Pergamon

Wat. Sci. Tech. Vol. 40, No. 4–5, pp. 223–233, 1999

0273–1223/99 $20.00 + 0.00

PII: S0273-1223(99)00504-1

ESTIMATION OF PATHOGEN REMOVAL IN AN ADVANCED WATER TREATMENT FACILITY USING MONTO CARLO SIMULATION

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ABSTRACT

Interest in water reuse for potable purposes has heightened the significance of evaluating the potential presence of microbial agents in treated water. Evaluating the public health risk from microbial agents in water after advanced water treatment (AWT) requires an estimate of the effectiveness and reliability of the treatment system in removing microbial agents. Indicator organisms such as total and fecal coliform do not provide sufficient basis to characterize the performance of the treatment system relative to the removal of pathogenic organisms such as enteric viruses and parasitic agents. Seeding studies provide an alternative experimental approach. However, when treatment systems are challenged using more specific indicators for enteric viruses, the results are often inconclusive because the organisms are reduced to non-detectable levels after the first few unit processes. In this study we provide a mathematical approach for estimating the effectiveness of the entire treatment train with respect to removal and/or inactivation of microbial agents. These estimates are insightful since standard monitoring of final effluent consistently yielded non-detectable results.

KEYWORDS

Advanced water treatment; challenge studies; coliphage; microbial removal; Monte Carlo simulation.

INTRODUCTION

The need to supplement local drinking water sources prompted the City of San Diego (City) to develop a unique water repurification project that would augment raw water to one of the City's reservoirs with water repurified at an AWT facility. The fundamental strategy of this reclamation concept is a treatment system composed of multiple barriers to contaminants, each of which provides significant and reliable rejection.

Based on Health Effects Studies (HES) conducted between the early 1980s and 1996, and a 1994 feasibility study, the California Department of Health Services (DHS) issued conditional approval of the San Diego Water Repurification Project (Cooper *et al.*, 1992; Montgomery Watson, 1994; Eisenberg *et al.*, 1996; Cooper *et al.*, 1997). Several of the comments in the conditional approval addressed the reliability of the disinfection strategy of the proposed AWT train.

In 1995, the City operated a pilot-scale AWT treatment train for a period of five months to address concerns raised by DHS in their conditional approval of the water repurification project. In October 1996, the City initiated a pilot program to prequalify microfiltration (MF), ultrafiltration (UF), and reverse osmosis (RO) membranes and to assure successful performance of the full scale AWT which is planned for construction by the end of 1999 (Montgomery Watson, 1997). As part of both programs, virus and parasite seeding studies were carried out to characterize removal rates through each of the proposed AWT unit processes.

Results from previous seeding studies conducted as part of the City's HES investigations, indicated that tertiary treatment (chemical coagulation and filtration post secondary treatment) plus the AWT unit processes (reverse osmosis, air stripping, and activated carbon) removed at a minimum 8.8 logs of MS-2 coliphage (99.9999998 percent) without final disinfection (Cooper *et al.*, 1997). This removal rate is considerably greater than that reported in either the Pomona virus study (LACSD, 1977) or the Monterey Study (Sheikh, 1987) which used filtration and chlorination of secondary effluent, but not reverse osmosis. These results demonstrate that it may not be physically possible to seed an integrated AWT train with a high enough concentration so that viruses are found in the final effluent. For this reason, this research focused on isolating and characterizing the removal of virus and parasites through individual unit processes rather than characterizing removal through the integrated AWT train.

Experimental results from the seeding studies were used to estimate the distribution of virus removal through each of the treatment units and the distribution of virus (bacteriophage) expected in the plant influent. Monte Carlo simulations were then run using the influent distribution and the individual unit process removal distributions to describe the expected cumulative removal of bacteriophage through an integrated AWT train. Simulations were conducted for a series of unit process combinations which are considered potential treatment combinations for full-scale implementation.

The results from the Monte Carlo analyses provide estimates for the expected distribution of removal of bacteriophage through several potential combinations of treatment processes. Through comparisons of these removal distributions to each other and to results reported previously, inferences were made regarding the relative effectiveness of the different treatment trains.

