REGIONAL WASTEWATER TREATMENT FACILITIES OPTIMIZATION BY SIMULATED ANNEALING

Enéas Souza Machado
Universidade de São Paulo, Departamento de Hidráulica e Saneamento, Cidade Universitária, SP.
sm.eneas@gmail.com
Monica Porto
Universidade de São Paulo, Departamento de Hidráulica e Saneamento, Cidade Universitária, SP.
mporto@usp.br
Eloy Kaviski
Universidade Federal do Paraná, Departamento de Hidráulica e Saneamento, Centro Politécnico, Curitiba, PR.
eloy.dhs@ufpr.br
Clarissa Scuissiato
Universidade Federal do Paraná, Departamento de Hidráulica e Saneamento, Centro Politécnico, Curitiba, PR.
clascui@pop.com.br

Abstract. Regional wastewater treatment systems are widely applied in urban regions, due to economic scale it provides. Since there is a large number of effluent discharges as well as potential sites for the location of treatment facilities, traditional engineering techniques can handle just a few of the possibilities of locating such facilities, sometimes missing the optimal facilities location, in terms of budget minimization. Traditional optimization techniques have been applied to this engineering problem, such as linear or non linear programming. This paper shows some initial results of applying simulated annealing, a metaheuristic derived from statistical mechanics, as an optimization tool for locating wastewater treatment facilities. The results show the potential possibilities of using such technique with near optimal results in a reasonable computer time.

Keywords. *simulated annealing, optimization, wastewater treatment systems.*

1. Introduction

One of the main environmental problems in less developed countries is the lack of adequate urban sewerage and sewage treatment, leading to poor water quality in rivers near urban and metropolitan areas. In Brazil, since such sewage works have not been built in the past decades, the estimated budget to cover the sanitary deficit is as high as R$150 billions until 2015.

Since the end of the Planasa (Brazilian's National Plan for Sanitary Works) in the late seventies, the country still doesn't have an institutional and financial arrangement for handling such a huge problem. Some bills have been discussed in the Congress, and sooner or later, the country will have to find an adequate framework for the problem. Independently of the political model to be chosen, the financial challenge will have to take into account least cost optimal regional solutions.

Economies of scale are an important characteristic of regional sewage works and engineers must seek a proper design of such regional works. Traditional engineering techniques are not adequate, since they can handle only a few alternatives. Instead, it is necessary to apply optimization procedures to facilitate the study of a large number of alternatives. The problem is that the objective function and the restraints lead to non linear equations. Real world problems contain hundreds of restraints that are very difficult ant time consuming to be solved by traditional optimization techniques such as Non Linear Programming.

This paper presents the formulation of the problem and its solution by use of simulated annealing (SA). SA is a metaheurístic technique that has been applied in the water resources field in the last years, with promising results. SA algorithm is presented and an application is showed and compared with traditional optimization results. A sensivity analysis of SA parameters is also presented.

2. Literature Review

Optimization models begun to be applied to regional water quality problems in the mid 1960s. Examples of such early models are Deininger (1965), Kerri (1966) and ReVelle, Loucks and Lynn (1967), all of them using Linear Programming. These first studies were applied to individual sewage treatment plants, and seek the minimum treatment efficiency in each plant to meet effluent standards or water quality objectives. Other optimization models have been widely used. Dynamic Programming was applied by Liebman and Lynn (1966), Converse (1972) and Rossmann (1978). Ecker (1975) and McNamara (1976) used Geometric Programming. Integer programming, with the decision to build or not a sewage treatment plant, has been widely used: Chang, Chen e Yang (1997), Chang, Brill, Jr. e Hopkins (1982) and Zhu and ReVelle (1988). Due to non-linearities of the problem, Non Linear Programming has also been extensively used: Nakamura e Brill, Jr. (1979), Ong (1983) and Carmichael e Strzepek (2000). These later studies deal

with regional treatment plants, where the objective is the size and location of the plants, some of them linked with a water quality simulation model to study water characteristics such as Dissolved Oxygen and Biological Oxygen Demand.

