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MODEL CALIBRATION FOR THE HIGH-PURITY OXYGEN ACTIVATED SLUDGE PROCESS – ALGORITHM DEVELOPMENT AND EVALUATION

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ABSTRACT

A model calibration algorithm is developed for the high-purity oxygen activated sludge process (HPO-ASP). The algorithm is evaluated under different conditions to determine the effect of the following factors on the performance of the algorithm: data quality, number of observations, and number of parameters to be estimated. The process model used in this investigation is the first HPO-ASP model based upon the IAWQ (formerly IAWPRC) Activated Sludge Model No. 1. The objective function is formulated as a relative least-squares function and the non-linear, constrained minimization problem is solved by the Complex method. The stoichiometric and kinetic coefficients of the IAWQ activated sludge model are the parameters focused on in this investigation. Observations used are generated numerically but are made close to the observations from a full-scale high-purity oxygen treatment plant. The calibration algorithm is capable of correctly estimating model parameters even if the observations are severely noise-corrupted. The accuracy of estimation deteriorates gradually with the increase of observation errors. The accuracy of calibration improves when the number of observations (n) increases, but the improvement becomes insignificant when n>96. It is also found that there exists an optimal number of parameters that can be rigorously estimated from a given set of information/data. A sensitivity analysis is conducted to determine what parameters to estimate and to evaluate the potential benefits resulted from collecting additional measurements.

KEYWORDS

Activated sludge; model; calibration; complex; oxygen; parameter estimation.

INTRODUCTION

The high-purity oxygen activated sludge process (HPO-ASP) was invented in the late 1960s, and has been widely used since then in large, mature cities with developed infrastructures and where land available for expansion is difficult to find. Many advantages of the HPO-ASP have been claimed over the air systems, such as more active biomass, better settling characteristics of sludge, etc. From the perspective of oxygen transfer, the most important advantage is the tremendous increase of oxygen transfer rate (OTR). The typical average oxygen transfer driving force for a HPO-ASP system operating at a mixed liquor D.O. level of 6 mg/l is approximately 25 mg/l as compared with 7 mg/l for an air system operating at a D.O. level of 2 mg/l.

This means that on an overall basis the high-purity oxygen activated sludge process will transfer about 3.6 times as much oxygen as an air system.

The HPO-ASP is more complicated than an air system. The complexity mainly results from the use of high purity oxygen (purity over 97%) and multi-stage (usually 3 to 4 stages), closed aeration tanks. Figure 1 shows the flow diagram of a typical HPO-ASP.

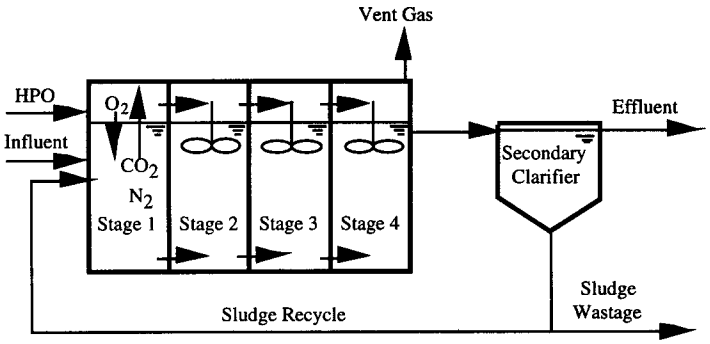

Fig. 1. High-purity oxygen activated sludge process.

The Sacramento Regional Wastewater Treatment Plant, which has a treatment capacity of approximately 6.57 m^3/sec, was used as a model for this investigation.

Process Model. Process models have been developed and applied to better understand and control the sophisticated process. An incomplete list of recent publications on this topic is Clifft and Andrews (1986), Stenstrom *et al.* (1989), Stenstrom (1990), Clifft and Barnett (1990), Clifft (1992), and Tzeng (1992).

The HPO-ASP model used in this study is a new process model which was developed based on the IAWQ Activated Sludge Model No. 1 (Henze, *et al.*, 1987; Yuan, 1993). None of the above publications used Activated Sludge Model No. 1.

The process model was applied to static conditions in this research. Sinusoidal excitation was applied to the process model to mimic the diurnal change in influent flow and substrate.

