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Uncertainty in pH and Temperature Corrections for Ammonia Toxicity

William J. Lewis, Jr.

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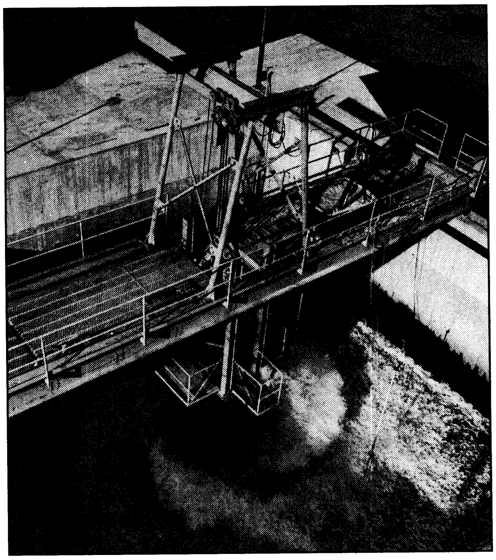
Nationwide, un-ionized ammonia and chlorine probably represent the two greatest challenges to aquatic life in the immediate vicinity of wastewater outfalls. Because these two substances are spontaneously and rapidly converted to non-toxic forms, they have often been given lower regulatory priority than more insidious toxins, such as metals or refractory organic substances, that persist in the environment. However, the general tightening of water quality standards is now causing many facilities to approach or exceed the allowances for discharges of un-ionized ammonia and chlorine. Particularly for ammonia, tightening of standards is of concern because of the vast costs that will ensue from nitrification of much of the nation's effluent.

Protection of aquatic life is mandatory, yet the basic requirements for protection are still being explored in very fundamental ways. Unlike residual toxins, which present the possibility for harm at some future time and place even when regulated to non-toxic levels, ammonia removal must be fully justified by immediate environmental benefits. In the face of uncertainty, regulatory authorities may favor conservative standards, while dischargers will typically favor more liberal ones. A central focus of the controversy over appropriate protection is the national criteria document, which defines the federal regulatory position and sets patterns for many state regulatory agencies.

In 1985, the U.S. Environmental Protection Agency issued a new national criteria document for un-ionized ammonia[1] that contains a comprehensive review of the toxicity of un-ionized ammonia to aquatic life. Using this information, the document proposes national criteria concentrations for exposures of aquatic life to un-ionized ammonia. Two sets of concentrations are proposed, one of which is applicable to waters containing salmonids (including trout and salmon) or other sensitive cold-water species, and the other to waters lacking such species. Each set of concentrations consists of chronic and acute limits of exposure corresponding to specific combinations of temperature and pH. Thus, application of the national criteria will depend on the pH and temperature characteristics of the environment. The criteria document also suggests a procedure for derivation of site-specific standards according to a pattern similar to that used in the establishment of the national criteria. If such procedures are used, the resulting site-specific standards will also be dependent on temperature and pH.

The incorporation of pH and temperature dependency into the national criteria tables and into the derivation of site-specific standards seems well-founded, given that toxicity experiments with numerous species of aquatic life have demonstrated changes in the toxicity of specific concentrations of un-ionized ammonia in relation to ambient pH and temperature. Although some experiments have failed to turn up evidence of pH or temperature dependency on ammonia toxicity,[2] the persistent occurrence of such effects in most experiments justifies the inclusion of

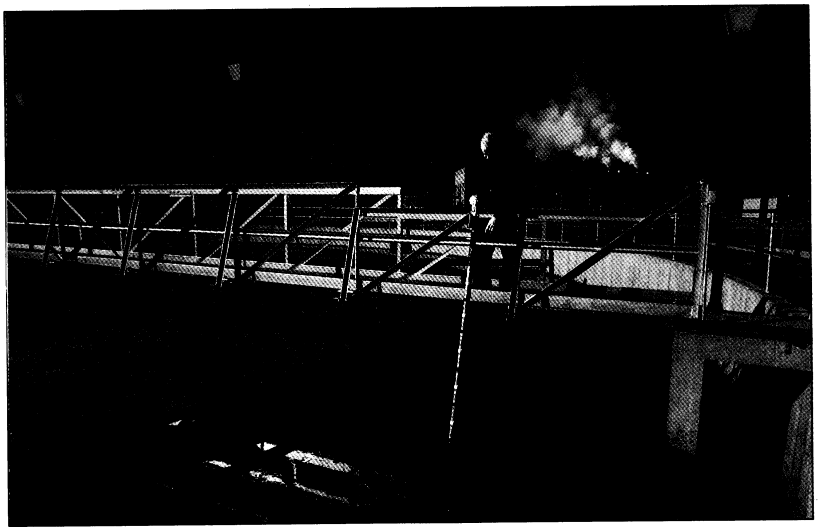


■ **Testing** effluents that are released into coastal waters can indicate whether ammonia toxicity will pose a future problem (center); trickling filter (right); sludge blanket depth is monitored following secondary treatment (bottom).

