complement of the reliability. Risk can be expressed with resistance(R) and load(L) as

$$Risk = P_f = P(L > R) \quad \cdots\cdots (1)$$

where P_f is the probability of failure and P (X) is the probability of an event X. Thus, the reliability of the system is

$$Reliability = 1 - P_f = P(Z \geq 0) \quad \cdots\cdots (2)$$

If Z=R-L is normally distributed

$$P_f = \Phi(-\beta) = 1 - \Phi(\beta) \quad \cdots\cdots (3)$$

where $\beta = \mu_Z / \sqrt{Var(Z)}$, μ_Z is mean value of Z, Var(Z) is the variance of Z, and $\Phi(\beta)$ is the cumulative standard normal distribution evaluated at β. β is called the reliability index or safety index and is a reciprocal of coefficient of variation of Z[1,11].

1. First-Order Reliability Analysis

This method utilizes a first-order approximation of Taylor series expansion. Taylor series expansion with respect to a point $P(x_{1p}, x_{2p}, x_{3p}, \cdots, x_{np})$ can be expressed as:

$$Y = G(x_{1p}, x_{2p}, x_{3p}, \cdots, x_{np}) + \sum_{i=1}^{n}(X_i - x_{ip}) \left(\frac{\partial G}{\partial X_i}\right)_p + \frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n}(X_i - x_{ip})(X_j - x_{jp}) \left(\frac{\partial^2 G}{\partial X_i \partial X_j}\right)_p + \text{higher order terms} \quad \cdots\cdots (4)$$

in which $G(\cdot)$ repressents estimation equation and the subscript "p" indicates the quantity Y is evaluated at the point of expansion P. The first-order approximation is formulated by truncating the second and higher order terms in the Taylor series expansion. Approximation including the second-order term is not only difficult to evaluate but also impractical except for the case where extreme risks (e. g., $< 10^{-4}$) highly nonlinear systems are of concern. The mean, E(Y), and variance[14] Var(Y), of Y by first-order approximation are

$$E(Y) = G(x_{ip}) + \sum_{i=1}^{n}(x_{mi} - x_{ip}) \left(\frac{\partial G}{\partial X_i}\right)_p 1:1 \quad \cdots\cdots (5)$$

$$Var(Y) = \sum_{i=1}^{n}\sum_{j=1}^{n} E[(X_i - x_{ip})(X_j - x_{jp})] \left(\frac{\partial G}{\partial X_i}\right)_p \left(\frac{\partial G}{\partial X_j}\right)_p \quad \cdots\cdots (6)$$

for dependent input parameters, or

$$Var(Y) = \sum_{i=1}^{n} Var(X_i) \left(\frac{\partial G}{\partial X_i}\right)_p^2 \quad \cdots\cdots (7)$$

for idependent input parameters, where x_{mi}= mean value of the variable i, and $\frac{\partial G}{\partial X_i}$ can be approximated numerically as $\frac{\partial G}{\partial X_i} \approx \frac{DY_i}{DX_i}$

Since first-order approximation involves only the first two moments (mean and variance) of the uncertaion parameters, this approach is aclled the first-order second-moment method.

Im the Mean-Value First-Order Second-Moment (MFOSM) method, Taylor series is expanded with respect to the mean of the variables, $X_m=(x_{m1}, x_{m2}, x_{m3}, \cdots, x_{mm})$. Therefore, the mean and variance of Y from Eqs. 5, 6, and 7 by MFOSM are

$$E(Y)=G(x_{m1}, x_{m2}, x_{m3}, \cdots, x_{mm}) \quad \cdots\cdots (8)$$

and

$$Var(Y)=\sum_{i=1}^{n}\sum_{j=1}^{n} Cov(X_i, X_j) \frac{\partial G}{\partial X_{i\,m}} \frac{\partial G}{\partial X_{j\,m}} \quad \cdots\cdots (9)$$

for dependent input parameters, or

$$Var(Y)=\sum_{i=1}^{n} Var(X_i, X_j) \frac{\partial G}{\partial X_{i\,m}}^{2} \quad \cdots (10)$$

