AUTOCALIBRATION OF CHLORINE TRANSPORT MODEL FOR STEADY STATE DISTRIBUTION SYSTEM BY GENETIC ALGORITHM

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ABSTRACT

The chlorine reaction kinetics within a distribution system is affected by the reactions occurring in the bulk flow in a pipe and at the pipe wall. The field determination of parameters governing the wall reactions of a pipe is difficult and hence these are a product of calibration. The autocalibration of a chlorine transport model consists of estimating these unknown parameters by comparing the measured and simulated chlorine concentrations at the monitoring nodes within the distribution system in a least square sense. The inverse model presented in the paper determines these unknown parameters by simulation-optimization procedure in which the Genetic Algorithm technique is used as an optimization module. The verification and application of the developed inverse model are illustrated using a large multiple source water distribution system under steady state. The developed inverse model is useful to the water supply agencies for calibration of the chlorine transport model for a water distribution system and hence to improve the operational strategies to maintain chlorine residuals within the system.

Key Words: Autocalibration, Genetic Algorithm, Wall reaction parameter and Optimization

1. INTRODUCTION

The forward simulation chlorine transport models predict the chlorine concentrations throughout the distribution system. The reliability of these predicted concentrations with respect to the field observations depends on the assigned parameter values involved in the type of reaction kinetics used in the model. The chlorine reaction kinetics within a distribution system is affected by the reactions occurring in the bulk flow in a pipe and at the pipe wall. The parameters controlling the chlorine reaction kinetics within the system can be broadly classified in to the bulk reaction parameters and the wall reaction parameters. Network chlorine transport models need to be calibrated by estimating the parameters which govern the simulation of chlorine concentrations. These governing parameters are associated with the first or non first-order bulk flow reactions and first- or zero-order wall reactions in the distribution system. The bulk reaction parameters can be estimated by the flask tests whereas the wall reaction parameters are difficult to estimate and hence are a product of calibration. The unknown wall parameters can be expressed in terms of first-order or zero-order wall reaction parameters. These wall reaction parameters are derived from mass transfer model proposed by Rossman et al. [1] and its modified version in Rossman [2].

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The field studies (Sharp et al. [3]) conducted on the determination of chlorine reaction parameters indicated the effect of pipe material, pipe diameter and flow rates on these reaction parameters. It should be noted that the above unknown reaction parameters can be estimated by trial and error procedure. Given sufficient number of observed chlorine concentrations at various locations throughout the system, initial values of global or zoned reaction parameters can be estimated and the simulation is performed. The observed chlorine concentrations and the corresponding simulated concentrations can be compared. If the two values do not agree within the acceptable limit, then the reaction parameters should be adjusted until a suitable match is found (Walski et al. [4]). But the above procedure, which is tedious, may not result in the evaluation of proper reaction parameters. Thus an autocalibration technique is desirable to avoid the tedious trial and error procedure. From the published literature, it is seen that the autocalibration of input-output chlorine transport model by Zeirolf et al. [5] and estimation of overall decay coefficients of a water quality model (FDM) by Al-Omari and Hanif Chaudhry [6] using a finite difference approach addressed the problem of parameter estimation methodically under dynamic conditions. And water quality reaction parameter estimation in a steady state distribution system has not been reported in the published literature. The algorithms developed by Zeirolf et al. [5] are applicable only for first-order (bulk and wall) reaction kinetics and the model does not consider the storage tanks and multiple water quality sources. The procedures described by Al-Omari and Hanif Chaudhry [6] are based on only overall first-order reaction kinetics and the work does not differentiate between bulk and wall related reactions. But a study by Maier et al. [7] showed that the two (bulk and wall) coefficients model represents the observed data better compared to single coefficient model. Also the Eulerian (finite difference) methods are less memory efficient in simulating the chemical transport in distribution systems (Rossman & Boulos [8]). Thus there is a need to develop the inverse modeling procedures, which are flexible enough to incorporate first- or non first-order bulk and wall reaction kinetics, for autocalibration of a typical water quality models. The splitting of overall reaction term into bulk and wall components is significant since bulk reaction parameters can be estimated by bottle tests whereas the wall reaction parameters are difficult to determine in the field.