Photo courtesy of the Massachusetts Water Resources Authority.

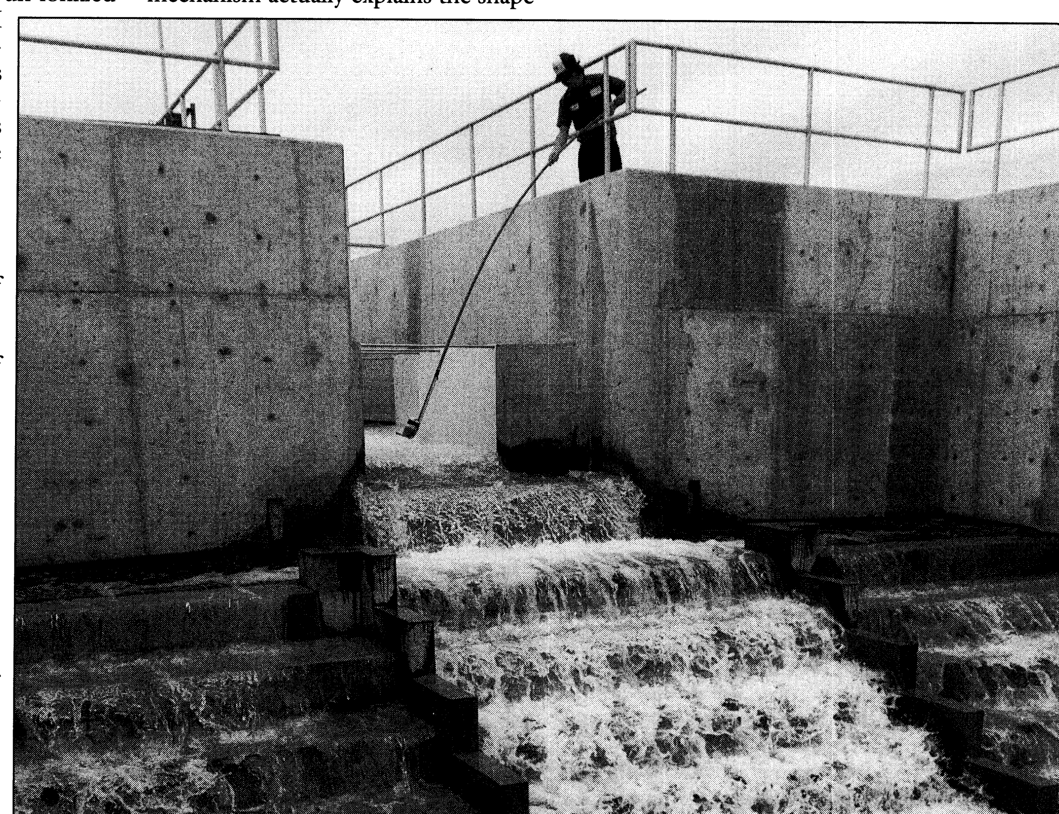
some kind of pH and temperature adjustment procedure. At least some of the species in most environments are likely to show the pH and temperature effects that have so often been documented in the literature.

The development of specific pH and temperature correction procedures as a component of the criteria document was handicapped to some degree by a restricted data base. The text of the criteria document acknowledges considerable uncertainty concerning the exact form of the relationships between ammonia toxicity. However, it does not provide any quantitative information on the degree of uncertainty that is associated with specific criteria concentrations. The absence of this information is of great practical importance because



the criteria concentrations will, in the absence of large amounts of dilution water, place stringent restrictions on the total ammonia concentrations of effluents, thus potentially leading to requirements for costly effluent nitrification. Furthermore, individual states may have adopted or may adopt in the future other kinds of pH and temperature corrections to serve as a basis for state standards or site-specific standards. In these instances, it will be useful to know whether given pH and temperature corrections are in conflict with the corrections given in the national criteria document, or whether they fall within the range of uncertainty that is inherent in the data base and underlying assumptions for pH and temperature corrections in the criteria document.

The purpose of the present analysis is to explore the major sources of uncertainty in the pH and temperature corrections of the new criteria document, and to present some estimates of the size of this uncertainty as applied to specific concentrations of un-ionized ammonia. First, the pH correction is analyzed, followed by a similar analysis of the temperature correction. A third section deals with the combination of the uncertainties.