for independent input parameters, in which the subscript "m" indicates the quantity being evaluated at the mean of the variables, and $Cov(X_i, X_j)$ is the covariance between X_i and X_j. The major advantages of this method are well explained by Yen et al.[11]. Particularly, this method requires only the mean and variance of the input parameters and it generates the uncertainty of the output variables from an explicit expression with a relatively simple formulation. However, it has certain disadvantages : a) ignorance of higher order terms, b) linearization of nonlinear behavior at the mean-values of uncertain parameters can cause large errors for conditions where failure involves parameter values significantly different from the mean values, and c) inability to incorporate probability distribution information.

Another approach to the first-order reliability analysis is an Advanced First-Order Second-Moment method (AFOSM). The basic concept of AFOSM is to reduce the error in the firstorder approximation due to nonlinearity by expanding Taylor series at a point of failure, $X^*=(x_1^*, x_2^*, x_3^*, \cdots, x_n^*)$, rather than at a mean value, $X_m=(x_{m1}, x_{m2}, x_{m3}, \cdots, x_{mn})$. At the failure point, the load (L) is the same as the resistance (R) and the performance variable (Z) is zero. The failure point (X^*) is located at the shortest distance from mean point (X_m) to the failure surface (Z=0) in standarized space, and this distance is β in Eq. 3.[1,11] Since the failure surface depends on both the load and the resistance in AFOSM, the performance variable Z can be used instead of L and R separately, where

$$Z=G(x_1, x_2, x_3, \cdots, x_n) \quad \cdots\cdots (11)$$

The first order expansion of Z for unrelated variables at a failure point is

$$Z=G(x_1^*, x_2^*, x_3^*, \cdots, x_n^*)+\sum_{i=1}^{n} C_i^*(X_i-x_i^*) \quad \cdots\cdots (12)$$

whrer $C_i^*=\partial G/\partial X_i$ evaluated at the failure surface. At the failure surface $G(x_1^*, x_2^*, x_3^*, \cdots, x_n^*)=0$, and the expected value of Z within the first-order approximation is

$$E(Z)\approx\sum_{i=1}^{n} C_i^*(x_{mi}-x_{mi}^*) \quad \cdots\cdots (13)$$

and corresponding standard deviation of Z for the case of independent variables is

$$\sigma_z = \sum_{i=1}^{n} \alpha_i C_i^* \sigma_i, \quad \cdots\cdots (14)$$

where, $\alpha_i = (C_i^* \sigma_i) / \left[\sum_{j=1}^{n} (C_j^* \sigma_j)^2 \right]^{0.5}$. Then the reliability index is

$$\beta = \frac{E(Z)}{\sigma_z} = \sum_{i=1}^{n} C_i^* (x_{mi} - x_i^*) / \sum_{i=1}^{n} \alpha_i C_i^* \sigma_i \quad \cdots\cdots (15)$$

Then the probability of facilure, for a normally distributed Z, can be easily evaluated by Eq. 3, $P_f = \Phi(-\beta) = 1 - \Phi(-\beta)$. Various techniques have been suggested to fine the failure point X* and reliability index β. The Generalized Reduced Gradient method, Rackwitz algorithm, and Shinozuka algorithm are examples of the techniques[1,10,11]. In this research, the Rackwitz[4] algorithm is used. More informations for AFOSM are available[1,11,12].

2. Monte Carlo Simulation

Monte Carlo simulation involves repeating a simulation process, using a set of values of random basic variables generated in accordance with the corresponding probability distributions of the random variables. By repeating the process, a sample of solutions for each corresponding set of random basic variables is obtained. This is similar to a sample of experimental observations. Therefore, the results of Monte Carlo simulation may be treated statistically, and methods of statistical estimation and inference are applicable[1]. In developing Monte Carlo simulation, it is necessary to generate random numbers from a prescribed probability distributions and for a given set of generated random numbers, the simulation process is deterministic because the generated random numbers are held constant during the simulation.