In the present study, the inverse models are developed for the autocalibration of steady state water quality model. The autocalibration problem is formulated in terms of minimizing the observed and computed chlorine concentrations in a least square sense. The models developed are based on the conventional inverse modeling approach which utilizes the steady state forward simulation water quality model as a routine in its simulation-optimization computational procedure. The solution methods used in the inverse model includes Genetic Algorithm Technique (GAT) which is a stochastic search method. Stochastic search methods are more robust and simpler to formulate and use, but are generally slower (Walski et al. [4]). The genetic algorithm is used for parameter estimation problems in ground water studies (Lingireddy [9]) and calibration (roughness parameter) of water distribution systems (Savic & Walters [10]; Walters et al. [11]). Application of the GA approach to water quality model calibration is in its infancy and hence provides a fertile area of research.

The inverse models developed in the present study compute the various water quality reaction parameters in a more direct fashion. The estimation of unknown reaction parameters and hence the prediction of chlorine concentrations by the inverse models is more accurate as the forward simulation steady state water quality model is an integral

part of the inverse model. In addition to the standard GA operators, the GA technique adopted utilizes the advanced GA operators such as fitness scaling, creep mutation and elitism. In the following sections the development, verification, applicability and usefulness of the inverse model are discussed for steady state distribution system. The application of the inverse model to identify and check the suitability of a reaction kinetics model for the given set of measurements is also illustrated.

2. DEVELOPMENT OF SIMULATION-OPTIMIZATION MODEL

In developing an inverse model using simulation-optimization procedure an efficient forward simulation water quality model is required. Thus in this section the forward simulation model developed is also discussed along with the inverse model.

2.1 Forward Simulation Model

The forward simulation model consists of two parts viz. hydraulic model and a water quality model. The hydraulic model, which computes the flows in the pipes of the system, is a prerequisite for the development of any water quality model. The available hydraulic model (Niranjana Reddy [12]) is used in the present study.

2.1.1 Water quality model

The principle of mass conservation along with the suitable bulk and wall chlorine reaction kinetics are used in formulating the water quality model. The basic governing equation required for water quality model to determine the steady state concentration of chlorine at any node j can be formulated as

$$Cnc_j = \frac{\sum_{i=1}^{Ninp_j} Cnc_{nu_i} \operatorname{Re} c_i Q_i}{\sum_{i=1}^{Ninp_j} Q_i}; \; j = 1, \cdots Njn \qquad (2)$$

where, Cnc_j= concentration at node j (mg/L); Cnc_{nui} = concentration at node nu_i (mg/L); $Ninp_j$= number of incoming pipes at node j; nu_i= upstream node of incoming pipe i; Q_i= flow in pipe i (m^3/s); Njn= number of nodes in the network; Rec_i= reaction coefficient for pipe i.

The expression for the reaction coefficient depends on the kinetics used for bulk and wall reactions. The details of the reaction coefficient are given in the reference (Munavalli & Mohan Kumar [13]). A steady state forward simulation water quality model is developed by integrating the hydraulic and water quality model.

2.2 Optimization Model

2.2.1 Objective function

The objective is to estimate the unknown reaction parameters so that the difference between the observed and the computed chlorine concentrations at the monitoring nodes are minimized in the least square sense. Thus the objective function is given by

$$E = \sum_{j=1}^{M} \left[Cno_j - Cnc_j \right]^2 \quad \text{.....(3)}$$

where, M = number of monitoring nodes; Cno_j = observed chlorine concentration at monitoring node j (mg/L).