Recently the so-called metaheuristics models have been applied to solve complicated models such as the one here described. Burn and Yulanti (2001) applied a genetic algorithm to solve a multiobjective location model for sewage treatment plants. Mujumdar and Vemula (2004) also applied genetic algorithm along with fuzzy sets to study multiple and conflicting objectives, with the variables treated as fuzzy ones. Cunha and Ribeiro (2004) used a tabu search algorithm for water network optimization. The same problem was solved by simulated annealing by Cunha and Souza (1999). The same metaheurístic has been used for siting and sizing regional sewage treatment plants: Souza et al. (2002) developed a model based on optimization by annealing, coupled with a GIS interface. The model was further developed by Cunha et al. (2004), incorporating water quality constraints.

3. Simulated Annealing

Simulated annealing algorithms can guarantee the near optimum global solution of any function, including discontinuous and non convex functions. Its main advantage is its characteristic of using a descent strategy that allows ascent probabilistic movements, thus avoiding being trapped in local optima. The concept was first introduced by Metropolis et al. (1953) and an algorithm was independently developed by Kirkpatrick et al. (1983) and Cerny (1985) to solve the traveling salesman problem.

The algorithm is based on the physical process of annealing. According to Cunha and Souza (1999), in this process, temperature is raised allowing mobility to the molecules. Then a cooling slow schedule is applied, when the molecules will end forming a crystalline structure. The high mobility of the molecules at a high initial temperature allows them to reach different states. Following an adequate cooling scheme the molecules will arrive at a minimum energy state and an ordered crystalline configuration. The Metropolis algorithm generates a sequence of states. If the energy of the initial state is E_i, then a perturbation mechanism is applied, generating an energy E_j in this second state. If $E_i - E_j \leq 0$, then j will be the second state. Otherwise, j can still be accepted as the next state according to a probability p given by: $p = exp(E_i - E_j)/k_\beta t$, where k_β is the constant of Boltzmann and t is the temperature of the process.

Aarts and Korst (1989) prove that the simulated annealing algorithm, formulated as a sequence of homogenous and finite length Markov chains converges in probability to the set of optimal solutions. In other words, asymptotically the algorithm finds an optimal solution with probability one. This result is achieved only after an infinite number of transitions, so that, in practical applications, one must resort to an approximation of the asymptotic convergence.

The algorithm can be described by the following steps:

(i) choose an initial configuration
(ii) test the viability of the initial configuration
(iii) set an initial temperature and a cooling schedule
(iv) for $j = 1$ to number of cooling states repeat (v) to (ix)
(v) generate a perturbation in the initial configuration to generate a candidate solution
(vi) test the viability of the candidate solution
(vii) if $E_2 < E_1$, the candidate solution is accepted
(viii) if $E_2 > E_1$, the Metropolis criterion is tested; if $p > 0$, the candidate solution is accept
(ix) repeat steps (v) to (viii) until number of simulations < maximum number of simulations or number of successes < maximum number of successes

The algorithm has the following parameters:

a) a the initial temperature of the process, representing the probability of accepting a transition from the initial configuration to a candidate solution with an higher energy;
b) n_1 the number of iterations in the same temperature, even if there is no gain in the optimal state of the configuration;
c) r cooling factor, representing the rate of temperature decreasing;
d) n_2 number of steps of temperature decreasing, performed without improvement in the optimum, before stopping the algorithm.

The values for initial temperature were used according to Press et al. (1992). In this paper n_2 was substituted by a maximum number of total iterations, $nmax$. The literature reports that n_1 and $nmax$ should be linked to the number of variables of the Objective Function. The study below presented uses n_1 and $nmax$ equal to 10 and 100 times the number

of variables, respectively. For the cooling factor *r*, Kirkpatrick et al. (1983) suggest a constant factor between 0.8 and 0.99, which were also used here.

3.1 Initial and candidate solutions

The initial solution was obtained through random sampling. For each one of the components of the variables vector, in an independent manner, uniformly distributed values are generated, within its respective validity limits. Then the restrictions are verified, repeating the process until reaching a viable random solution.