Selection of an appropriate probability distribution for a given random variable in a simulation requires gathering and evaluating all the available facts, data, and knowledge concerning each variable. Choosing the form of probability distribution is often a trade-off between theoretical justification and empirical evidence. Dawson and Wragg[13] have shown that, when the first two moments only are specified, the maximum entropy distribution on the interval $(-\infty, +\infty)$ is the normal distribution. The Normal distribution is used in the reliability analysis of model output in this study.

The following equation from Park and Miller[14] was used to generate uniform random numbers U(0.1)

$$Z_i = (16807\ Z_{i-1}) \pmod{2147483647} \quad \cdots\cdots (16)$$

Once the uniformly distributed random numbers (U) are generated between 0 and 1, an appropriate transformation is necessary to generate random numbers for other distributions.

For uniform distribution $U(r_1, r_2)$,

$$X = r_1 + (r_2 - r_1)U \quad \cdots\cdots (17)$$

For normal distribution $N(\mu, \sigma^2)$[15],

1. Generate U and U from U(0, 1)

2. $X_1 = \mu + \sigma\sqrt{-2\ln U_1}\ \mathrm{Cos}\ 2\pi U_2$

$X_2 = \mu + \sigma\sqrt{-2\ln U_1}\ \mathrm{Sin}\ 2\pi U_2 \cdots$ (18)

Once random numbers are generated, data set can be formulated with random numbers and simulation results from each data set can be treated like experimental result for further analysis.

Ⅲ. Methods

The reliability analysis methods (Monte Carlo Simulation and First-Order Reliability Analysis) were applied to the QUAL2E. QUAL2E model has been nolified and calibrated[16] for application to the Passaic River located in northeastern New Jersey, USA, and this modified model (QUAL2E-Passaic) is used in this research. QUAL2E-Passaic has 32 reaches, they are divided into 257 elements in total, and the length of each element is 0.4km. It can simulate up to 15 water quality constituents in any combination desired by the user. The total length of the study sectioni s about 100km, with a total drainage area of about 2188km^2, and study area includes 27 wastewater treatment dischargers. The average annual precipitation over the study area is about 120cm. The water quality response varies greatly from section to section due to the topographic, geographic, and hydrologic conditions; and types of land use[16]

Reliability analysis methods are applied to determine the cumulative distribution functions (CDF_S) for the critical dissolved oxygen (DO), maximum biochemical oxygen demand (BOD), maximum ammonia (NH3), and maximum chlorophyll a (CHL) concentrations along the river. QUAL2E has its own uncertainty analysis subroutine (QUAL2E-UNCAS) which employs options for sensitivity analysis, first-order error analysis, and Monte Carlo simulation. However, they are not used in this research because the QUAL2E-Passaic model cannot use QUAL2E-UNCAS due to a different input data format and also the results from QUAL2E-UNCAS do not provide all the necessary information for the reliability analysis approach developed in this study. Therefore, FORTRAN programs were developed for random number generation using the concepts and ideas described earlier and batch program was used for 2,000 Monte Carlo simulation. Detail procedure is availabel[17]

Ⅳ. Results and Discussion

The key input parameters which affect output variance of the four constituents were identified in Table-1 from variance calculation using Eq 7. They affect dominantly on the output variances, therefore, random variables for the four constituents were limited to these key input parameters. The uncertainty involved in each key input parameters was estimated from literature review and summarized in Table-1[17]. Reliability analyses were performed with the information of these key input parameters. Many sets of random data were generated with the uncertainty data of key input parameters and 2, 000 simulations were run for Monte Carlo method.