Model Calibration. Model calibration represents the process of assigning values to the parameters used in the model such that the error between the model predictions and the observations from the real plant is minimal. Model calibration has been done by hand in many cases in the past, but is difficult for process models that have a large number of parameters. Activated Sludge Model No. 1, after being simplified for the HPO-ASP, has 11 biokinetic parameters - 4 stoichiometric coefficients and 7 kinetic coefficients. The total number of parameters of the process model is well over 30. The necessity for developing a model calibration algorithm is obvious. Tzeng (1992) performed the first model calibration that used observations from a full-scale oxygen activated sludge treatment plant. The particular process model that Tzeng calibrated uses the Clifft and Andrews structured activated sludge model (Clifft and Andrews, 1986).

Many questions need to be answered before a model calibration algorithm is developed and the corresponding calibration is implemented, such as: What observations are to be used in the calibration? How many data points are adequate for the calibration? How many parameters can be rigorously estimated from a given set of observations? The answers to these questions are crucial to the success of the calibration.

The objective of this study is to present the development and evaluation of a model calibration algorithm for the high-purity oxygen activated sludge process. More specifically, we intend to find out the effects of the following factors on the performance of the calibration algorithm: data quality, number of data points, and

the number of measured variables. The investigation is accomplished through numerical experiments in which the observations are generated numerically by corrupting model predictions with Gaussian noise. By doing so, we guarantee that the model is not the cause if a good fit is not achieved. We also have the advantage of knowing the 'true' values of the parameters and have the flexibility of adjusting the data quality (e.g. greater or lesser variability in data).

MODEL CALIBRATION METHOD

The basic approach in all calibrations is usually the same: An objective function (or merit function) is designed that measures the agreement between the data and the model with a particular choice of parameters. The objective function is conventionally arranged so that small values represent close agreement. The parameters of the model are then adjusted to achieve a minimum in the objective function. The adjustment process is thus a problem in minimization in many dimensions.

Objective function. Least-squares is the most common form of objective function used. Three kinds of least-squares objective functions can be used: absolute least-squares (ALS) (Eq. 1), weighted absolute least-squares (WALS) (Eq. 2), and relative least-squares (RLS) (Eq. 3). ALS is not appropriate for the activated sludge process because the magnitudes of observations differ significantly. For example, the ranges of some observations in a full-scale HPO-ASP are: DO 5-12 mg/l; vent gas oxygen purity 0.40-0.80 (oxygen mole fraction); MLSS 1000-2000 mg/l. One possible solution to the uneven-weight problem associated with the ALS objective function is WALS which solves the problem by assigning an appropriate set of weights to different variables measured. Another possible solution is to normalize the function by dividing the difference between the model-predicted and observed values by the model-predicted value. This is RLS (Eq. 3). Eq. 4 represents the relative least-squares objective function that uses observations of 1st stage DO, 4th stage DO, vent gas oxygen purity, and MLSS.

$$f = \sum_{j=1}^{m}\left(\sum_{i=1}^{n}\varepsilon_{a_{ij}}^2\right) = \sum_{j=1}^{m}\left(\sum_{i=1}^{n}\left(S_{ij} - S_{ij}^*\right)^2\right) \qquad \text{(Eq. 1)}$$

$$f = \sum_{j=1}^{m}\left(\sum_{i=1}^{n}\gamma_{ij}\varepsilon_{a_i}^2\right) = \sum_{j=1}^{m}\left(\sum_{i=1}^{n}\gamma_{ij}(S_{ij} - S_{ij}^*)^2\right) \qquad \text{(Eq. 2)}$$

$$f = \sum_{j=1}^{m}\left(\sum_{i=1}^{n}\varepsilon_{r_{ij}}^2\right) = \sum_{j=1}^{m}\left(\sum_{i=1}^{n}\left(\frac{S_{ij} - S_{ij}^*}{S_{ij}^*}\right)^2\right) \qquad \text{(Eq. 3)}$$

$$f = \sum_{i=1}^{n}\left(\left(\frac{p_{O_{2_4}}^* - p_{O_{2_4}}}{p_{O_{2_4}}^*}\right)_i^2 + \left(\frac{S_{O_{2_1}}^* - S_{O_{2_1}}}{S_{O_{2_1}}^*}\right)_i^2 + \left(\frac{S_{O_{2_4}}^* - S_{O_{2_4}}}{S_{O_{2_4}}^*}\right)_i^2 + \left(\frac{MLSS^* - MLSS}{MLSS^*}\right)_i^2\right) \qquad \text{(Eq. 4)}$$

