Modelling and simulation of a municipal WWTP with limited operational data

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Abstract Mathematical modelling and simulation of activated sludge systems have gained increasing attention in wastewater treatment within the last years. In particular, standardized mathematical models implemented in several simulation platforms are applied in design, optimization, control and research of activated sludge systems. In this paper, the developed model for the wastewater treatment plant (WWTP) in Verona, Italy is described and the results of the steady-state simulation are discussed. The model of the plant was based on the state–of-the-art Activated Sludge Model No.1 (ASM1) combined with the Takács model for the secondary clarifier and was implemented in the WEST® Software version 3.7.5. The focus of this work was to evaluate the applicability of the conventional construction and operational data of the plant for modelling and simulation. In order to increase the predictive power of the simulation results selected parameters of the ASM1 were adjusted during the model calibration. The opportunities for further applications of the plant model are discussed.

Keywords wastewater treatment; simulation; model calibration; mathematical modelling; ASM1

INTRODUCTION

Mathematical modelling of activated sludge processes became a popular tool in the last decade and has wide application in research, plant design, optimisation, training, and model-based process control (Henze et al., 2000; Langergraber et al., 2004). The by far mostly used and best known are Activated Sludge Models (ASM) developed by the International Water Association (IWA). The Activated Sludge Model No.1 (No.1 was used to indicate further development of this model), proposed by the IWA in 1986, allows the dynamic simulation of organic matter degradation and nitrification/denitrification processes (Gujer, 1991, 2006). Increasing popularity and understanding of the biological phosphorus removal phenomena led to the development of the ASM2 (published in 1995). In 1999 the Activated Sludge Model No.2 was further expanded to ASM2d, where denitrifying phosphorus-accumulating organisms were included (Henze et al., 2000). The last, but neither *final* nor *general*, ASM3 model was presented in 1999, which can be seen as a revision of the ASM1 expanded for some new conceptions of the activated sludge processes.

Numerous mathematical models of the activated sludge, apart from the ASMs, are reported in literature, eg. the ASAL models (Jones,1978; Chambers and Jones, 1988) and the TUDP model (Murnleitner i in. (1997); Van Veldhuizen i in. (1999)). Most of these models are able to simulate organic matter removal, nitrification, denitrification and some of them also phosphorus removal by bio- and physical-chemical methods. However, the large number of processes which are described by even more parameters results in a high model complexity. But, several studies indicated that only a few of the model parameters have to be adjusted during model calibration (Mino et al., 1997; Makinia et al., 2002; de la Sota et al., 1994). Most of these parameters can be derived from specialized studies such as batch test or concentration profiles along the bioreactor. However, traditional plant operation provides only routinely performed analyses of conventional parameters (e.g. BOD_5, TSS) which are not directly applicable for modelling purposes (Makinia et al., 2002). Only a few examples are given in the literature where plant operating data were used directly as model input. Çinar et al. (1998) and Makinia et al. (2002) investigated such an opportunity with partly successful results.

The objectives of the study were to evaluate the applicability of the Verona full-scale plant operational data to the activated sludge models, and to study the feasibility of setting up the model of the WWTP based only on the typically available construction and operational data without performing specialized studies for more detailed plant characterization.

METHODS

Description of the Verona WWTP

The wastewater treatment plant (WWTP) investigated in this study is located in the city of Verona, Italy. The Verona plant is designed for an average influent dry-weather flow rate of 92 000 m^3 d^{-1} and is composed of four parallel lines of preliminary and primary treatment units comprising screens and rectangular aerated grit chambers; three parallel circular primary clarifiers; five parallel activated sludge basins (total volume V_R = 23 777 m^3, water head H_R = 4.08 m; design aerated volume is 70% of V_R); six parallel secondary clarifiers (total area A_{SC} = 8 688 m^2; total volume V_{SC} = 26 064 m^3; depth at the overflow H_{SC} = 3 m) (Zambarda, 2008a). The plant was designed for the removal of organic matter and nitrogen by denitrification followed by nitrification. Wastewater containing nitrates generated in the aerated zone is recirculated to the anoxic zone. Phosphorus removal by excess uptake was not taken into account during design stage, therefore in the Verona plant phosphorus is removed mainly by biomass metabolism. For the simulation study only routine operational data from the Verona plant were used; no additional measurements were performed. The raw data collected from the plant were examined to extract several sets of data representing approximately 30-day periods of steady state operation. These data were elaborated (statistically and using mass balances) and averaged, assuming that this average represents steady state. The average data from two different periods were used in this simulation study for model calibration (Table 1) and for verification of the calibrated model.