Ammonia toxicity and pH correction

Variation in toxicity of total ammonia with pH has long been recognized.[3] However, the separation of this pH dependency into two components is more recent. Because the proportion of total ammonia that is un-ionized varies markedly with changing pH, the decrease in toxicity of a given amount of total ammonia with decreasing pH was at first interpreted simply as a reflection of the decreasing dominance of the un-ionized form at lower pH, given the assumption that the un-ionized form accounts for virtually all of the toxic effect. However, toxicity tests with a number of freshwater species have demonstrated a residual trend in toxicity with pH after the proportional change in the un-ionized component has been considered. This trend takes the form of an increase in toxicity with declining pH for a given amount of un-ionized ammonia.

The relationship between pH and toxicity for a given concentration of un-ionized ammonia is nonlinear.[3] Although very few of the curves for individual species are sufficiently well-defined to show the details of curvature, it appears that the relationship between pH and the logarithm of the LC50 (lethal concentration for 50% of the population) for un-ionized ammonia has four regions: a region of linearity or near linearity at low to moderate pH (generally pH 5 to 7); a region of pronounced curvature causing a stabilization of the LC50 with increasing pH (generally in the range of pH 7 to 8); a plateau over which the LC50 remains nearly constant (generally pH 8 to 8.5); and a downward inflection of the curve, suggesting increased toxicity with further pH rise (pH 8.5 to 9.0). The first three regions of the curve are well accounted for by a joint toxicity model in which both ionized and un-ionized ammonia are toxic, but with differing potency.[3] The ratio of potencies in relationship to the ratio of the ionized and un-ionized fractions controls the shape of the curve. It has not been conclusively demonstrated that this mechanism actually explains the shape of the curve relating pH and LC50 for un-ionized ammonia, but it is not necessary that the mechanism be fully understood for the formulation of criteria based on empirical toxicity data. The increase in toxicity at high pH does not conform to the joint toxicity model or to a closely related empirical model that was used in developing the national criteria.[3] This difficulty is circumvented by the assumption of a fixed toxicity above pH 8. The practical implications of this assumption are discussed below in greater detail.

The empirical equation that serves as a basis for the pH correction is

$$LC50 = LIM\,[1 + 10^{SLP(PHT-pH)}] \quad (1)$$

Where

LC50 = 50% lethal un-ionized ammonia concentration,
LIM = asymptote,
SLP = slope shown by the initial, linear position of the curve,
PHT = transition pH for curvature, and
pH = ambient pH.

Because the equation is used only up to a pH of 8 (above pH 8, the LC50 is set to that of pH 8), the equation is reformulated in the criteria document by substitution:

$$LC50 = \frac{(LC50_{pH8})[1 + 10^{SLP(PHT-8)}]}{(1 + 10^{SLP(PHT-pH)})} \quad (2)$$

Except for the LC50 at a reference pH, all parameters must be fixed in any equation representing the relationship between pH and toxicity. Parameters controlling curvature or asymptotes simply cannot be evaluated case-by-case because this would require sufficient experimental data to define the shape of the pH-toxicity response curve for individual species. For this reason, EPA simplified Equation 2 before using it in the development of the national criteria for ammonia: SLP was assigned a value 1.0, and PHT was assigned a value of 7.4 across all species. The basis for these simplifications will be examined in further detail below.

To summarize, Equation 1 was simplified by EPA in developing the national criteria for un-ionized ammonia in three major ways: by the imposition of an abrupt asymptote at pH 8.0 for the curve relating pH to LC50; using the assumption that the variable SLP can be assigned a constant value of 1.0; and using the assumption that the variable PHT can be assigned a constant value of 7.4. These simplifications, as well as the curve-fitting procedures themselves, are sources of uncertainty in the final criteria numbers.

Curve fitting. The data that was used in quantifying the relationships between pH and toxicity of ammonia was first logarithmically transformed to achieve greater homogeneity of variances.[3] Logarithmic transformations are commonly used for such purposes, but transformation of the LC50 data has some important consequences for uncertainty in the final criteria numbers. It reduces the apparent variability, and thus increases the apparent certainty of the statistical relationships. However, final criteria numbers are retransformed to arithmetic form, and thus carry the correspondingly greater uncertainty of the arithmetic scale.

The criteria document for ammonia reports that the final curve fitting was from data for four taxa (rainbow trout, coho salmon, fathead minnow, and *Daphnia*). The R^2 value of 96% suggests that the curve explains most of the variation in the data (over 90%). One might therefore assume that the degree of variation around the curve is very small for practical purposes, such as predicting criteria concentrations. However, this assumption would be incorrect.