The Metropolis algorithm can be used for generating a set of points in a space with $\boldsymbol{X}$ variables with a distributed density function $f_{\mathbf{X}}(\mathbf{X})$. A sequence of points $\mathbf{X}_0, \mathbf{X}_1, ...,$ is generated, representing a random walk moving through the $\boldsymbol{X}$ space. The rules by which this random walk is made are as follows:

- Consider that the random way is on point $\mathbf{X}_n$.
- An iterative process is applied for generating the $\boldsymbol{X}_{n+1}$ point. The new point can be randomly chosen over the surface of a hypersphere with a small radius δ, around the $\boldsymbol{X}_n$ point. The methods used for the random variables generation are presented in the appendix.
- A sampled point $\boldsymbol{X}_t$, is accepted, considering the following ratio:

$$r = \frac{f_{\mathbf{X}}(\mathbf{x_t})}{f_{\mathbf{X}}(\mathbf{x}_n)}. \tag{1}$$

- If $r>1$, then the point $\mathbf{X}_t$ is accepted ($\mathbf{X}_{n+1} = \mathbf{X}_t$), while if $r<1$, the point $\mathbf{X}_t$ is accepted with probability *r*. In this procedure r is compared to *r* an uniformly distributed number u, in the interval [0,1], $\mathbf{X}_t$ being accepted if $u<r$. When the point $\mathbf{X}_t$ is not accepted, the random way keeps on point $\mathbf{X}_n$ ($\mathbf{X}_{n+1} = \mathbf{X}_n$).
- By using the same procedure the $\mathbf{X}_{n+2}$ point is generated.
-

The value of δ should be chosen in such a way that 1/3 to 1/2 of the generated configurations are accepted; in other way, the method becomes less efficient. (Koonin e Meredith, 1990). If there is a large number of rejected configurations, this means that the value of δ is too large; in other way, if δ is too small, then one will have a large number of accepted configurations, but the explored region will be small. The best choice to the initial point $\mathbf{X}_0$ lies where the probability distribution is at a maximum.

4. Model application and results

The simulated annealing algorithm was applied to a hypothetical regional sewage treatment plant location problem, formulated by Deinenger and Su (1971) and also applied by Ong (1983). Given a set of seven communities located along a river and its tributary, there are seven potential sites available for the construction of wastewater treatment plants. The objective is to find the size and location of wastewater treatment plants and the interconnecting conveyance system which will minimize the total construction cost. The problem is depicted in Fig. 1.

The objective function has the following mathematical formulation:

$$\text{Min} \sum_{i=1}^{6} CP_i(Y_i) + \sum_{i=1}^{6} CP_i(Z(_i) + \sum_{i=1}^{7} CT_i(X_i) \tag{2}$$

Subject to:

a) Flow balance at each source node

b) Upper and lower bound constraints

Where:

Y_i: amount of wastewater carried by the i-th section of conveyance (in the direction from upstream to downstream). Considered as dependent variable;
Z_i: amount of wastewater carried by the *i-th* section of conveyance (in the direction from downstream to upstream); Considered as dependent variable;

X_i: amount of wastewater to be treated at plant *i*. Considered as independent variable;
$CP_i(Y_i)$, $CP_i(Z_i)$: cost of piping (gravity sewer or forcemain) as a function of Y_i or Z_i;
S_i: amount of wastewater generated at source *i* (Y_i, Z_i, X_i and S_i are used in the flow balance at each source node);
XU_i, YU_i, ZU_i: maximum amount of flow at the treatment plants and the conveyances; these are the upper and lower bound constraints.