2.2.2 Solution Method by Genetic Algorithm

A genetic algorithm (GA) is a member of a class of search algorithms based on artificial evolution (Holland [14]). GA simulates mechanisms of population genetics and natural rules of survival in pursuit of the ideas of adaptation. GA, a search and optimization tool, work differently compared to classical search and optimization methods. GA has been increasingly applied to various search and optimization problems because of their broad applicability, ease of use, efficiency and global perspective. The efficiency indicates the robustness of the search method that underlies the GA approach and the flexibility of the formulation itself (Goldberg [15]). GA optimization is not a replacement for traditional simulation modeling; instead, it is performed as a next step after simulation modeling since GA is not an analysis model but is a inverse model which can be used to simulate system parameters. Goldberg [15] and Michalewicz [16] have given an excellent introduction to GA and it can drive the solution search towards the optimum objective function value starting from an initial set of randomly generated decision variables. Genetic algorithm does not necessarily guarantee that the global optimum solution will be reached, although experience indicates that they will give near-optimal solutions after a reasonable number of evaluations (Simpson et al. [17]). Previously genetic algorithm has been used for the water distribution system optimization problems (Murphy et al. [18]; Simpson et al. [17]; Dandy et al. [19]; Savic & Walters [20]). These works on optimization of water distribution systems solved by GA included the determination of pipe diameters so that the cost of the system is minimum. Savic & Walters [10] applied GA for calibrating the network models. Reis et al. [21] addressed the problem of appropriate location of control valves in a water distribution system and their settings via GA to obtain maximum leakage reduction for given nodal demands and reservoir levels. Mulligan & Brown [22] demonstrated that the GA is a useful calibration tool in water quality modeling that is used for predicting dissolved oxygen concentration in streams, calibration applications using synthetically generated data with and without error. And GA was found to be a useful tool to estimate water quality parameters in a calibration scenario. Meier & Barkdoll [23] applied GA to optimize the sampling design in water distribution system.

The basic steps involved in the GA approach are: (i) Representation of the decision variables by a coding scheme; (ii) Random generation of initial population of trial solutions. Each trial solution consists of a set of coded decision variables of the optimization problem; (iii) Evaluating the fitness of each individual trial solution (string) in a population after translating each string in to corresponding set of decision variables and (iv) Applying the GA operators (reproduction, crossover and mutation) to generate new improved population set. Apart from the above three basic operators of the simple GA, the operations such as fitness scaling, niching, creep mutation and elitism are applied to improve GA convergence characteristics. The solutions with higher fitness will survive and the weak fitness solutions are eliminated.

As formulated above in the Equation (3), the parameter estimation is an unconstrained optimization problem. And GA is naturally cast as an unconstrained search technique (Goldberg [15]). The various unknown reaction parameters constitute a set of decision variables to be evaluated by GA and this can work by evaluating the fitness of each potential solution consisting of values for the set of unknown reaction parameters. Fitness is determined by comparing how well the simulated chlorine concentrations resulting from the candidate solution match the measured values collected in the field. The computationally intensive step involved in GA technique is the determination of fitness that is somehow related to the objective function value. The GA continues to spawn generations of potential solutions until comparison of solutions from successive generations no longer produces a significant improvement. In addition, GA process eliminates most of the routine and tedious aspects of the calibration process. GA will generally achieve better fits to the available data if the correct set of variables is included in the solution and can establish the correct range of possible solutions. The GA implementation procedure is also illustrated in Figure 1.