The "exceedance probability", the cumulative distribution function expression, is used rather than "probability of failure" or "reliability", because the concern is the probability that constituents exceed a certain level of concentration. Reliability analyses were made for the lowest DO, highest BOD, highest NH3, and highest CHL of the system. The exceedance probability by Monte Carlo (MC) simulation is estimated as follows :

$$P_e = \frac{\text{number of model outcomes with } Z<0}{\text{total number of simulations}} \quad \cdots\cdots (19)$$

and the exceedance probability by MFOSM is estimated as follows :

$$P_e = \Phi(-\beta) = 1 - \Phi(\beta) \quad \cdots\cdots (20)$$

where Z=R-L, R is a concentration level of concern which is fixed for any evaluation of Eqs. 19 and 20, L is conentration simulated by the model, $\beta = E[R-\mu_L]/\sigma_L$, σ_L is the estimated standard deviation of the output concentration, μ_L is the estimated mean of the output concentration, and $\Phi(\cdot)$ is the cumu-

Tabel-1. Key Input Parameters to the Output Variance of QUAL2E-Passaic

Parameter	Contribution(%)	Remarks	CV(%)*
Variance in the Lowest Dissolved Oxygen(Geach 3)			
Reaeration Coefficient(Reach 3)	49.351	Reach of interst	50
Reaeration Coefficient(Reach 2)	25.087	One reach upstream	50
NH3 Oxidation Rate(Reach 3)	12.299	Reach of interest	25
NH3 Oxidation Rate(Reach 2)	4.015	One reach upstream	25
TOTAL	90.752		
Variance in the Highest Biochemical Oxygen Demand(Reach 2)			
BOD Decay Rate(Reach 2)	81.800	Reach of interest	25
BOD Settling Rate(Reach 2)	13.088	Reach of interest	25
TOTAL	94.888		
Variance in the Highest Ammonia(Reach 2)			
NH3 Oxidation Rate(Reach 2)	96.162	Reach of interest	25
Sediment Oxygen Demand Rate(Reach 2)	3.848	Reach of interest	30
TOTAL	100.000		
Variance in the Highest Chlorophyll a(Reach 32)			
Algal Maximum Specific Growth Rate	93.170	System wide	10
Algae/Temperature Solar Radiation Factor	5.655	System wide	10
TOTAL	98.825		

*Coefficient of Variation (CV) = standard deviation/mean.

lative standard normal distribution. The μ_L and σ_L for the MC method are obtained from statistical analysis of the simulation results, and they can be determined by Eq. 8 and 11 for MFOSM, respectively. The exceedance probability by AFOSM is also estimated by Eq. 15, the Rackwitz algorithm[12].

Table-2 shows the comparison of the reliability analysis results from MC, MFSOM, and AFOSM methods, for the lowest DO, highest BOD, highest NH3, and highest CHL, respectively. For the lowest DO, the exceedance probabilities from the three methods are close to each other at higher concen

Tabel-2. Comparison of the Results from the Three Methods of Reliability Analysis

Constituent Concentration (mg/L)	Exceedance Probability(%) MC	MFOSM	AFOSM
Lowest DO			
1.10	98.50	90.78	92.24
1.25	96.40	87.88	89.07
1.50	89.65	81.81	82.64
1.75	81.20	74.12	74.42
2.00	71.50	65.01	65.45
2.25	59.55	54.81	55.40
2.50	49.20	44.62	44.60
2.75	37.30	34.61	34.62
3.00	26.80	25.56	25.60
3.25	18.05	17.96	17.39
3.50	11.20	11.91	11.79
3.75	6.75	7.48	7.16
4.00	4.30	4.45	4.08
4.25	2.25	2.49	2.09
4.50	1.05	1.31	1.03
4.74	0.45	0.65	0.46
Highest BOD			
11.80	90.90	99.96	99.9
11.90	99.00	99.19	98.91
12.00	91.65	93.081	92.10
12.10	68.45	71.04	69.15
12.15	50.25	50.0	53.98
12.17	42.55	49.70	46.02
12.20	32.60	35.56	34.46
12.28	11.70	13.33	15.56
12.35	3.55	3.93	4.79
12.40	1.60	1.31	2.00