METHODS

1997 Microbial challenge studies

The AQUA 2000 Research Center is located at the San Pasqual. Water Reclamation Plant in Escondido, CA and was established to provide a venue to test operating conditions and treatment combinations to assure the successful design and performance of the full scale AWT facility. The AQUA 2000 AWT treatment train takes tertiary treated water as influent and treats the water with unit processes as shown schematically in Figure 1. A detailed description of the unit processes in the AQUA 2000 treatment facility and unit process specifications are found under separate cover (Montgomery Watson, 1997). The microbial challenge studies conducted at the Aqua 2000 Research Center are described in detail under separate cover (Soller *et al.*, 1997; Olivieri *et al.*, 1998). A summary of those studies follows.

MS-2 bacteriophage was employed as the model virus because it is not a pathogen to humans and is an RNA virus of similar size and shape to poliovirus and hepatitis A virus. Coliphage seed was prepared by inoculating a log-phase culture of *E. coli* F^+ Amp into a flask of growth medium containing MS-2 coliphage and, with constant mixing, incubated for 18 hr at 35°C. The resultant culture was centrifuged at 3500 R-PM for 20 minutes and the supernate was retained as the seed material. The seed concentration was determined by plaque assay and contained between 10^{10} and 10^{11} phage plaque forming units (pfu) per ml (WCPH, BioVir, 1995).

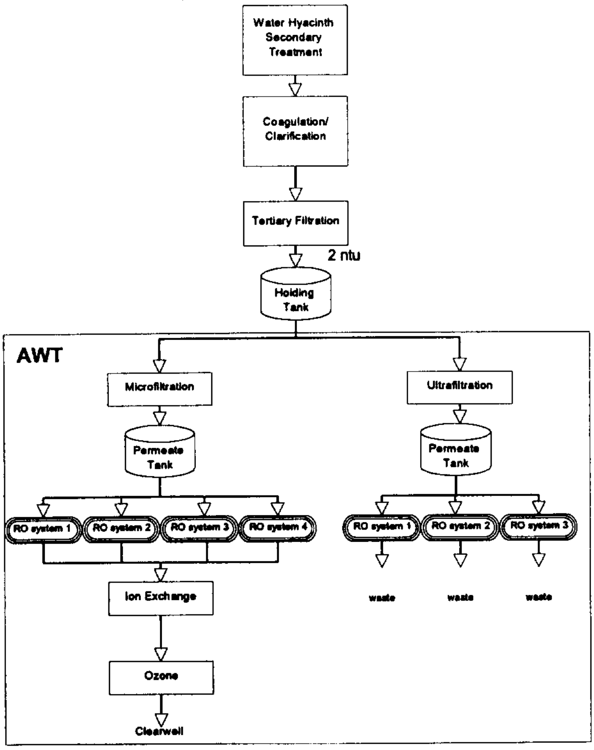

Figure 1. AQUA 2000 Research Center 1997 process train.

Separate virus challenge studies were conducted on the selected treatment processes to allow the evaluation of the rejection capabilities of each unit process. Moreover, the seeding experiments were conducted in reverse order of unit processes (e.g. ozone, before reverse osmosis, before pretreatment) to minimize potential downstream contamination.

Seeding was conducted on MF, UF, RO (4 membranes), and ozone treatment units, and samples were collected and analyzed as 100 mL grab samples (Soller *et al.*, 1997). To determine if the various sample waters could have a detrimental effect on the phage used in the seeding studies, a die-off study was conducted on each water type. Results of the die-off study indicate that the results of the experiments would not be impacted by the inoculation method (WCPH, BioVir, 1995). Seed solution concentrations were also measured at the beginning and at the end of the experimental time period for each unit process to further confirm seed challenge concentrations. The methods used to determine the presence and number of microorganisms are found under separate cover (WCPH, BioVir, 1995).