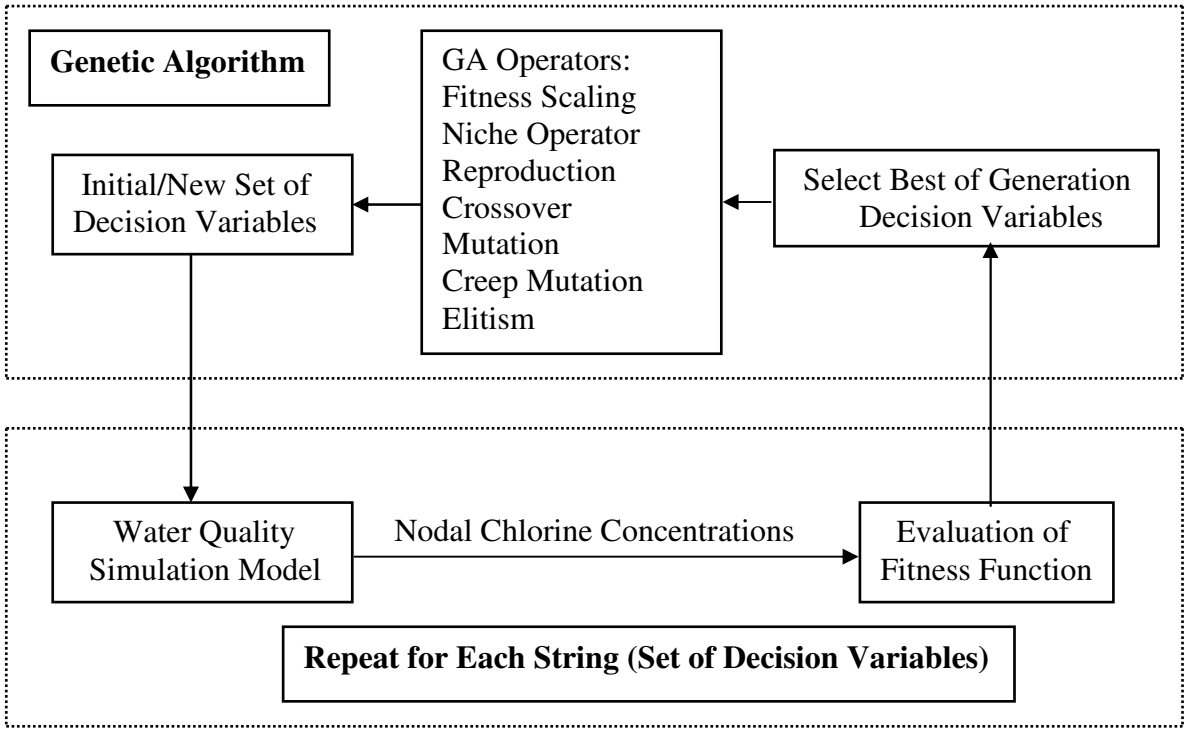

Figure 1. GA Implementation Procedure

3. MODEL APPLICATION: RESULTS AND DISCUSSION

3.1 Verification and Application

The verification and application of the model is illustrated using the water transmission main network of Bangalore city in India. The details of the system are given in the reference Munavalli & Mohan Kumar [13]. To summarize briefly, the whole

system is grouped based on the age of the pipes in to three zones and the network is shown in the Figure 2. The pipes 1 to 36, 37 to 71 and 72 to 94 with Hazen-Williams Coefficient (HWC) of 106.90, 127.50 and 103.60 (Datta & Sridharan [24]) form the three groups respectively. The first-order kinetics for both bulk and wall reactions is used for this application. The reaction parameters used for illustration are assumed to be hypothetical. The first-order bulk reaction parameter used is 2.0 d^{-1} and the wall reaction parameters assigned are 0.75 m/d, 0.50 m/d and 1.0 m/d for the three groups of pipes respectively. A constant chlorine concentration of 0.75 mg/L is assumed to be injected from all the three sources of supply.