It is not possible to obtain precise confidence limits for most relationships that are intrinsically nonlinear.[4] However, various approximations are possible. For present purposes, it suffices to calculate a minimum value for confidence limits; the actual confidence limits are then known to be at least this broad.

For a linear least-squares regression of Y on X, the 95% confidence interval for a specific predicted value of Y ($\hat{Y}_o$) for a particular value of X ($X\hat{o}$) will be

$$Y_o \pm t_{n,0.975} \cdot s \; \frac{(1 + 1/n + (X\hat{o} - \bar{X})^2)^{0.5}}{\Sigma (X_i - \bar{X})^2}$$

Where

t = t statistic for n degrees of freedom at probability 0.975, and
s = root mean square residual variation.

The minimum value of $(Xo - \bar{X})^2$ is 0 (when $X_o = \bar{X}$); thus the confidence limits are never smaller than

$$Yo \pm t_{n,0.975} (1 + 1/n)^{0.5} \qquad (4)$$

Or, for reasonably large values of n when n is greater than 20,

$$Y \pm 2s \qquad (5)$$

Similar reasoning applies to confidence limits for a least-squares fit to a curvilinear relationship. The true confidence limits will be determined by multiple components, including uncertainty in Y in relation to the mean $\bar{Y}$, and uncertainty in Y as affected by position along the axis of the independent variable. Thus, the 95% confidence interval for predicted value of Y (as in the case of a criteria number predicted from a reference LC50 and a pH) will be at least as large as shown by Equation 5.

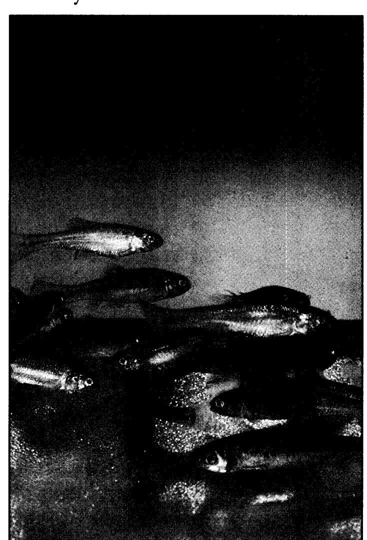
The root mean square residual (s) is not given in the criteria document for the pH curve. However, measurements of distances of points from a data plot of the criteria document lead to an estimate of 0.10 for s. Thus, the 95% confidence band is no closer than 0.2 log units to the curve; the actual limits will be broader, especially near the ends of the curve.

To illustrate the uncertainty in terms of LC50 concentrations on the arithmetic scale, as used in the criteria tables, it is instructive to work through an example. A useful example can be taken from an LC50 of 0.5 mg/L NH_3-N, which would fall within the range of LC50 concentrations for each of the three fish species used in the criteria document over the range of pH that is most common in freshwater environments (pH 7 to 8). The logarithm of 0.5 is -0.30. Adding and subtracting 0.2 log units yields the minimum boundaries for the 95% limits: —0.50 to -0.10. On an arithmetic basis, the corresponding limits would be 0.32 to

0.79 mg/L (the limits are not symmetrical about the mean on an arithmetic scale because of the logarithmic transformation). Thus, the zone of uncertainty ranges from 63 to 159% of the nominal value, 0.5 mg/L. Expressed in terms of percentage, this degree of minimum uncertainty applies across the entire range of LC50 values calculated from the curve (Figure 1).

The foregoing calculation of minimum confidence limits shows that specific criteria concentrations, deviating as much as half from the table values, could not be considered distinct from the table values, even if all other assumptions leading to the derivation of the table values were free of uncertainty. This is simply the variation inherent in the data base from which the pH correction is derived. A similar degree of uncertainty would be applicable to any other specific set of numbers incorporating the pH correction as derived in the national criteria document.

Another aspect of the use of logarithmic transformations is the uneven spread of uncertainty above and below the estimated mean LC50 based on a given pH. As illustrated in the example given above, the boundary for a given confidence band, expressed as a percentage of the estimated value, extends further above