The results of the MS-2 bacteriophage seeding studies of the MF, UF, and RO membrane systems are summarized in Figures 2 and 3, which are cumulative probability plots based on the removal of MS-2 during the respective seeding experiments. Ozone experimentation was carried out at four different doses of ozone ranging from 0.3 mg/L*min to 1.7 mg/L*min with all experiments yielding results below detectable limits.

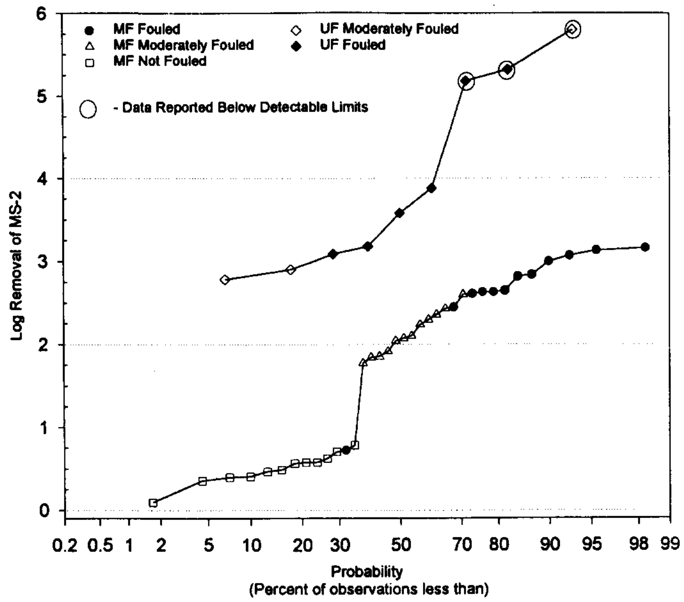

Figure 2. Cumulative probability plot of pretreatment performance during 1995 and 1997 MS-2 seeding studies.

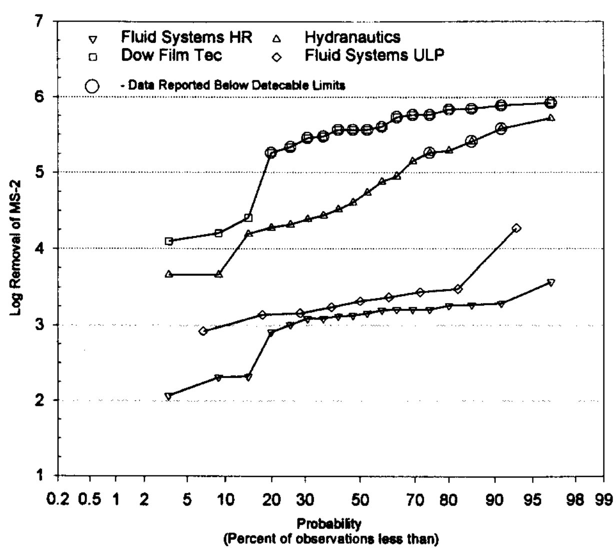

Figure 3. Cumulative probability plot for reverse osmosis membranes used during 1997 MS-2 seeding studies.

Bench scale experiments were also carried out on Aqua 2000 AWT effluent to establish inactivation curves for virus exposure to free chlorine (Soller *et al.*, 1997). The results of the experiments are shown in Figure 4. Results indicate that 6 logs of MS-2 bacteriophage are inactivated quickly (CT of ~55 mg/L*min) after which the inactivation rate seems to slow somewhat. Bacteriophage was reduced to the limit of the assay in all experiments utilizing a CT higher than 150 mg/L*min.