Constituent Concentration (mg/L)	Exceedance Probability(%) MC	MFOSM	AFOSM
Highest NH3			
13.20	99.60	99.99	99.21
13.25	97.55	99.84	96.76
13.30	90.35	97.50	89.93
13.35	76.90	83.65	73.20
13.39	59.80	57.78	57.93
13.41	50.05	42.22	42.07
13.45	31.70	16.34	31.30
13.50	14.50	2.49	13.70
13.60	1.45	0.01	1.18
Highest CHL			
20.00	99.90	92.59	99.79
30.00	98.90	89.93	98.63
40.00	95.45	86.65	95.80
50.00	89.30	82.76	91.20
60.00	82.55	78.08	84.97
70.00	74.95	72.81	77.82
80.00	67.35	66.97	70.07
90.00	59.50	60.62	62.21
100.00	51.30	54.13	54.50
110.00	42.30	47.45	47.29
120.00	35.55	40.84	40.52
130.00	29.35	34.48	34.39
140.00	24.45	28.55	28.88
150.00	19.75	23.12	24.02
160.00	15.25	18.35	19.71
170.00	12.00	14.23	15.95
180.00	8.35	10.79	12.69
190.00	5.55	8.01	9.85
200.00	2.80	5.78	7.39
210.00	0.90	4.08	5.15
215.00	0.05	3.40	4.13

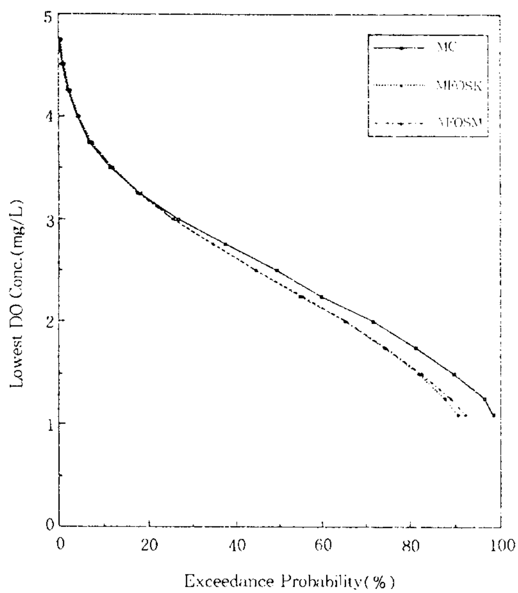

Fig. 1. Comparison of the Lowest DO exceedance probability curves estimated by Monte Carlo, MFOSM, and AFOSM

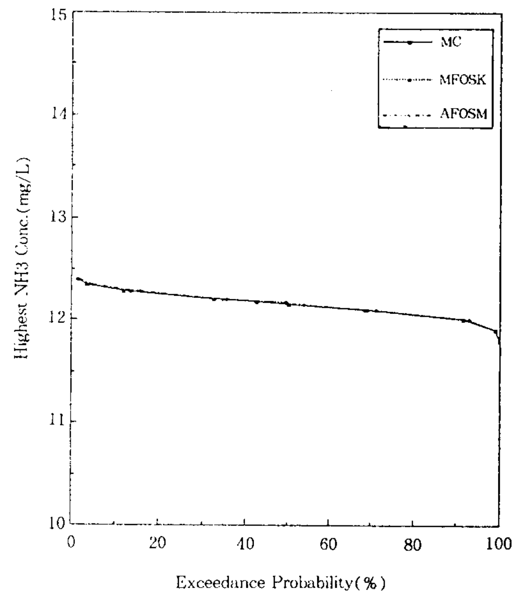

Fig. 2. Comparison of the Highest BOD exceedance probability curves estimated by Monte Carlo, MFOSM, and AFOSM