where S - the observed variable; i - as subscript, denotes the ith observation; j - as subscript, denotes the jth observed variable; * - as superscript, denotes predicted values; m - total number of observed variables; n - total number of observations; γ - weight; ε_a - absolute error; ε_r - relative error. The model includes a mass balance on the gas phase so that the oxygen uptake rate (OUR), which is frequently used by other investigators for parameter estimation, is not linearly independent, and its inclusion would not add further information, except to identify errors in other data. Only limited OUR data are available from the plant, and is of questionable value since it is infrequently collected.

Most measurements in biological systems have normally or log-normally distributed relative errors instead of absolute errors. Saez and Rittmann (1992) demonstrated that the relative least-squares objective function (Eq. 3) is superior to the absolute least-square criterion (Eq. 1) where observations (state variables) differ significantly in magnitude, such as in the activated sludge process.

Constraints. The parameters in the HPO-ASP model have clear physical implications. For example, the heterotrophic yield Y_H must have a value between 0 and 1. In reality, Y_H has an even narrower bound, such as between 0.5 and 0.8. This is true for all parameters in the process model. To ensure that the parameter values selected by the calibration program are physically feasible, it is necessary to impose constraints on them. In the calibration program, the constraints are given in the form of upper and lower bounds. With well defined parameter bounds, it takes less iterations for the objective function to converge to its minimum. However, if the calibration algorithm is robust, the constraints should not be too stringent, that is, the range between the upper and lower bound should not be too narrow.

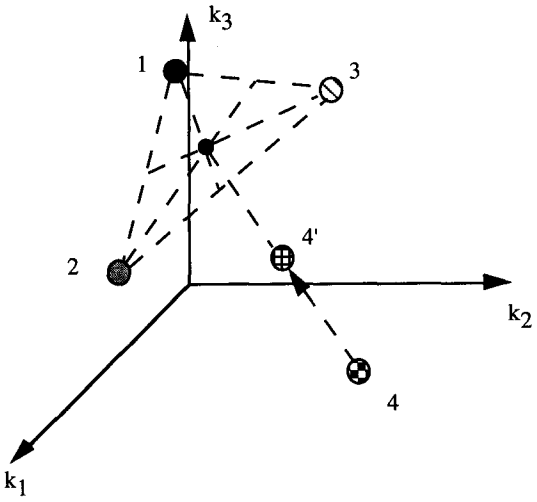

Fig. 2. Illustration of the complex method.

Observations. The observations used in this study are generated mathematically as follows. For a state variable S at time t, the relative error of the observation, S_i, to the exact solution S_i^*, is defined as:

thus $S_i = S_i^* + \varepsilon_r S_i^*$. If ε_r is normally distributed, with mean $\mu = 0$ and variance = τ, then the observation S_i is also normally distributed, with mean $\mu = S_i^*$, and variance = τS_i^*. If $\tau = 0.10$, this means the variance of the observation equals to 10% of the exact solution S_i^*.

Optimization method. After the objective function and constraints of parameters are defined, the calibration problem is transformed into a nonlinear, constrained optimization problem. Many optimization techniques are available for this purpose, such as the Gauss-Newton method. The particular algorithm used in the research is the Complex Method. The Complex method was developed in 1965 by Box (Box, 1965). Its derivation is not rigorously based on mathematical theory. It is an empirical method. It, however, has been proved to be a very robust optimization algorithm for many engineering problems (Little and Williams, 1992). The Complex method is derivative-free, and thus remarkably robust to messy problems such as discontinuities and difficult-to-evaluate or nonexistent derivatives.