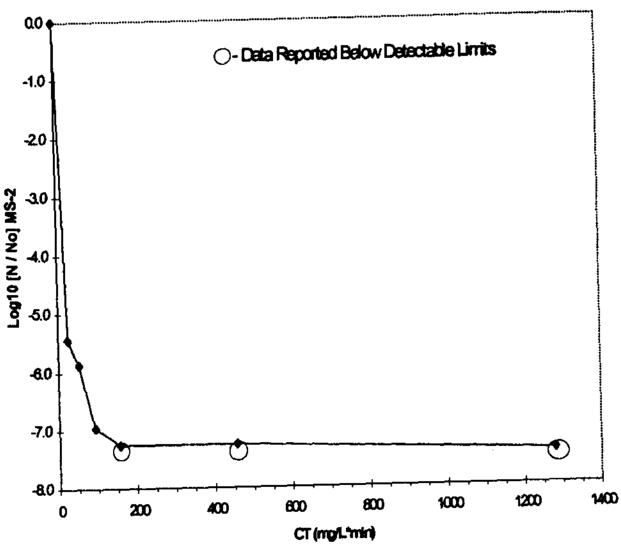

Figure 4. Free chlorine inactivation curve for MS-2 bacteriophage in RO effluent.

RESULTS AND DISCUSSION

Quantifying the removal of MS-2 through each unit process

To estimate process train performance, probability distributions of removal through each of the unit processes and the plant influent were identified using a Maximum Likelihood Estimate (MLE) approach (Ott, 1995). The identified probability distributions were then used in a Monte Carlo simulation model to estimate the distribution of coliphage removals and associated variability in each of a series of integrated treatment systems. It should be understood that this approach is stochastic by nature and incorporates the observed variability in the experimental data (Sakaji *et al.*, 1998). Moreover, it should be noted that the quality of the experimental data is crucial to estimating coliphage removal as the collection of the data is costly, and thus the estimates are based on a limited number of observations.

The first step in creating a model to estimate treatment train performance was to characterize virus removals through each of the unit processes of interest. Families of distributions which best described the experimental data were chosen for each unit process (and the plant influent), and then the experimental data were used to estimate the parameter values. Because the data for each treatment unit were not sufficient to choose explicitly one distribution over another based on a statistical test, skewness was chosen as the significant criterion for distribution family selection. If the treatment unit experimental data were left-skewed a gamma distribution (Ott, 1995) was selected for further characterization. Whereas, if the treatment unit experimental data were right-skewed, a Weibull or lognonnal distribution (Ott, 1995) was selected. Once the distribution family was selected for each treatment unit, the seeding study data (and routine monitoring data, if appropriate) were used to calculate the MLEs and the 95% confidence regions of the "best fit" distribution. The Weibull, lognormal, and gamma distributions are described by two parameter functions. Therefore, the 95% confidence regions are described by a two-dimensional closed surface. For the purposes of the simulations, the values of the parameters which corresponded to the MLEs were used.

The following is a brief description of the distributions of removal used to describe the experimental results in each of the unit processes.