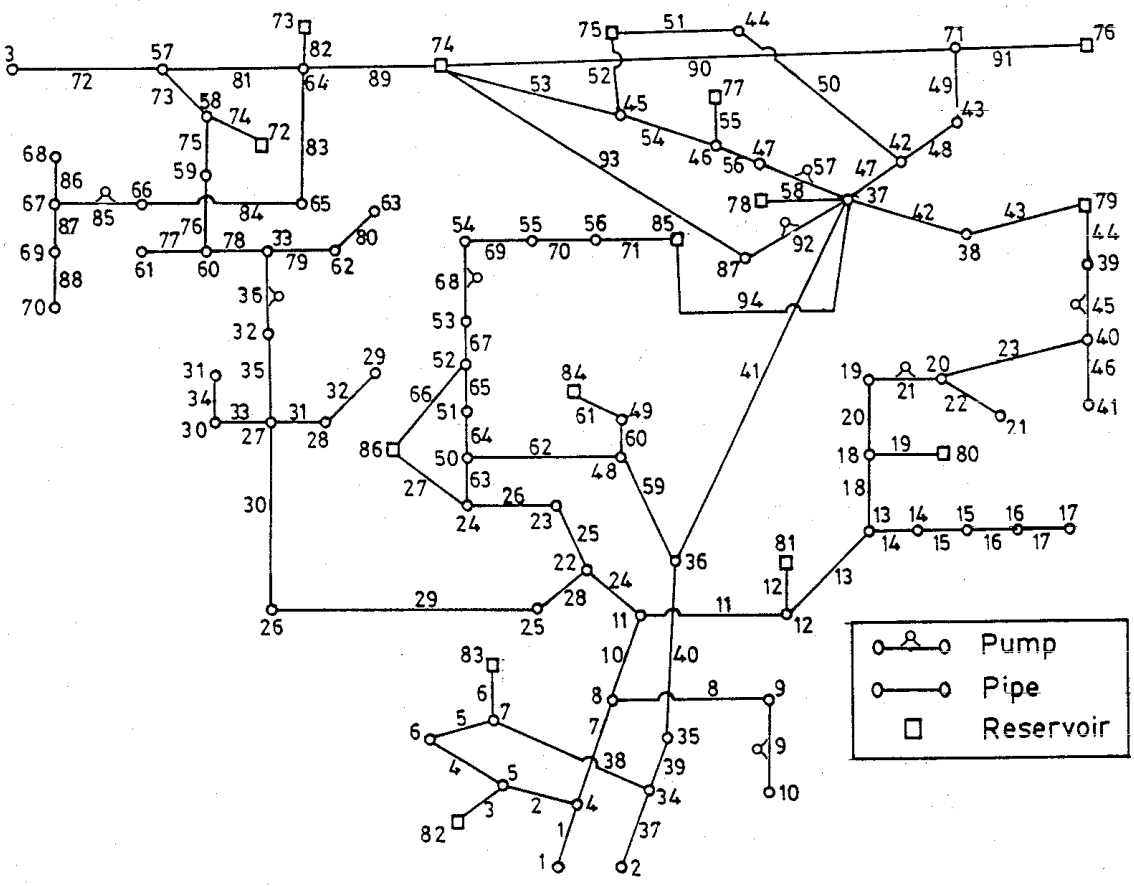

Figure 2. Schematic of Bangalore Water Transmission Main Network

The verification of the model is done in two steps. In the first step, the steady state forward simulation water quality model is run for the network and the ultimate chlorine concentrations are obtained at all the nodes. In the second step the chlorine concentrations at some nodes are assumed to be the input observations for the inverse simulation and the water quality parameters (used in the forward simulation and considered to be unknown in the inverse model) are estimated by the inverse model. For this system the parameters to be determined are the three group wall reaction parameters and these are estimated using GAT. The chlorine concentrations simulated by the forward simulation model at the reservoir nodes are given in the column two of Table 1. The inverse model is run using these concentrations and GA parameters given in Table 2 as the inputs to the model. The

run of the inverse model essentially reproduced the parameters that are used in the forward simulation. Figure 3(a) shows the rapid convergence in the value of objective function for best of generation and average generation results. These results verify the inverse model and also illustrate the capability of the inverse model to produce the system parameters from the measurements (which are synthetically generated) using GAT.