Table 1 Operational and performance characteristics of the Verona WWTP during the investigated period

Parameter	Unit	Value	
Influent flow rate (Q)	m^3 d^{-1}	92 434	
MLSS[1] conc.	g L^{-1}	4.5	
Return sludge ratio	% of Q	1.8	
Nitrate recycle rate	% of Q	4.5	
Waste sludge flow rate	m^3 d^{-1}	1 366	
RAS[2] conc.	g L^{-1}	5.8	
DO[3] conc. in the aerobic tanks	mg L^{-1}	1.3	
Concentration of:		Settled wastewater	Final effluent
COD_{tot}[4]	mg L^{-1}	320	29
Total Kjeldahl Nitrogen (TKN)	mg L^{-1}	49.0	6.1
Ammonia nitrogen($N\text{-}NH_4$)	mg L^{-1}	-	3.0
Nitrate nitrogen ($N\text{-}NO_3$)	mg L^{-1}	-	4.1
Total Suspended Solids (TSS)	mg L^{-1}	98	12.0

[1] Mixed Liquor Suspended Solids; [2] Return Activated Sludge; [3] Dissolved Oxygen; [4] Total Chemical Oxygen Demand;

Simulation environment

In this work simulations were carried out in the WEST® (World Wide Engine for Simulation, Training and Automation) Software Package version 3.7.5. The WEST® simulator was chosen as a modelling and simulation environment because of the in-house experience, direct application to WWTP and possibility to reuse previously developed models. WEST® is a user-friendly platform for modelling and simulation of any kind of process that can be described by a structured collection of differential algebraic equations. Presently, WEST® is mainly applied to the modelling and simulation of wastewater treatment plants (Vanhooren et al., 2003).

Model configuration

The simulation of the activated sludge WWTP of Verona was based on the standard ASM1 combined with the Takács (Takács et al., 1991) secondary clarifier model. Simulation of the wastewater pre-treatment and sludge processing was not performed, since the relevant data were not available. Additionally, it should be stressed that inclusion of the primary treatment and sludge processing models into the overall WWTP model would increase its complexity substantially, which, considering the limited set of data, may lead to unreliable simulation results. The biochemical reactions occurring in both bioreactors are described by the ASM1, whereas their hydraulic behaviour is represented by ideal continuous stirred tank reactors (CSTR) models. The ASM1 is still extensively used in the wastewater community and has become the standard model for simulation of activated sludge plants, which resulted in a long list of references reporting experience with its application. Over two decades after the introduction of ASM1, several more complex models are available (e.g. ASM2d, ASM3), which include more recent findings in the activated sludge process and fix some of the ASM1 defects (Langergraber et al., 2004; Henze et al., 2000; Alex et al., 2008; Gujer, 2006). In this study ASM1 was selected, especially due to its relatively low complexity, which appeared essential since limited data is available for its calibration, and its extensive description in literature. These two features of ASM1 appeared to overweight its limitations regarding the purposes of this simulation study. The assumption of an ideal CSTR is that it has a uniform concentration within its confines i.e. the influent is mixed instantaneously and completely. Hydrodynamic scheme of the biological reactor was assessed by means of experimental tests (tracer addition and detection of effluent concentration time profile): the anoxic tank was simulated with a single CSTR and the aerobic tank was simulated with two CSTRs, both characterised with 50 % of the original design volume (Zambarda, 2000) (Figure 1). The average concentration of DO is 1.3 mg L^{-1}. The DO concentration in the single aerobic reactor model was assumed, according to suggestion of Zambarda (2008b), at the level of 0.8 and 1.8 mg L^{-1}, in the downstream order (in Figure1 labelled: ‘Aer1’ and ‘Aer2’, respectively). The DO concentration in the aerobic tanks is fixed at the specified levels by a Proportional-Integral (PI) controller which is altering the value of the oxygen mass transfer coefficient (k_La) to reach constant oxygen concentrations.