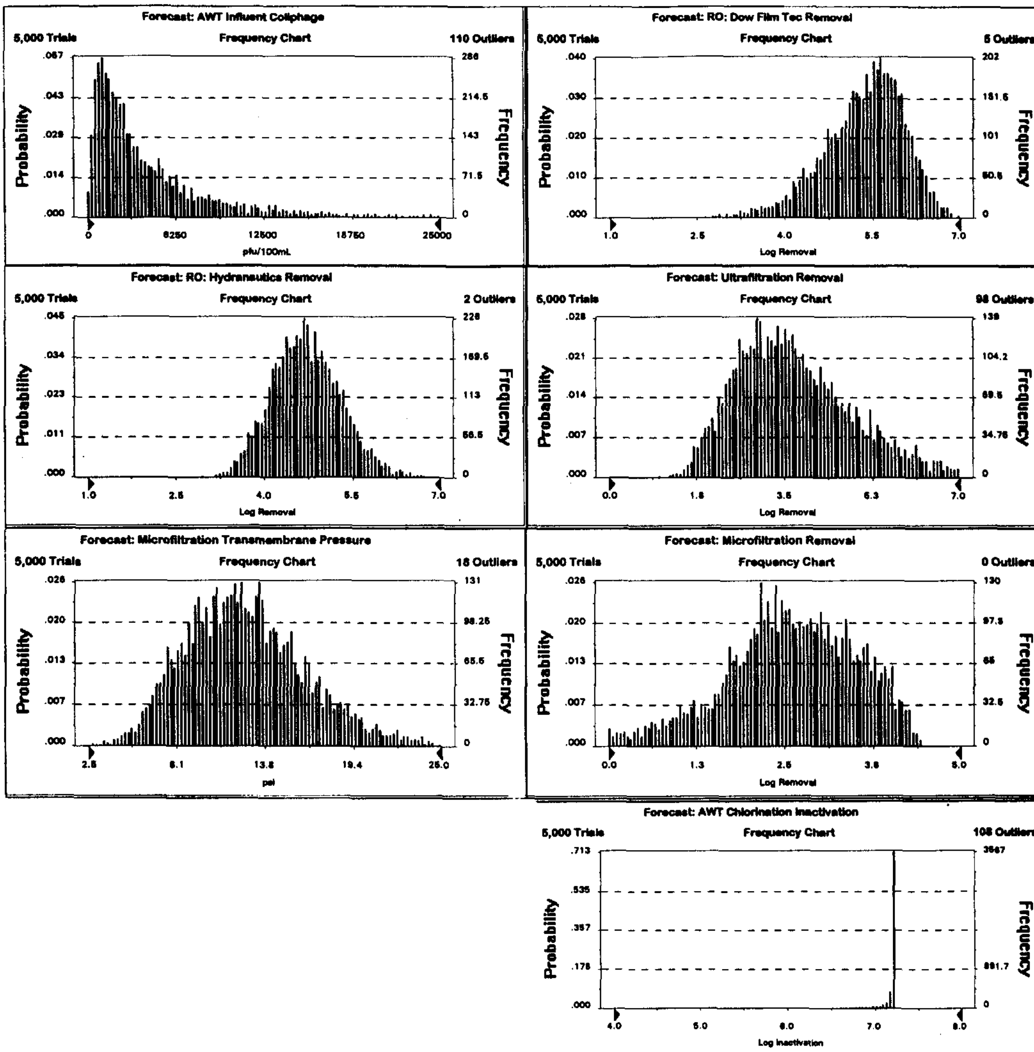

Figure 5. Representative frequency charts used for evaluation of process train performance with respect to coliphage removal.

Influent and RO. MLEs for the plant influent and RO units (four membranes) were generated as described above. Representative results are shown in Figure 5 (Soller *et al.*, 1997). Twenty-nine data points representing influent to the AWT were collected during the study period. Using these data, the lognormal MLE corresponded to a distribution with geometric mean of 3074pfu/100mL and geometric standard deviation of 2.84. Similarly, using the approach described above estimates for the Fluid Systems HR and Dow Film Tec RO membranes were found to be Weibull distributions with scale and shape equal to (3.16, 10) and (5.65, 9.3), respectively. MLEs for the Hydranautics and Fluid Systems ULP RO units were found to be Gamma distributions with scale and shape equal to (0.0744, 63.48) and (0.07, 50.0), respectively.

UF. The ultrafiltration unit process was challenged on six separate occasions. It was reported that the UF membrane used during the first three seeding events was compromised due to broken fibers (Montgomery Watson, 1997). Therefore, results from the first three seeding events (shown in Figure 5) are modeled independently from the last three, which were conducted on a membrane which was known to be intact. Using the criteria described previously, the MLE for coliphage removal through the UF unit during the first three seeding events corresponded to a lognonnal distribution with mean 3.83 logs and standard deviation of 1.3 logs. The last three seeding experiments of the UF unit resulted in seven of nine observations with concentrations below the limit of the assay (1 pfu/100 mL). With this limited amount of quantifiable data, it was not possible to generate an MLE for removal of coliphage. However, given the results of these three seedings, it is clear that at least 6 logs of coliphage were removed in each of the experimental samples.

Results from the ozone, micro filtration, and chlorination experiments required further investigation to characterize the removal of MS-2 through these unit processes.

Ozone. Seeding studies on the ozone unit process were conducted at four different CTs ranging from 0.3 to 1.7 mg/L*min, the results of which always resulted in concentrations below the limit of the assay (1 pfu/mL). Based on these results and influent concentrations, it was concluded that at least 6.2 logs of coliphage were removed during each of the experimental observations. Because endpoints were never reached in ozone effluent samples, it was not possible to generate an MLE for removal of coliphage through the ozone treatment unit.