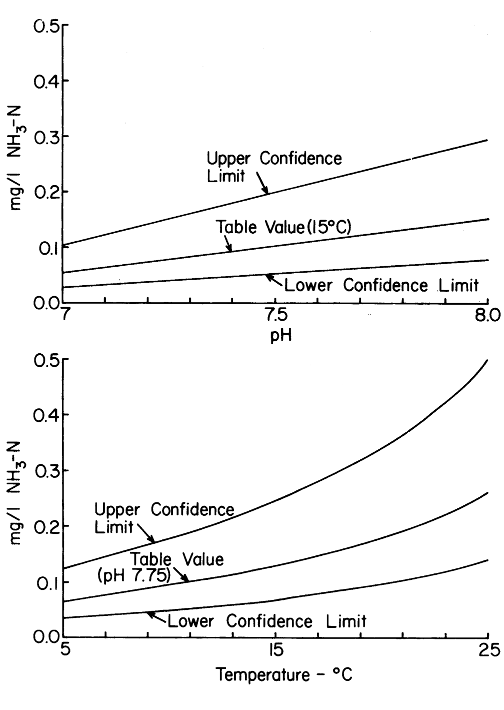


■ **Proper plant maintenance (left and top right) is essential in sustaining acceptable effluent ammonia concentrations; fathead minnows were the only warm-water species represented in the pH and temperature correction procedures (above).**

the estimated value than below the estimated value. Thus, on an arithmetic scale, there is more up- than down-scale uncertainty for a given criterion concentration.

The constant SLP assumption. The optimal value of the parameter, SLP, was determined empirically[3] using Marquardt's algorithm. For data on rainbow trout and coho salmon, the empirically-determined value of SLP approached 1.0 very closely (1.01, 1.02). Thus, it seems reasonable to assume that the value of SLP for these species is exactly 1.0. This assumption is only slightly less reasonable for *Daphnia*, which shows an SLP of 1.13.

The empirical fit for the fathead minnow, which provides one of the four strongest data sets relating pH to LC50, leads to a SLP value of 0.65 that deviates considerably from 1.0 . However, because of the small amount of underlying data, even such a large deviation from 1.0 cannot be considered statistically meaningful.[3] On the other hand, such a large deviation from 1.0 does suggest considerable uncertainty about the most appropriate fixed value of SLP. In terms of applications, the curve for the fathead minnow has particular significance because the fathead is the only warm-water fish species in the group of taxa from which the pH corrections were derived. The rationale in defense of fixing SLP at 1.0 is that R^2 shows little deterioration for individual species if the value of SLP is assumed to be 1.0 in all cases. Although this is correct, a deterioration in the explained variance that is relatively small in terms of R^2 actually has considerable practical significance because of the logarithmic transformation of the LC50 values, as discussed above. The decline in R^2 from 0.97 to 0.93 for the fathead minnow when SLP is assumed to be 1.0 represents approximately a doubling in the amount of variance that cannot be accounted for by the curve. Because an R^2 of 0.96 corresponds to 95% uncertainty bands extending approximately 50% around a nominal LC50 value, the implications of doubling the unexplained variance of points from the line are considerable. Thus, while it is true that the absolute decrease in R^2, caused by the assumption of constancy in SLP is small, the practical implications for uncertainty in actual LC50 values are considerable.



Given the need to select a single SLP value, it seems logical to set SLP equal to 1.0 because the value 1.0 is not only near the mean value of all the individual SLP determinations, but also is consistent with a plausible mechanism (the joint toxicity model) for the toxicity of ammonia. However, the choice of a fixed value introduces uncertainty, particularly because the fathead minnow data did not conform well with the assumption. Two other species, the green sunfish and the smallmouth bass, show good explanation of variance (R^2 = 99%) combined with values of SLP below 1.0: 0.3 for the smallmouth bass and 0.9 for the green sunfish. Thus, of the three nonsalmonid species that conform well with the empirical model, all have SLP values below 1.0. While this easily could be explained by chance, it illustrates uncertainty in the assignment of a constant value to SLP.

Use of a constant value for PHT. The criteria document uses a constant value of 7.4 for the parameter PHT. As explained in the criteria document, this parameter value was obtained by pooled regression analysis of data for four taxa: *Daphnia*, fathead minnow, rainbow trout, and coho salmon. The criteria document acknowledges that uncertainty results from the assumption that PHT is constant at 7.4. It is possible that PHT differs across species. Also, even if PHT were constant across species, the assumed value of PHT is subject to error because it is based on only 38 data points, the combined size of the data set for the four species.

In addition to these acknowledged sources of uncertainty, there are two other sources not expressedly acknowledged. First, the use of a pooled regression approach to estimate PHT, in effect, does not equally weigh the taxa that contribute to the overall pool of data. This is so because the number of data points for individual taxa are not the same. Second, the restriction of the pooled regression analysis to only four species implies that the individual data points for other species are not valid for determining the shape of the pH-LC50 relationship.

According to the criteria document, a pooled regression was used in obtaining the lowest value to be used for a constant for PHT. This pooled regression was evidently based on data for four species: *Daphnia*, coho salmon, rainbow trout, and fathead minnow. Although the method for pooling is not given, a pooled regression for a combination of species is likely to be influenced by each species in proportion to the number of data points for that species. The data points for the four species used in the pooled regression for the criteria document are as follows: *Daphnia*, 18 points; coho salmon, 7 points; rainbow trout, 7 points; fathead minnow, 6 points. Thus, *Daphnia* accounts for almost half of the pooled data set, and has an accordingly disproportionate influence on the determination of PHT. The value of PHT for *Daphnia* is within the mid-range for the four species, but is substantially greater than the PHT value of 7.79 for the fathead minnow.