Figure 2 illustrates the basic idea of the Complex method for a 3-parameter system. Each point (k_1,k_2,k_3) in 3-D space represents a set of parameters to be estimated. The method requires at least four sets of parameters to be initially selected, and scatters them randomly in the domain. For this 3-parameter system, four sets of parameters are chosen. They are denoted as points 1, 2, 3, 4 in Figure 2. Mathematically, this is implemented as:

$$\theta_{i,j} = L_i + r_{i,j} (U_i - L_i)$$

where

i = as subscript, denotes the ith parameter ($i=1,2, ..., N$),
j = as subscript, denotes the jth set of parameter ($j=1, 2, 3, ..., K$),
N = number of parameters,
K = number of parameter sets,
$r_{i,j}$ = a random real number between 0 and 1,
$\theta_{i,j}$ = value of the ith parameter in the jth set of parameters,
U_i = upper bound of the ith parameter, and
L_i = lower bound of the ith parameter

Each point (each set of parameters) is used to make predictions and the objective function is calculated from model predictions and observations. The point (set of parameters) which causes the largest objective function (largest error) is identified, say, as point 4. Point 4 is then moved half way to the middle point between the centroid of points 1, 2, and 3 and point 4. Now point 4 becomes point 4'. The parameter values of point 4' are used to make predictions, the objective function is calculated and its value is compared to those of points of points 1, 2, and 3. A highest value is found, and that point is adjusted through the same procedure as described. This is iterated again and again, until all sets of parameters give the same function value (Kuester and Mize, 1973).

Other. The initial conditions and inputs used for observation generation and prediction are the same. Sinusoidal inputs are used to represent the diurnal changes in influent quantity and quality. Tabulated in Table 1 are the values of the stoichiometric and kinetic coefficients used for observation generation.

ALGORITHM EVALUATION

The effects of the following factors on the performances of the calibration algorithm - quality of observations, number of observations, number of measured variables, and number of parameters estimated- are evaluated in the following case studies.

Quality of observations

The quality of observations is indicated by the values of the variances of the Gaussian noises. Hourly observations of 1st stage DO, 4th stage DO, vent gas oxygen purity, and MLSS are used for calibration. A total of 60 hours of hourly observations is used. The variance of the Gaussian noises is set to 0.10, 0.20, 0.30, and 0.40 respectively.

Number of observations

The observations used are the same as in A except the number of observations are changed from 24, 48, 72, to 96. This analysis is intended to find the optimum sampling period which meets the requirement of correctly calibrating the model but avoids wasting resources by not taking too many observations. The variance of the Gaussian noise is fixed as 0.20 in this analysis.

TABLE 1. Parameters in the simplified IAWPRC Activated Sludge Model Symbol.

Symbol	Name	Unit	Value[a]
Stoichiometric parameters			
Y_H	yield for heterotrophic biomass	g Cell COD formed/g substrate COD oxidized	0.67
f_p	fraction of biomass yielding particulate products	dimensionless	0.08
i_{XB}	mass N/Mass COD in biomass	g N(g COD in biomass)-1	0.086
i_{XP}	Mass N/Mass COD in products from biomass decay	g N (g COD)-1 in endogenous mass	0.06
Kinetic Parameters			
μ_H	Maximum specific growth rate of heterotrophs	day-1	6.0
K_S	Half-velocity coefficient of heterotrophs	g COD m^{-3}	20.0
K_{OH}	oxygen half-saturation coefficient for heterotrophs	g O_2 m^{-3}	0.20
b_H	decay coefficient of heterotrophic biomass	day^{-1}	0.62
k_a	ammonification rate	$m^3 \cdot (g\ COD.day)^{-1}$	0.08
k_h	maximum specific hydrolysis rate	g slowly biodegradable COD (g cell COD · day)$^{-1}$	3.0
K_X	half-saturation coefficient for hydrolysis of slow biodegradable substrate	g slowly biodegradable COD (g cell COD)$^{-1}$	0.03

[a] typical value at 20°C

Number of measured variables

The observations used here are the same as above except that the measurements of ammonia nitrogen are added. The results obtained are compared with those in which ammonia nitrogen is not considered in the objective function.

RESULTS AND DISCUSSION

A. The relationship between the variances of the relative errors and the quality of data may be explained as follows: the larger the values of the variances are, the worse the quality of the data. The results of this study are shown in Figure 3. The line denoted as 'exact' represents the exact solution of process model. The line denoted as 'predicted' represents the solutions of the process model using the estimated parameter values. For a given set of observations of reasonable quality, with a reliable calibration, the 'estimated' should be very close to the 'exact'. As we can see from Figure 3, the 'estimated' fits the 'exact' quite well in all cases, though it deteriorates gradually and slowly with increasing τ.