MF. The generation of a maximum likelihood estimate for coliphage removal through the microfiltration unit is somewhat more complex than those described above. As shown in Figure 2, there is a relationship between MF membrane fouling, as indicated by transmembrane pressure and the removal of coliphage by the MF unit (Soller *et al.*, 1997). This observation is corroborated by the fact that MF seeding study observations and routine monitoring data are consistent with each other, once this factor is accounted for.

The relationship between transmembrane pressure and the observed removal of coliphage was quantified by using a Marquardt-Levenberg optimization algorithm to fit an exponential function to the experimental data (Press *et al.*, 1986; Nash, 1979). The optimal exponential function was compared to n^{th} order polynomial fits of the data, and was found to compare favorably in terms of R^2. In contrast to the best fit polynomial model, the exponential model saturates at high levels of transmembrane pressure. This result is consistent with the reality of the physical system; as membrane fouling increases, the maximum obtainable log removal is achieved and then maintained. The exponential function best describing the relationship between membrane fouling and removal of coliphage is as follows:

$R_{\log 10} = 3.35 - 14.71 \times e^{(-0.27 \times Ptm)}$ where:

$R_{\log 10}$ is the log removal; and *Ptm is* the observed transmembrane pressure.

A maximum likelihood estimate of the distribution describing nine months of transmembrane pressure data was generated, based on a gamma distribution with scale and shape equal to (1.19, 10.583), respectively (Refer to Figure 5). This transmembrane pressure distribution is used in conjunction with the relationship between membrane fouling and removal of coliphage, as presented above, to generate the expected removal distribution of coliphage through the microfiltration unit.

Specifically, the following procedure is used to generate the expected distribution of coliphage removal in the microfiltration unit, the results of which are shown in Figure 5:

A transmembrane pressure value is randomly sampled from the maximum likelihood gamma distribution;
The result of that sampling is then mapped into a log removal value using the exponential formula given above. This computed removal represents the expected mean removal given the transmembrane pressure;
A final log removal then is generated from the expected mean removal by uniformly sampling the 99% confidence region of the mean value; and
This process is repeated 5000 times.

Free Chlorine Contact. The purpose of the AWT chlorination experiment was to develop an inactivation curve for virus contact with free chlorine. Those results are shown in Figure 4. A Marquardt-Levenberg optimization algorithm was used to fit an exponential function to the experimental data. The results of the optimization yielded the following equation ($R^2 = 0.985$):

$I_{log10} = 7.208 - 7.145 \times e^{(-0.04424xCT)}$ where: I_{log10} is the log inactivation.

Because the contact time to be used at the North City AWT has yet to be determined, a conservative approach was taken in estimating the inactivation of coliphage in the relative estimation of process train performance. Using the exponential model described above, the CT was sampled uniformly between 5 and 500 mg/L*min. The resultant frequency distribution for inactivation of coliphage from contact with free chlorine is shown in Figure 5.

Comparison of MS-2 removal through selected treatment trains

The cumulative removal (and inactivation) of coliphage was estimated for the six treatment systems shown in Figure 6 using the distributions of removal described above. These estimates were obtained through a series of Monte Carlo simulations where for each trial, the simulation model generated an influent concentration and appropriate removals for each unit process. Using these values, the resultant effluent concentration was computed along with a cumulative removal for the entire treatment train. Each simulation was composed of 5000 individual trials.