Even more significant than the disproportionate influence of *Daphnia* is that the PHT determination did not consider PHT values for other taxa. The exclusion of other taxa is justified by the insufficient range of pH or the insufficient number of data points represented for the other taxa. However, of the other taxa examined, four show values of R^2 equal to or greater than 98%.[3] Because the R^2 value is used as an indicator of satisfactory fit, it seems arbitrary to exclude some taxa for which the R^2 value is high, particularly because it is suspected that PHT may vary among species. If PHT varies among species, it is important to include as many different species-specific estimates as possible. Exclusion of species is done on a rational basis, but there are equally valid arguments for the inclusion of a broader range of species, which would almost certainly broaden the confidence limits for variation around a curve based on constant PHT. While restriction of the curve-fitting to the four species represented by the best data sets results in the best fit of data to the final curve, this may give an errone-

■ **Tighter water quality standards, particularly for ammonia, are forcing treatment facilities to operate at or above accepted limits.**

ous impression of the goodness of fit for species in general because the four species selected for use in curve fitting are also those that deviate least from each other in curve parameters. For this reason, the pooled 0.96 R^2 value for the final relationship with constant SLP and PHT may be misleadingly high.

Flattening of the curve at pH 8. As explained in the criteria document, there is evidence for increasing toxicity of un-ionized ammonia as pH increases above 8.5. This phenomenon cannot be identified unequivocally because of the small number of data points within this range. An empirical model could be formulated to reflect the suspected reversal in slope in the vicinity of pH 8.5. However, this would involve the introduction of at least one more parameter, which could scarcely be justified in view of the small number of points available for estimating the values of multiple parameters. Consequently, as a practical expedient, the national criteria numbers are based on the assumption that the LC50 value flattens at a pH of 8.0. The criteria document acknowledges that this will cause a fitted curve to pass slightly below the apparent peak at pH 8.5, but closer to the data at 9.0. The flattening of the curve introduces bias involving underestimation of LC50 at pH 8.0 to 8.5 and overestimation somewhere above pH 8.5.

Bias in the curve relating pH to LC50 is of much greater practical importance for pH values between 8.0 and 8.5 than it is at higher pH because of the smaller percentage of surface waters in the U.S. with pH above 8.5. Thus, while the simplifying assumption for flattening the pH-LC50 curve seems to be rational or fair in the sense that it balances underestimation of the LC50 in one pH range with overestimation in another pH range, the practical effect is to ensure consistently low LC50 values within the pH range occupied by a substantial proportion of surface waters. While the magnitude of this bias cannot be specified precisely, an estimate can be made based on available data.

Only four values shown in the previously referred to figure in the criteria document fall between pH 8.1 and 8.4 (between 8.0 and 8.5, but exclusive of the boundaries). As expected, all four of these lie above the fitted curve used in developing the criteria numbers. The probability of this occurring by chance is $(1/2)^4$, suggesting that the suspected bias does appear. The mean deviation between the fitted curve and the available LC50 estimates from pH 8.0 to 8.5 is 0.07 log units, or 17%. The bias will not be uniform within that pH range, however, and the data base is not large enough to define the bias well.

The temperature correction

Temperature affects the ionization of ammonia. Thus, increasing temperature is typically accompanied by increasing toxicity for a given concentration of total ammonia. However, after a correction is made for the ionization effect, there is a residual trend toward higher toxicity of ammonia at lower temperatures for most fish species that have been tested over a range of temperatures.[3] Generally speaking, the LC50 changes three-to-four-fold over temperature ranges of 10° to 20°C, which are typical environmental temperature ranges for most fish species. Given this indication of higher toxicity for un-ionized ammonia at lower temperatures, some adjustment of criteria numbers for temperature is appropriate.

The temperature adjustment used in the national criteria document is based on data assembled from 13 studies, including six species.[3] As in the case of the pH studies, the LC50 data were logarithmically transformed.[3] Plots of the transformed data indicated an essentially linear relationship between temperature and LC50. The line of best fit for each species was reported, and statistical information was given on a species-by-species basis.[3]

The national criteria document uses a temperature correction based on an equation of the form[3]

$$LC50 = LCR\,[10^{SLT(T-20)}] \qquad (6)$$

Where

LCR = LC50 at a reference temperature of 20°C,
SLT = slope of the relationship relating the logarithm of LC50 to the temperature, and
T = temperature.