B. The results of this analysis are shown in Figure 4 and Table 2. There is no significant difference between n=24 and n=96 so far as the fit between the 'predicted' and the 'exact' solutions is concerned, but it is true the fit improves as the number of observations increases. The estimated parameters show the same pattern: the relative error between the estimated value and the 'true' value decreases when the number of observations increases (Table 2).

Theoretically, for a longer observation period, a more accurate calibration should be obtained. In the real world, however, the observation period is always limited to a finite time interval due to the limitation in resources. This analysis provides useful information when a decision needs to be made on a possible tradeoff between accuracy and resources.

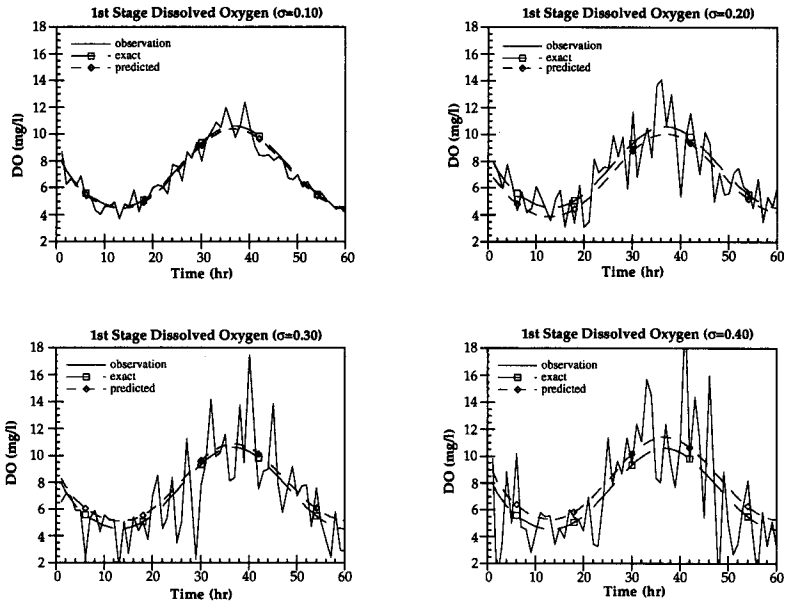

Fig. 3. Effect of on 1st stage DO calibration.

TABLE 2. Relative Error of Parameter Estimation for Different n (Number of Observations).

parameter	n=24	n=48	n=72	n=96
Y_H	5.76%	2.05%	1.34%	0.36%
μ_H	8.50%	4.34%	2.61%	0.79%

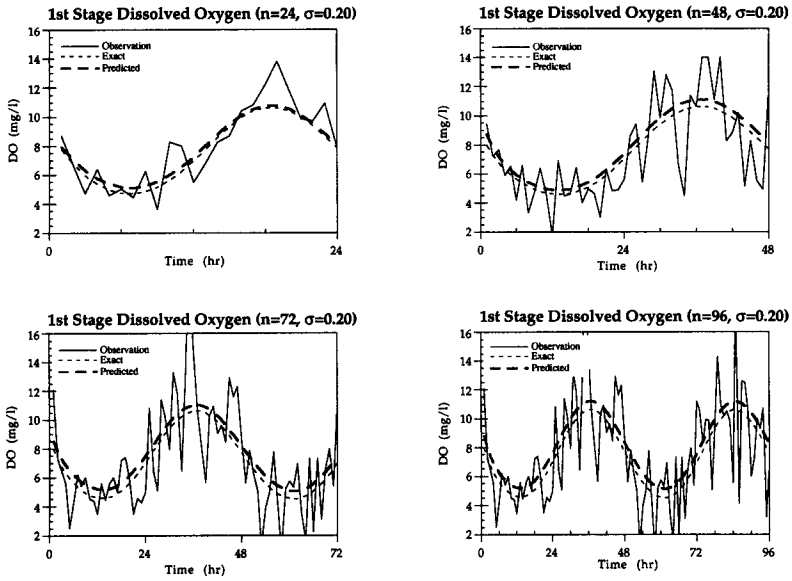

Fig. 4. First stage dissolved oxygen for different n.

C. The results of A and B reveal that some parameters, such as i_{XB} and i_{XP}, cannot be accurately estimated if the objective function only includes 1st stage DO, 4th stage DO, vent gas oxygen purity, and MLSS (Table 3).