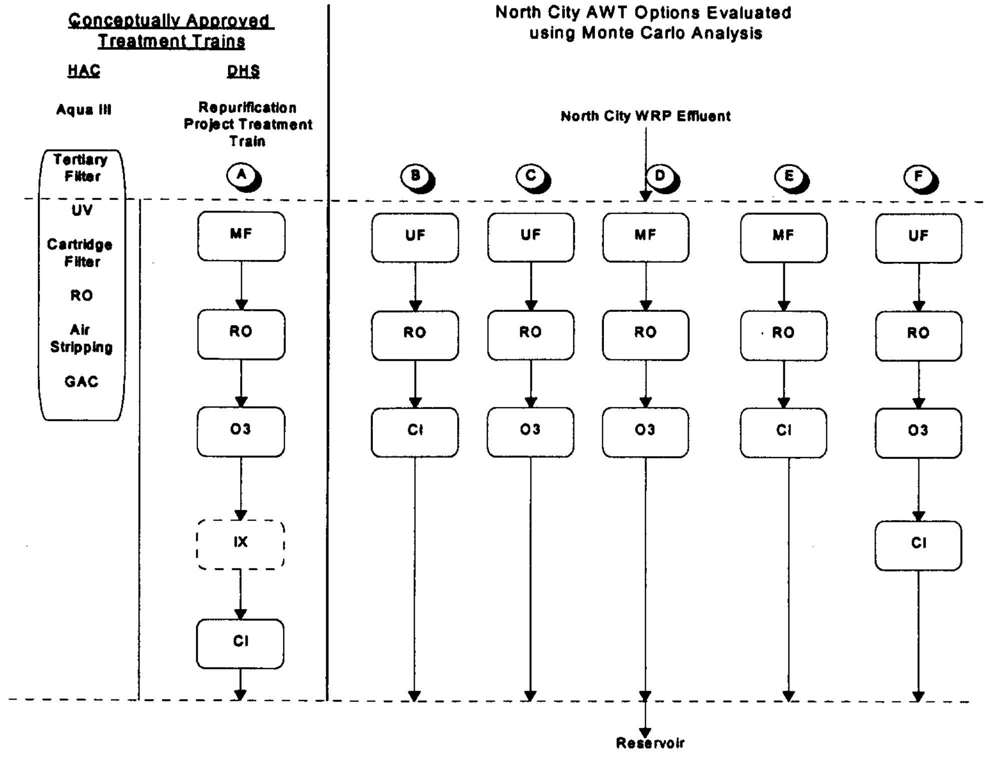

Figure 6. Treatment trains to be evaluated.

To investigate the sensitivity of the methods used, simulations were conducted using the results for two different RO membranes as recommended by the City and an independent Health Advisory Committee. Based on the results of previous HES investigations and the results of the Monte Carlo simulations, a comparison of process train performance is presented in Figure 7. Specifically, the relative performance during the challenge studies of the treatment trains outlined in Figure 6 are presented along with results from the 1997 HES and the estimated microbial inactivation for the DHS conceptually approved treatment train (Figure 6, treatment train A) from the 1994 Feasibility study.

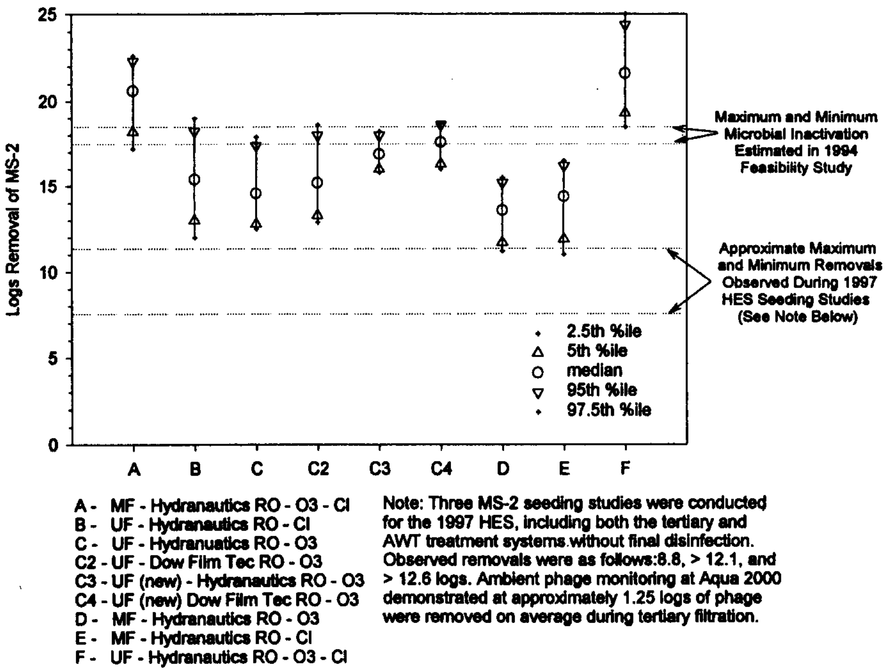

Figure 7. Summary of Monte Carlo analysis. Log removals of investigated treatment trains based on MLE predictions for each individual treatment unit and 5000 trials for each treatment train.