The criteria document fixes the value

of SLT at 0.03, which is the arithmetic mean of the individual values of SLT across the 13 studies.[3] Some special conditions are then set for application of the equation at high temperatures. These special conditions, which differ for cold- and warm-water species, acknowledge flattening of the LC50 at the upper temperature ranges and prevent application of increasing LC50 concentrations at temperatures that become inherently stressful to fish.

As in the treatment of pH, the criteria document acknowledges the need for more extensive information and uncertainty concerning the precise form of the relationship relating temperature to LC50. However, the criteria document does not specify the degree of uncertainty that should be attached to the temperature corrections.

Uncertainty in SLT. Whereas the pH corrections were made on the basis of the four strongest data sets, the temperature corrections were made on an entirely different basis, using arithmetic averaging across all available data sets, including those incorporating only two points. This inconsistency calls into question the philosophy underlying the treatment of the parameter values. If species are suspected of differing in their parameter values, or if experimental conditions may have influenced the parameter values in unknown ways, it is more appropriate to average parameter values than to select strong data sets or to pool data sets. Consequently, the determination of SLT is probably more appropriate than the determination of parameters for the pH correction. However, in both instances, uncertainty is introduced by the need to choose between the strongest data sets and an adequate representation of variation among species or across experimental conditions.

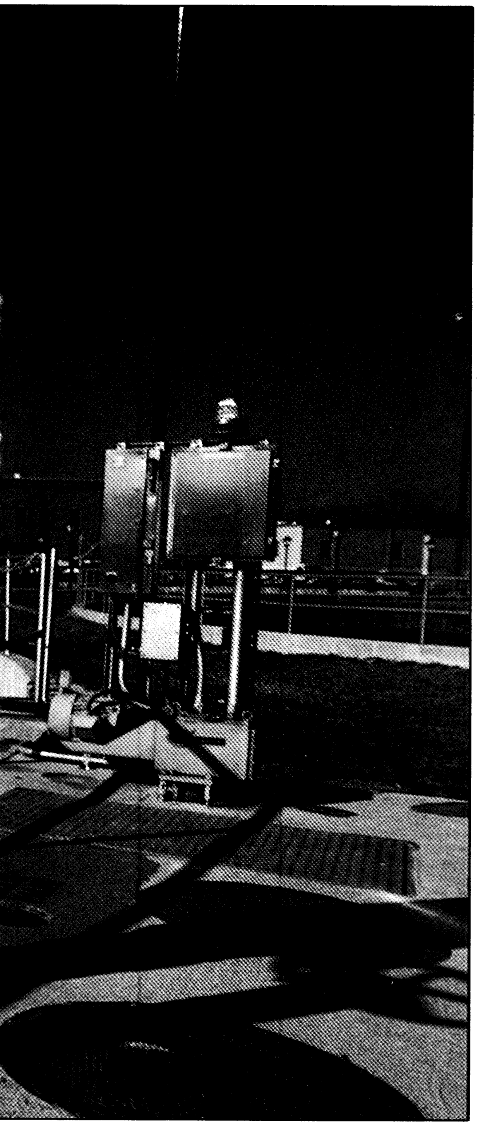
The criteria document states that there are no statistically significant differences among slopes for different species. This might be taken as an indication of strong uniformity across species. Instead, it is more a reflection of the weakness of the data set, and particularly of the sparse number of points for some of the species.

As noted in the criteria document, the values of the slopes for individual species vary from 0.016 to 0.054 around the arithmetic mean of 0.03 used in the criteria document. The uncertainty associated with this range of variation in slopes should be clarified. For this purpose, we may consider a hypothetical example in which the reference LC50 (at 20°C) is 1 mg/L, and the environmental temperature is 10°C. For this combination of conditions, the LC50 is 0.50 mg/L if the slope is 0.03. However, at a slope of 0.054, the LC50 would be 0.69, and at a slope of 0.016, the LC50 would be 0.29. Thus, the differing slopes correspond to a range of 58 to 138% around the value predicted by the mean slope (Figure 1).

■ **Until the requirements for the protection of aquatic life are known, dischargers will likely favor more liberal operating standards.**

Uncertainty for individual species. The degree of uncertainty in the relationship between LC50 and temperature for individual species is surprisingly high. The three strongest data sets used in the derivation of the temperature correction are for the fathead minnow, rainbow trout, and channel catfish.[3] Each of these relationships is based on 15 or more data points over a good range of temperatures. The R^2 values are, however, surprisingly low: fathead minnow, 53%; rainbow trout, 44%; and channel catfish, 76%. Thus, as much as half of the variance in these relationships cannot be accounted for by temperature. Higher values of R^2 for other species are not meaningful in most cases because of the very small number of points. In a number of cases, only two points were used. Thus, the data demonstrate a large amount of scatter around the relationships that serve as a basis for the temperature correction. On a relative basis (R^2), the scatter for data applicable to individual species is much larger than it is for the pH relationship.