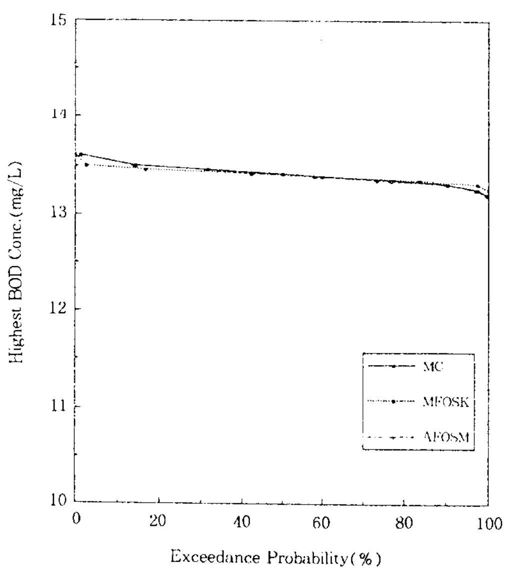

Fig. 3. Comparison of the Highest NH3 exceedance probability curves estimated by Monte Carlo, MFOSM, and AFOSM

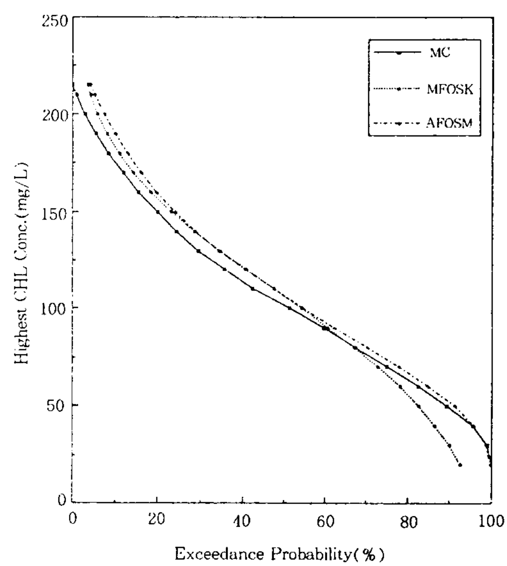

Fig. 4. Comparison of the Highest CHL exceedance probability curves estimated by Monte Carlo, MFOSM, and AFOSM

trations, but those of MFOSM and AFOSM deviatie from that of MC as concentration decreases. Among the methods, AFOSM result is slightly closer to MC result than that of MFOSM. For the highest BOD and NH3, generally, tne AFOSM result is colser to the MC result than MFOSM result. However, the range of variation is so small that the difference is not apparent in Figures 2 and 3. For the highest CHL, MFOSM result deviates from the MC result apparently at lower concentrations while AFOSM result is close to MC result. Overall, AFOSM result is closer to MC result than MFOSM result. This implies that AFOSM is the better substitute for MC simulation, the reason being reduction of linearization error by expansion of Taylor series at a failure point rather than at the mean values.

During MC simulation, about 300 random data sets were physically unrealistic and could not be used for model running. However, the recommended data range information was not incorporated in the calculation of the first-orliability analysis because the probability was calculated based on mathematical manipulation. This can partly explain why larger deviations are expected in extreme values rather than around the mean value, because the values around the mean are assumed to be inside the recommended range.

V. Conclusions

Three reliability and analysis methods (Monte Carlo, MFOSM, and AFOSM) were applied to the QUAL2E-Passaic model and the results were compared each other. The results of 2,000 Monte Carlo simulations were considered a good representation of the stochastic properties of the system and were used as a reference for comparison with oter methods. Overall, AFOSM result is closer than MFOSM result to that from Monte Carlo mthod. The differences between the three methods are small in the central portion of the exceedance probability curve, and more significant at the tails but it is not too large. AFOSM method is more complicated than MFOSM in algorithm and slightly reduce the error from linear approximation. However, MFOSM is relatively simple and the performance of it is adequate from the decision making point of view, therefore, it can be used as a a practical alternative to Monte Carlo method in stream water quality modeling.

VI. Acknowedgement

The work reported here was partially supported by the New Jersey Water Resources Research Institute under U.S. Geological Survey Grant Number INT-14-08-0001 G2034. The assistance and encouragement of Dr. Joan Ehrenfeld, Institute Director, are greatly appreciated.

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(접수일자 : 1995년 7월 8일)