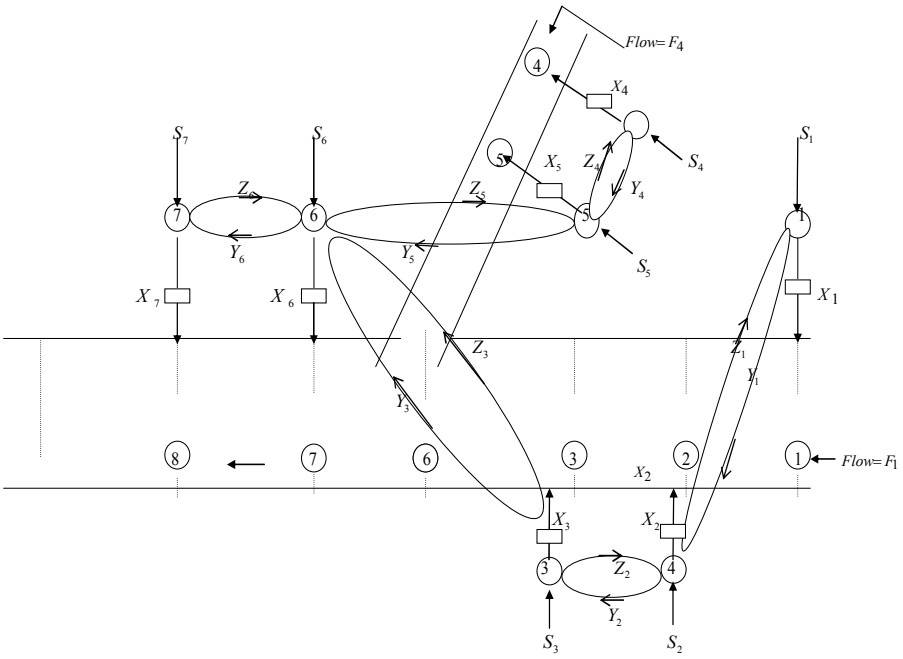

Figure 1 – River, sewerage and treatment plants system

The objective function has the following mathematical formulation:

$$\text{Min} \sum_{i=1}^{6} CP_i(Y_i) + \sum_{i=1}^{6} CP_i(Z(i) + \sum_{i=1}^{7} CT_i(X_i) \quad (2)$$

Subject to:

a) Flow balance at each source node

b) Upper and lower bound constraints

Where:

Y_i: amount of wastewater carried by the i-th section of conveyance (in the direction from upstream to downstream). Considered as dependent variable;
Z_i: amount of wastewater carried by the *i-th* section of conveyance (in the direction from downstream to upstream); Considered as dependent variable;
X_i: amount of wastewater to be treated at plant *i*. Considered as independent variable;
$CP_i(Y_i)$, $CP_i(Z_i)$: cost of piping (gravity sewer or forcemain) as a function of Y_i or Z_i;
S_i: amount of wastewater generated at source *i* (Y_i, Z_i, X_i and S_i are used in the flow balance at each source node);
XU_i, YU_i, ZU_i: maximum amount of flow at the treatment plants and the conveyances; these are the upper and lower bound constraints.

The cost functions, either for the wastewater conveyance or for the treatment plants are of the type:

$$CT = (a - b*X_i)*X_i \quad (3)$$

Where *a* and *b* are coefficients of the equation.

Table (1) presents the SA results, compared to the results found by Ong (1983), by means of a heuristic technique called Random Polyhedron Search (RPS). The optimal solution calls for a single regional treatment plant located at site 6. The parameters' values for the lowest Objective Function value are: *dx1*=0.0090, *fat*=0.902 and *t1*=0.43.

Table 1. Results of the regional treatment plant location problem

	Objective Function (US10^6)	X_1 (mgd)	X_2	X_3	X_4	X_5	X_6	X_7
Simulated Annealing	2.734	0.0	0.0	0.0	0.0	0.0	6.6	0.0
RPS heuristic	2.730	0.0	0.0	0.0	0.0	0.0	6.6	0.0

5. Sensivity Analysis

A sensivity analysis was performed, verifying the results of the Objective Function, with varying values of the cooling factor (*fat*), the initial temperature (t_1) and the change of the radius of the hypersphere, when looking for a candidate solution (*dx*). In all simulations, the number of steps to decrease the temperature was 100. The results are shown in Tab. (2). Lower temperatures resulted in most of the minimum values for the Objective Function. Also, lower values of the cooling factor led to better values of the Objective Function, showing that a slower cooling can find near optimal results. When *t1* and *dx* are maintained fixed, changing the values of *fat* gives higher changes in *fmin* in comparison with fixing *fat* and *dx* and changing the values of *t1*. Changing *dx*, with fixed values of *fat* and *t1*, gives small variations to the value of *fmin*. In other words, the model is less sensible to *dx* and *t1* variations, and a more sensible to the cooling factor *fat*.