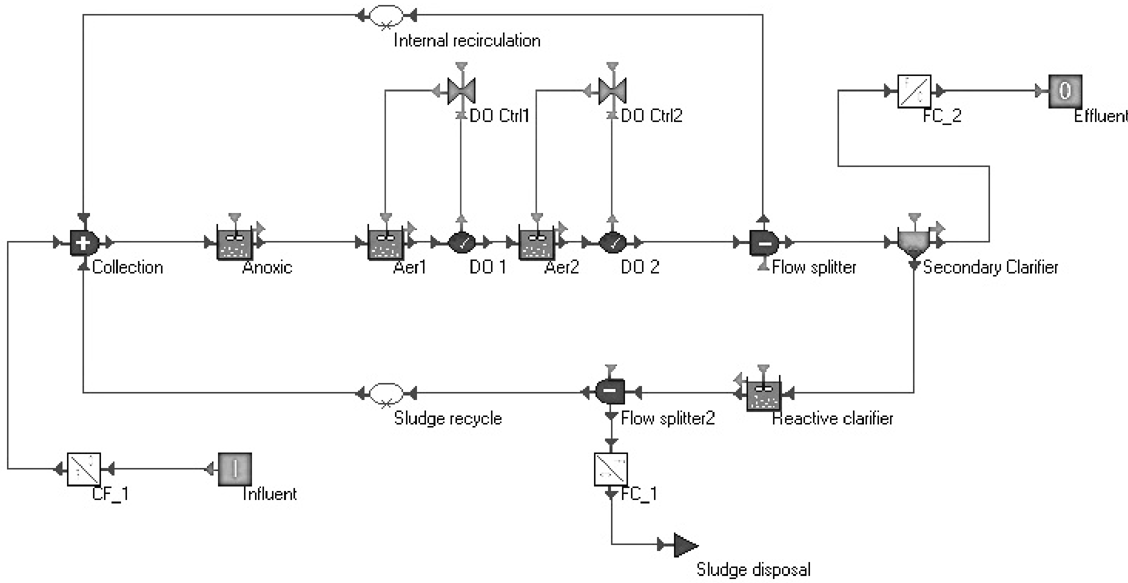

Figure 1 The Verona WWTP model configuration in the WEST® Software

The Takács model was selected to describe the settling-thickening process occurring in the secondary clarifier. In the evaluation of six one-dimensional settler models performed by Grijspeerdt et al. (1995) it was identified to give the most realistic results for ten sets of experimental data, both for steady-state and dynamic conditions. The used secondary settler in this case is a non-reactive (no biological reactions take place) unit consisting of 10 horizontal layers, of which the 5th (counting from the surface) is the feed layer. Since it was confirmed by the plant operators that denitrification processes occurs in the secondary clarifiers (available data cannot assure this phenomena) an anoxic virtual tank was placed in the sludge loop of the model to describe the biochemical processes occurring in the real settler (labelled 'Reactive clarifier' in Figure 1). The biochemical processes in the additional reactor were described by ASM1 and its hydraulic behaviour by a CSTR. The assumed volume of the reactive clarifier is equal to the volume of the sludge blanket in the real clarifier, this is 20% of V_{SC}.

Influent fractionation

The ASM1 was used to simulate organic matter and nitrogen removal in the activated sludge process. An application of this model requires the influent characterization on a COD_{tot} basis, which is then divided into a variety of fractions according to the model variables (see Henze et al., 1987). For the modelling purposes, the operational routine data of the Verona plant were used (Table 1). In order to generate the model influent, a conversion of the conventional plant parameters described by primary effluent concentrations was performed for the ASM1 model components. A standardized and a modified procedure according to Makinia et al. (2002) were used (procedure A and B), whereby the latter one is more classical and takes the specific process conditions of the Verona plant into account. The resulting model inputs are listed in Table 2. In both cases, the input parameters for the applied fractionation procedures are TSS and COD_{tot} of the real primary effluent. These parameters are subsequently used to calculate, by the use of the relevant assumed or calculated stoichiometric parameters the concentrations of the required ASM1 carbonaceus components. The values of the stoichiometric parameters varied for each procedure, therefore the generated model inputs differ in terms of soluble COD (SCOD)/particulate COD (XCOD) ratio, however their biodegradable COD (BCOD) content is equal (Table 2).