Uncertainty associated with scatter around the final temperature correction. The 95% limits of LCR and SLT for individual species are quite broad,[3] even for the most favorable determinations, and thus indicate considerable uncertainty for any specific determination of the temperature correction. However, of greater direct relevance to the final criteria values that incorporate temperature corrections would be the confidence limits that should be attached to temperature corrections across all species based on the fixed 0.03 value for SLT, as adopted in the criteria document. Because the data



points are drawn from different populations, a precise determination of confidence limits is impractical. However, as in the case of confidence limits for pH, it is possible to calculate minimum confidence limits from the residual sum of squares. The actual confidence limits will be broader than this calculated minimum.

The deviation of each of the data points from the common temperature correction line was estimated by measurement on the graphs. These deviations, expressed in logarithmic units, were squared, summed, and divided by degrees of freedom. The square root of this quantity, which is the root mean square residual, is 0.1 log units of LC50. As shown by Equations 3 to 5, the minimum 95% confidence interval for a predicted value is plus or minus two times the root mean square with respect to the regression line; this minimum will be approached most closely near the center of the data set ($\bar{X}$, $\bar{Y}$). For example, if a temperature-corrected LC50 is predicted to be 0.5 mg/L, the minimum confidence limits would extend -0.2 to +0.2 log units; converting to an arithmetic scale, the limits would be 0.32 to 0.79 mg/L. Thus, the minimum confidence limits extend from 63 to 159% of the predicted value. At some distance from $\bar{X}$, confidence will be lower because uncertainties associated with the determination of the slope have a greater effect on Y at greater distances from the center. As in the case of the pH correction, the band of uncertainty is broader above the predicted LC50 than below the predicted LC50 because of the logarithmic transformation of data that is used in making arithmetic projections.

Combinations of pH and temperature

The criteria document acknowledges that interactions between pH and temperature are not quantifiable using present information. Any such interaction would introduce bias into the combined temperature and pH corrections.

In addition to direct interaction, there is a compounding of variance in the pH and temperature corrections when the two are used together in making individual LC50 estimates for specific combinations of pH and temperature. For a particular estimate, the sums of squares are additive (assuming no interaction). As shown in the preceding analysis, the minimum standard deviation around an individual prediction would be 0.1 for pH and 0.1 for temperature. The underlying sums of squares are 0.01 for pH and 0.01 for temperature; the combination is thus 0.02. The square root is 0.14, which corresponds to 95% limits of ± 0.28 log units. For an LC50 of 0.5 mg/L, the minimum 95% limits would be 0.26 to 0.95 mg/L, or 52 to 190% of the nominal value. On a percentage basis, these minimum limits apply to all predictions. This is a minimum approximation of the confidence limits because higher individual variances will apply for most combinations of pH and temperature correction. In addition, sources of uncertainty that cannot be quantified are not fully represented in these estimates of variance. This is particularly true for chronic criteria, which are subject not only to the same uncertainties as the acute criteria, but also to variance associated with estimates of the acute:chronic ratio. Some uncertainties are likely to introduce bias, while others will magnify scatter.

Conclusions

The new national criteria for ammonia, unlike previous criteria, acknowledge a relationship between pH, temperature, and the toxicity of a given concentration of un-ionized ammonia. Because of the incorporation of factors that modify toxicity, the new criteria are more realistic and better justified from a conceptual viewpoint than simpler criteria. This improved realism is desirable, and may even be considered essential if both environmental protection and the cost-effectiveness of wastewater treatment are to be maximized. More simplistic standards cannot accommodate variations in toxicity, and therefore may be wasteful of either economic or environmental resources, or both.

Although more complex criteria, such as those for ammonia, are more realistic, they are also more difficult to evaluate. Whereas the conformance of individual species with simplistic standards is relatively easy to judge from inspection of empirical data on which criteria are based, sources of error for more complex standards become more obscure, and there is a greater danger that new errors will be introduced through compounded variances or through erroneous modeling assumptions that introduce bias. Thus, a more complete treatment of error is a desirable adjunct of future criteria documents. For ammonia, until the data base improves, the national criteria should be viewed as a set of rational guidelines, from which the ideal criteria may ultimately be found to deviate considerably. ■

William J. Lewis, Jr., is professor and director of the center for limnology at the Univ. of Colorado at Boulder.

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