Table 1. Error Free and Noisy Concentrations for Verification and Application

Reservoir Node	Error Free Conc. (mg/L)	Noisy Conc. Data Set 1	Error (%)	Noisy Conc. Data Set 2	Error (%)	Noisy Conc. Data Set 3	Error (%)
72	0.4533	0.4535	0.05	0.4452	1.78	0.4486	1.03
73	0.6330	0.6671	5.11	0.6465	2.13	0.6503	2.74
74	0.5863	0.5783	1.38	0.5982	2.03	0.6302	7.49
75	0.3541	0.3639	2.69	0.3229	8.80	0.3359	5.15
76	0.2626	0.2471	6.27	0.2462	6.25	0.2415	8.03
77	0.3587	0.3631	1.22	0.3705	3.28	0.3564	0.65
78	0.3895	0.3852	1.13	0.4145	6.43	0.4002	2.74
79	0.2440	0.2675	8.78	0.2733	12.03	0.2593	6.26
80	0.3815	0.3812	0.07	0.3875	1.57	0.3996	4.76
82	0.6535	0.6642	1.61	0.6788	3.87	0.6233	4.62
83	0.6177	0.6168	0.14	0.6001	2.84	0.6030	2.38
84	0.5765	0.5814	0.85	0.6096	5.74	0.5785	0.36
85	0.4181	0.4260	1.85	0.4082	2.36	0.3954	5.43
86	0.5391	0.5451	1.10	0.5244	2.72	0.5662	5.02

Table 2. GA Parameters

GA Parameter	Value
Population size	30
Number of generations	100
Probability of crossover	0.70
Probability of mutation	0.01
Probability of creep mutation	0.70
Conditional probability of downward adjacency mutation	0.50

The above network is also used to illustrate the application of the inverse model to estimate the wall reaction parameters under synthetically generated noisy measurements. The error free data at the reservoir nodes used for verification is corrupted to generate noisy measurements. The source strength of chlorine (0.75 mg/L) at all source nodes is known, the