Table 2 Selected results for the model influents composition

	COD_{tot} [mg L^{-1}]	TSS [mg L^{-1}]	BCOD /COD_{tot}	SCOD /COD_{tot}	XCOD /COD_{tot}	TSS /XCOD
Influent A	320[1]	98[1]	0.85	0.42	0.58	0.53
Influent B	320[1]	98[1]	0.85	0.59	0.41	0.75

[1] measured value

The concentrations of nitrogenous components of ASM1 were calculated using the formulae proposed by Vanhooren and Nguyen (1996).

RESULTS AND DISCUSSION

Model calibration

The model predictions for effluent quality and sludge concentration in the biological reactors as well as in the returned sludge flow were used as a measure for the model accuracy to mimic the plant performance. The initial biological parameters used in the simulation correspond to their typical values at 20°C and neutral pH suggested by Henze et al. (1987). The initial simulation results, in Figure 2 denoted as 'simulated', were obtained by a calculation based on the default kinetic and stoichiometric parameter set of the ASM1.

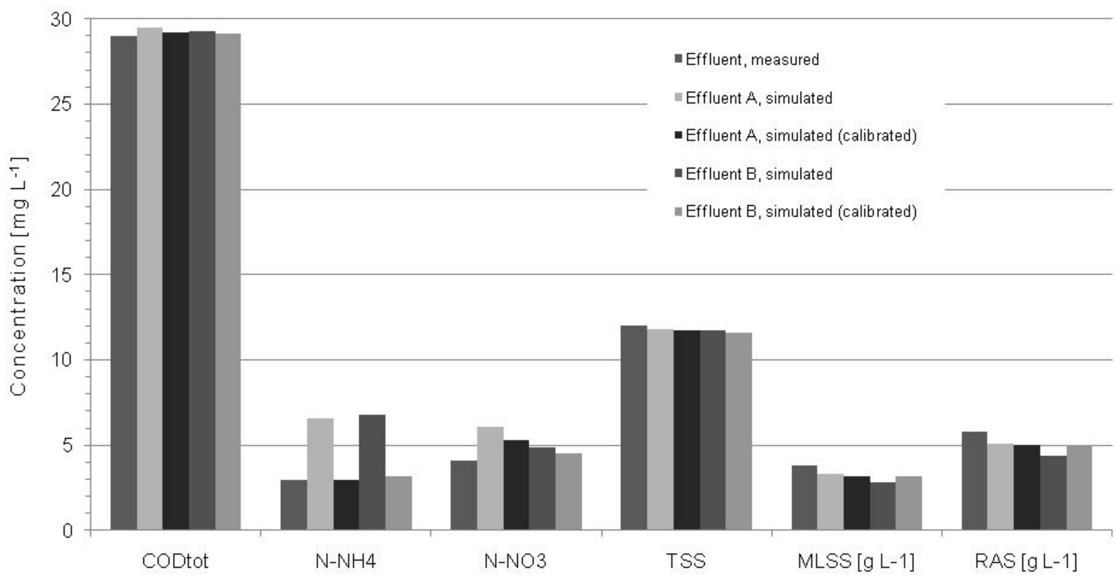

Figure 2 Comparison of measured and simulated effluent concentrations

The effluents A and B are the results of the simulation using the influents A and B, respectively. The significant discrepancies between measured values and simulated predictions, especially in terms of nitrogen removal, were noted for both effluents (Figure 2). Thus, in order to obtain a reasonable fit between simulated values and actual observations the model parameters were calibrated. The model calibration was performed in a step-wise adjustment manner based on knowledge and experience of the modeller. This 'human expert method' (term coined by Çinar et al., 1998) was continued until a satisfactory match, in modeller's judgment, between simulated (calibrated' in Figure 2) and measured values was obtained. The instructions provided in the 'calibration protocols' (Langergraber et al., 2004; Vanrolleghem et al., 2003; Hulsbeek et al. 2002; Melcer et al., 2003) were taken into account during the model calibration. In order to meet the real effluent characteristics with sufficient accuracy the following ASM1 kinetic parameters were adjusted: K_S, K_{NO}, $K_{O,A}$, k_A, K_{NH} (Table 3).