Results from the full scale plant seeding studies conducted during the 1997 HES investigations indicated that the combined tertiary and AWT processes removed between 8.8 and greater than 12.6 logs of seeded MS-2 without final disinfection (Cooper *et al.*, 1997). Because the 1997 HES results represent removals from the combined tertiary and AWT processes, an estimate of tertiary treatment efficiency was needed to compare the 1997 **HES results with** the Aqua 2000 AWT results.

Review of the Aqua 2000 routine coliphage monitoring data, indicated that tertiary treatment removed approximately 1.25 logs of coliphage on average between October 1996 and June 1997. Therefore, it is assumed that the1997 HES minimumand maximum removals without tertiary treatment corresponded to 7.55 and 11.35logs, respectively (i.e. 8.8-1.25 and >12.6-1.25).

As shown in Figure 7, all of the treatment systems investigated removed significant quantities of coliphage. It can also be noted that the methodology used is sensitive enough to account for relatively small differences between treatment systems. The predicted median log removals of the treatment trains of interest varied between 13.6 and 21.6 logs. Based on influent data generated from routine monitoring and the predicted treatment train removal rates, the median predicted effluent concentrations ranged from 8.5×10^{-11} to 8.0×10^{-19} pfu/100mL of coliphage.

Since many of the unit process distributions are based on seeding study data which were observed below detectable limits, it should be understood that the results for all of the simulations should be viewed as conservative. Moreover, the correct interpretation of the results is as a relative comparison of performance rather than an absolute estimate of microbial removal through the treatment systems. Modification of the current methodology to estimate more accurately the absolute removal of a particular treatment systems is a topic of current research.

An independent Health Advisory Committee assembled to review this work concluded that all treatment trains with predicted microbial removal greater than or equal to the removal reported during the 1997 HES are at least as effective as that treatment train with respect to microbial removal and/or inactivation. Examination of Figure 7 reveals that only process alternatives D and E failed to match the maximum performance observed during those investigations. Note however that even alternatives D and E exceeded the maximum removals observed during the 1997 HES more than 95% of the time. On the other hand, only one of the process trains (Alternative F) met or exceeded the performance of the process train proposed by the City of San Diego and approved by the CA DHS (Alternative A).

CONCLUSIONS

The work described above will be used by decision-makers including the City of San Diego and the California Department of Health Services to evaluate and select the configuration for the planned Advanced Wastewater Treatment System. As shown by this work, the use of multi-stage Monte Carlo simulation appears to be a viable technique for comparison of relative effectiveness of treatment systems involving multiple treatment units in series, each of which is capable of removing virtually all of a constituent of concern, In such cases, the potential removal capability of the entire treatment system cannot be directly measured, and this method of estimation provides a reasonable quantitative measure for relative comparison. Although this work was directed at virus removal, the methodology could also be applied to organic chemicals or other constituents which are effectively removed by a series of treatment processes, to less than detection limits in the plant effluent.

ACKNOWLEDGEMENTS

This research was conducted as a collaboration between the Public Health Institute, EOA, Inc., BioVir Laboratories, and Montgomery Watson under contract to the City of San Diego. The authors would like to acknowledge their collaborators, Robert Hultquist, Richard Sakaji, and Toby Roy of the California Department of Health Services, as well as Samer Adham and Joan Oppenheimer of Montgomery Walson. The authors would also like to gratefully acknowledge Richard Danielson, David Ross and Daniel Smith for their considerable help with this research. This research was funded by the City of San Diego Metropolitan Wastewater Department.

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