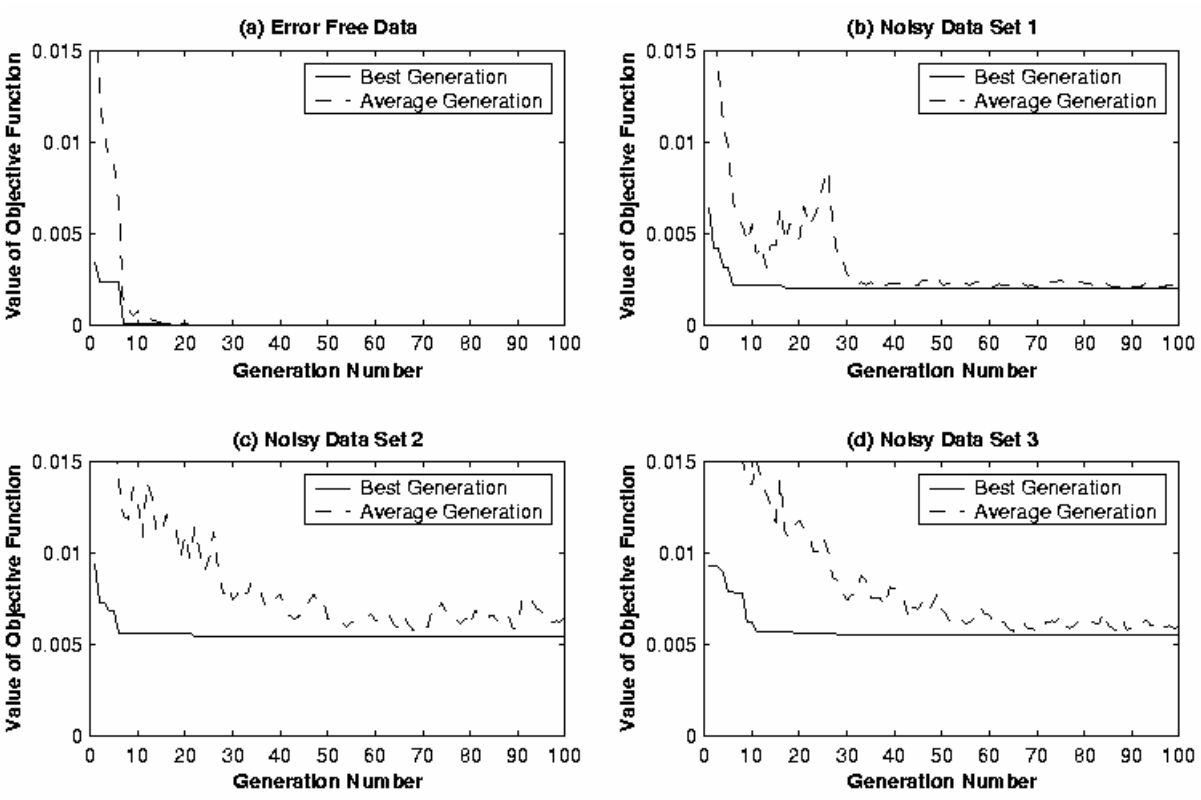

Figure 3. Variation of Objective Function Value With Generation Number

wall reaction parameters are evaluated for noisy data. Three sets of normally distributed random numbers with mean zero and standard deviation of 0.02 mg/L are used to create three different sets noisy measurements which are given in Table 1 along with the percentage errors introduced with respect to the error free data.

Table 3. Estimated First-order Wall Reaction Parameters by GAT - Noisy Data

Parameter	True Value (m/d)	Estimated Value (m/d)
Data Set 1		
1	0.75	0.7206
2	0.50	0.4555
3	1.00	1.0255
Average Error (%)		5.11
Data Set 2		
1	0.75	0.7560
2	0.50	0.4630
3	1.00	1.0415
Average Error (%)		4.09
Data Set 3		
1	0.75	0.6686
2	0.50	0.5376
3	1.00	0.9283
Average Error (%)		8.44

It can be seen that the actual errors introduced at some nodes are as high as 12%. The inverse model is run using GAT with these noisy chlorine concentrations and the GA parameters listed in Table 2 as inputs. The estimated wall reaction parameters by are GAT are given Table 3. It can be seen from the table that the unknown parameters are well estimated. The convergence in the value of objective function with generation, for best of generation and average generation results, is shown in Figures 3(b)-(d) for the three data sets respectively. It can be seen that the there is not much improvement in the best generation value of objective function after 10 generations indicating the rapid computation of the parameters.

3.2 Performance of Reaction Kinetics

The objective of this section is to identify appropriate reaction kinetics for a given set of observed data. The applicability of the developed model to carry out this procedure is illustrated using four hypothetically generated sets of observations that are given in the Table 4. It is assumed that the bulk flow reactions are governed by either first- or second-order kinetics and the corresponding reaction parameters are 2 d^{-1} and 4.5 L/mg/d respectively. In the process of identification the first- or zero-order wall reaction parameters are also estimated. The inverse model is applied on to each of the data sets for the various combinations of bulk and wall reactions. The same GA parameters are used as given in Table 1. The appropriate reaction kinetics model is selected based on the goodness of fit between the observed concentrations at the monitoring nodes and the concentrations computed by the inverse model at these nodes. The goodness of fit between the two observations is interpreted in terms of average absolute error and Root Mean Square (RMS) error. The wall reaction parameters computed for various reaction kinetics and the corresponding error statistics of best fits with respect to each hypothetical data set are given in Table 5.