Table 3 Comparison of the default and adjusted kinetic parameters

Model parameter	Symbol	Unit	Values	
			Default	Adjusted
Half-saturation coefficient (hsc) for heterotrophs	K_S	$gCOD\ m^{-3}$	20.00	5.00
Nitrate hsc for denitrifying heterotrophs	K_{NO}	$gNO_3\text{-}N\ m^{-3}$	0.50	0.10
Autotrophic ammonia hsc	K_{NH}	$gNH_3\text{-}N\ m^{-3}$	1.00	0.80
Autotrophic oxygen hsc	$K_{O,A}$	$gO_2\ m^{-3}$	0.40	0.30
Ammonification rate	k_A	$m^3\ (gCOD\ d)^{-1}$	0.08	0.04

The half-saturation coefficient for heterotrophs (K_S) was decreased from 20 to 5 gCOD m^{-3}, causing a decrease of effluent nitrate and COD_{tot} concentration. The decreased value of the K_S implies an increased affinity of the biomass for substrate which may be caused by several factors: elevated concentrations of readily biodegradable compounds in wastewater, since 25 % of the Verona WWTP influent is industrial discharge from food-processing industries (Zambarda, 2008b); influences of the aerated grit chambers and primary clarifiers performance.

The nitrate half-saturation coefficient (K_{NO}) for denitrifying heterotrophs was decreased from 0.5 to 0.1 gN-NO_3 m^{-3} assuming improved nitrate transfer into bioflocs due to their size and structure.

The oxygen half-saturation coefficient for autotrophs ($K_{O,A}$) was decreased from 0.4 to 0.3 gO_2 m^{-3}. The adjustment of this parameter resulted in significantly lower ammonia concentrations in the effluent. The calibrated value of the oxygen half-saturation coefficient for autotrophic biomass indicates improved oxygen transfer into bioflocs. This may be caused by the specific size and structure of the bioflocs and also a high efficiency of the aeration system due to the installation of new rectangular diffusers (Zambarda, 2008b)

The ammonia half-saturation coefficient for autotrophs (K_{NH}) was decreased from 1.0 to 0.8 gN-NH_4 m^{-3} to display significant lower ammonia concentrations in the effluent which concurrently increases the nitrate concentration in the effluent. The increase of the K_{NH} value may be related also to the biofloc size and structure, which increases the substrate affinity of biomass.

It should be noted that the values of the four (of six) calibrated model half-saturation coefficients were lower than the default ASM1 values, which indicates improved biomass affinity for the substrates. This may be related to the relatively small average size of the biofloc, which was not measured during the investigated periods but was confirmed by the plant operators to be the typical feature of the plant. According to Marquot et al. (2006) the half-saturation coefficients can be regarded as compensation parameters for the occurrence of dead zones within the activated sludge tank, in which concentrations of soluble and particulate components differ from the well mixed zone. Lower values of half-saturation coefficients may indicate that no significant dead zones occur in the plant reactors due to uniform hydrodynamics of the reactors.

The ammonification rate (k_A) was decreased from 0.08 to 0.04 m^3 (gCOD $d)^{-1}$. The adjustment of this parameter led to the decrease of the ammonia and organically bound nitrogen ratio in the effluent. Lower values of k_A lead to more organic soluble substances containing nitrogen which remain in the treated wastewater because the ammonification rate is slower. The organic nitrogen fraction of the analysed effluent constitutes over 50 % of TKN which implies that the ammonification rate is lower than typical.

As depicted in Figure 2, the calibration of the ASM1 improved the accuracy of the nitrogen removal predictions. There are only slight differences between the calibrated model predictions considering the model influent used. It is noticeable that the simulation, with influent A resulted in a $N\text{-}NH_4$ effluent concentration which is closer to the measured value than with influent B. On the contrary, the use of the influent B allowed to predict the $N\text{-}NO_3$ concentration in the effluent with higher accuracy.

Model verification

In order to verify the predictive power of the calibrated parameters simulations were run using a new set of influent data from other time periods. The main principle of the calibrated model verification is to keep all the adjusted model parameters constant so that obtained results are comparable. However, additionally in order to achieve more satisfactory results of the verification, the volume of reactive clarifier and influents components were adjusted. Adaptation of the influent composition consisted in the adjustment of the S_I and S_S in order to achieve acceptable results in terms of predicted effluent COD_{tot} concentration. Particulate fraction of influent COD_{tot} was adjusted to increase MLSS and RAS concentrations. However, it should be stressed that the results obtained after such an adjustment should be treated with caution and their reliability may be questionable. The results of the model verification (for the model input calculated using procedure A) are presented in Figure 3.