TABLE 3. Relative errors between the 'true' and 'estimated' values of parameters

parameter	s=0.10	s=0.20	s=0.30	s=0.40
Y_H	0.60%	1.34%	0.10%	2.30%
i_{XB}	25.47%	35.58%	49.88%	49.19%
i_{XP}	2.83%	12.30%	49.83%	16.00%

A steady-state sensitivity analysis is then conducted to systematically identify the sensitivities of observations to the changes of parameters. The sensitivity of the *ith* state variable S_i with respect to the j_{th} parameter τj is defined by the following formula:

$$\Sigma(S_i,\theta_j)=\frac{\dfrac{\partial S_i}{S_i}}{\dfrac{\partial\theta_j}{\theta_j}}\cong\frac{\dfrac{\Delta S_i}{S_i}}{\dfrac{\Delta\theta_j}{\theta_j}}$$

From the definitions of i_{XB} and i_{XP}, it is natural to conclude that i_{XB} and i_{XP} have little effect on 1st stage DO, 4th stage DO, and 4th stage oxygen purity (vent gas oxygen purity), but strongly affect the nitrogen balance in the system. Table 4 confirms this point. In contrast, DO_1 and DO_4 are much more sensitive to Y_H and μ_H. Vent gas oxygen purity is not sensitive to any parameter, thus its measurements are of limited value for model calibration.

TABLE 4. Sensitivities

$\Sigma(DO_1,i_{XB})=5.8306\times10^{-4}$	$\Sigma(DO_4,i_{XB})=6.1926\times10^{-4}$	$\Sigma(p_{O_{2_4}},i_{XB})=1.6484\times10^{-4}$
$\Sigma(DO_1,i_{XP})=-1.9889\times10^{-4}$	$\Sigma(DO_4,i_{XP})=-4.3348\times10^{-4}$	$\Sigma(p_{O_{2_4}},i_{XP})=3.5604\times10^{-3}$
$\Sigma(DO_1,Y_H)=2.4264\times10^{-2}$	$\Sigma(DO_4,Y_H)=6.0553\times10^{-2}$	$\Sigma(p_{O_{2_4}},Y_H)=4.6264\times10^{-3}$
$\Sigma(DO_1,\mu_H)=7.6667\times10^{-3}$	$\Sigma(DO_4,\mu_H)=-3.5814\times10^{-3}$	$\Sigma(p_{O_{2_4}},\mu_H)=5.0330\times10^{-3}$

It is obvious that for a given set of information (observations) only a certain number of parameters can be rigorously estimated. If the observations are not sensitive to a parameter, then the parameter cannot be rigorously estimated from the given observations. On the other hand, if a parameter is to be estimated, only observations sensitive to the parameter should be used. If we intend to estimate i_{XB} and i_{XP}, additional observations, such as measurements of ammonia nitrogen, should be used.

This analysis is useful to the design and implementation of a model calibration. It provides insights into the algorithm, and lets one know what parameters can be reliably estimated from given observations, and what possible improvements may be attained by adding additional measurements.

SUMMARY AND CONCLUSIONS

A model calibration algorithm is developed for the high-purity oxygen activated sludge process. The objective function is formulated as a relative least-squares function and the optimization method is the Complex Method. The effects of the following factors on the performance of the algorithm are evaluated: data quality, number of observations, and number of estimated parameters.

The following conclusions are drawn from this study.

1. The model calibration algorithm is robust to the quality of observations. As long as the errors are random (no systematic errors), the algorithm is capable of estimating the parameters to an acceptable accuracy.

2. The accuracy of calibration improves as the number of observations increases. However, the improvement slows down as the number of observations increases. No significant improvement is observed beyond n = 96 (hourly observations of 4 days). In this study n = 24 (hourly data of 1 day) was able to estimate Y_H and μ_H within 10% of their true values. For applications in which 10% is an acceptable estimation error, hourly sampling for 24 hours should be an adequate sampling scheme.

3. For a given set of observations, only a certain number of parameters can be reliably estimated. A sensitivity analysis should be performed before the calibration is performed to determine what parameters are to be estimated. If additional variables are to be measured and used for calibration, the potential benefits resulted from the addition should be quantitatively evaluated in advance.

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