Table 4. Hypothetical Data Sets

Reservoir Node No.	Data Set 1	Data Set 2	Data Set 3	Data Set 4
72	0.5046	0.4014	0.4349	0.3777
73	0.6161	0.6010	0.5849	0.5992
74	0.5480	0.5984	0.6396	0.5539
75	0.3823	0.3996	0.3558	0.5019
76	0.2914	0.3349	0.2408	0.2333
77	0.3740	0.3198	0.3776	0.3109
78	0.3042	0.3632	0.4233	0.4303
79	0.2614	0.2249	0.1820	0.2241
80	0.4152	0.4069	0.3679	0.3960
82	0.6247	0.6625	0.7147	0.6918
83	0.5691	0.5362	0.5915	0.6555
84	0.6318	0.6166	0.5439	0.4683
85	0.3949	0.4806	0.4722	0.4468
86	0.5337	0.5598	0.5175	0.5592

It is seen from Table 5 that any of the reaction kinetics can be fitted to the hypothetical data since the average absolute error and RMS error are relatively comparable for all the reaction kinetics models used. Thus the choice of proper reaction kinetics model becomes all the more difficult. Such situation may arise in the field condition also.

Table 5. Performance of Reaction Kinetics Models and Estimated Reaction Parameters

Data Set	Reaction Kinetics		Wall Reaction Parameter m/d (I-order) mg/m^2/d (0-order)			Average Absolute Error (mg/L)	R.M.S Error (mg/L)
	Bulk Order	Wall Order	Group 1	Group 2	Group 3		
1	first	first	0.6858	0.5028	0.8906	0.0340	0.0390
	first	zero	284.39	200.11	253.28	0.0448	0.0506
	second	first	0.4502	0.3726	0.7278	0.0272	0.0353
	second	zero	198.89	149.34	208.88	0.0345	0.0397
2	first	first	0.7048	0.4492	0.8580	0.0371	0.0429
	first	zero	311.74	193.84	264.07	0.0367	0.0457
	second	first	0.4655	0.3027	0.7388	0.0384	0.0429
	second	zero	224.26	122.42	249.68	0.0360	0.0412
3	first	first	0.7885	0.4931	1.1066	0.0316	0.0379
	first	zero	350.18	200.30	349.71	0.0293	0.0354
	second	first	0.5413	0.3598	0.9668	0.0350	0.0439
	second	zero	256.41	153.62	306.66	0.0311	0.0371
4	first	first	0.5734	0.4260	1.834	0.0384	0.0551
	first	zero	291.63	167.55	446.47	0.0442	0.0601
	second	first	0.3363	0.2977	1.638	0.0435	0.0563
	second	zero	200.72	124.57	437.79	0.0421	0.0565

4. CONCLUSIONS

An integrated hydraulic and water quality forward simulation model is developed. The autocalibration of chlorine transport model is formulated in terms of observed and computed chlorine concentrations in a least square sense. The optimization model is solved using simulation-optimization technique with GA in its optimization module. The GA procedure utilizes advanced operators in addition to the standard operators. The verification of the model is carried out using the synthetic error free measurements and the application part consists of estimating the value of unknown reaction parameters for synthetic noisy measurements using a large multiple source network. The network used for the above processes is divided into three zones based on age of the pipes. The model verification shows the capability of the model to estimate correctly the unknown parameters for a given error free data. The application of model illustrates the rapid estimation of the reaction parameters with a reasonable degree of accuracy. The model developed can also be used for any combination of bulk and wall reaction kinetics. The convergence characteristics of this improved GA are much better compared to the standard GA procedure. It can be concluded that the GA technique is best suitable for

autocalibration of water quality models. The model provides a useful tool to the water supply authorities to calibrate the water quality models of their systems.

NOMENCLATURE

Cnc_j = concentration at node j (mg/L);
Cnc_{nui} = concentration at node nu_i;
Cno_j = observed chlorine concentration at monitoring node j (mg/L);
M = number of monitoring nodes;
nu_i= upstream node of incoming pipe i;
$Ninp_j$ = number of incoming pipes at node j;
Njn = number of nodes in the network;
Q_i = flow in pipe i (m^3/s);
Rec_i = reaction coefficient for pipe i.

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