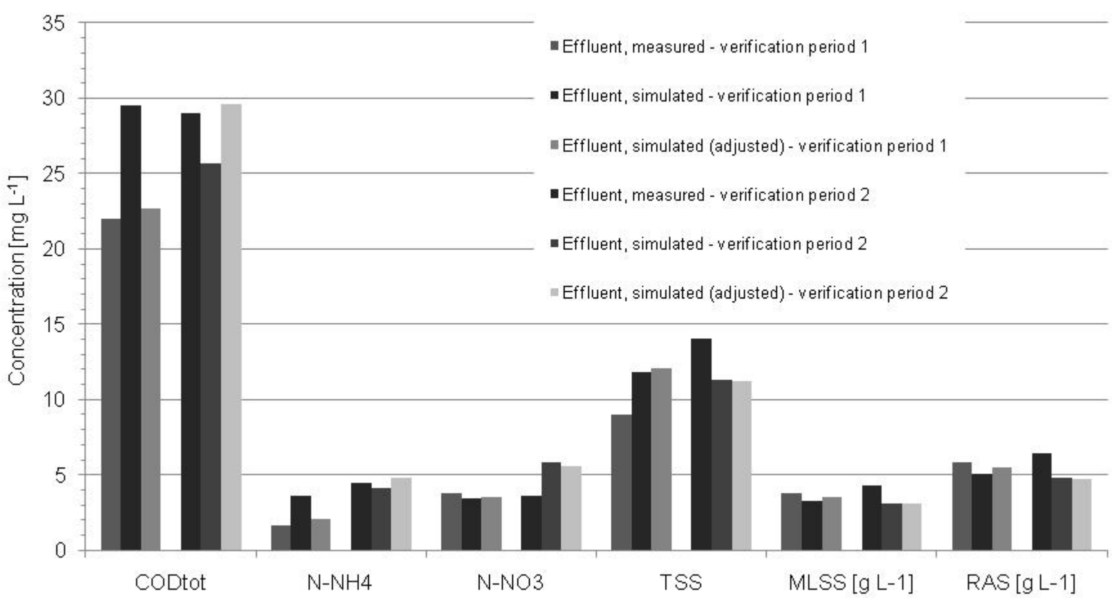

Figure 3 Results of the calibrated model verification

The results of the verification show that the calibrated model is able to characterize the general trend of the plant performance using influent and operational data from different time periods; however, agreement between measured and simulated values for some parameters is mediocre. After the adjustment of the abovementioned model parameters, the quality of the simulation results improved significantly. This may be related, amongst others, to modifications of the process configuration at the plant (e.g. alteration of the aerated volume which was confirmed by the plant's operators), changes in the influent composition (due to periodic and changeable loading and composition of industrial discharge) and the fact that average data were used for the simulation.

CONCLUSIONS

Based on the obtained results of the Verona plant simulation and modelling, the following conclusions can be derived:

- the typical operating and construction data, despite their informative limitations, can be successfully applied to model and simulate the performance of the municipal-industrial WWTP in Verona;
- the study indicates that a useful model can be developed for municipal activated sludge systems using ASM1 as a basis;
- the model developed and verified during this study is able to predict the Verona plant behaviour with acceptable accuracy. Modelling with limited operational data is feasible to indicate the trends of the effluent concentrations. However, to achieve a better concordance additional research is needed to determine special aspects of the specific plant behaviour, e.g. the oxygen profile within the bioreactors, detailed wastewater characterization or RAS composition. The calibrated model parameter set obtained in the static (steady-state) simulation should be subjected to validation with the results of additional studies, such as lab-scale experiments and/or extensive monitoring of the plant for dynamic simulations.

The model developed in this study can be used for various purposes:

- for the Verona plant operators as a useful and practical tool for prediction of the results of changing operation parameters, such as, recycle ratios, waste sludge flow rate, the DO concentration etc.
- for optimization of the plant in terms of energy conservation (associated with aeration and recirculation), minimisation of the waste sludge flow, enhancing the contaminants removal.
- for further development into a model which could be used for dynamic simulation and applied as an element of a real time control system of the plant performance.

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