Table 3 shows the results for the mean value of the Objective Function (*fmed*), its Coefficient of Variation (*cv*) and the ratio between the number of simulations of accepted solutions in the Metropolis algorithm and the total number of simulations (*pac*). The same variations for the parameters were used as above. The values for the Coefficient of Variation were all less than 0.30, showing a smooth surface of the Objective Function. The values of the ration *pac* were not higher than 10%, showing that the range of simulated temperatures was quite near the optimal final temperature.

6. Conclusions

Simulated Annealing seems to be a promising optimization tool for the regional planning of wastewater treatment plants, as was already shown by Cunha et al. (2004). Such problems have nonlinear objective functions and constraints, being difficult ones to be solved by traditional non linear programming. Further investigations are needed to get a good knowledge of the parameters' behavior. The authors are also studying the addition of other constraints such as water quality constraints and budget considerations. The Simulated Annealing algorithm, maybe coupled with Dynamic Programming seems to be an adequate tool for the dynamic schedule of such engineering works.

Table 2. Objective Function Values for Different Cooling Schedules (fat and t_1) and Hypersphere Radius (dx_1)

fmin	dx1 = 0.0090						fmin	dx1=0.0096					
fat/t1	0.35	0.37	0.39	0.41	0.43	0.45	fat/t1	0.35	0.37	0.39	0.41	0.43	0.45
0.890	2.827	2.964	3.064	2.955	3.119	2,783	0.890	2.781	3.148	2.959	2.990	3.262	3.039
0.894	2.791	3.130	3.029	2.940	2.932	2,790	0.894	2.983	3.188	2.908	2.810	2.810	2.907
0.898	2.951	2.921	2.813	2.922	2.962	3,196	0.898	3.279	2.836	2.838	2.858	3.016	2.993
0.902	2.846	2.860	3.191	2.828	2.734	2,966	0.902	3.122	2.817	2.963	2.742	2.921	2.768
0.906	2.915	2.870	3.203	2.836	2.909	2,814	0.906	2.830	2.924	2.830	3.292	2.959	2.913
0.910	2.951	2.901	2.737	2.974	3.187	2,739	0.910	2.940	2.808	2.829	2.795	2.937	2.899

Table 2. Objective Function Values for Different Cooling Schedules (fat and t_1) and Hypersphere Radius (dx_1) (Cont.)

fmin	dx1=0.0102						fmin	dx1=0.0108					
fat/t1	0.35	0.37	0.39	0.41	0.43	0.45	fat/t1	0.35	0.37	0.39	0.41	0.43	0.45
0.890	2.760	2.971	2.908	3.006	2.765	2,740	0.890	2.882	2.954	2.839	2.973	3.056	3.002
0.894	2.791	3.260	3.056	3.124	2.748	2,737	0.894	2.820	2.947	2.972	2.840	2.822	2.921
0.898	2.804	2.903	2.916	2.916	2.909	2,826	0.898	2.776	3.003	2.984	3.248	3.265	2.965
0.902	2.908	2.909	2.829	2.872	2.797	2,991	0.902	3.039	2.758	2.776	2.954	2.919	3.327
0.906	2.992	2.983	2.814	2.867	2.910	2,989	0.906	3.432	2.867	2.737	2.768	2.911	3.187
0.910	2.915	2.915	2.888	2.803	3.065	2,935	0.910	3.278	2.910	2.826	3.014	2.849	2.961

Table 2. Objective Function Values for Different Cooling Schedules (fat and t_1) and Hypersphere Radius (dx_1) (Cont.)

fmin	dx1=0.0114						fmin	dx1=0.0120					
fat/t1	0.35	0.37	0.39	0.41	0.43	0.45	fat/t1	0.35	0.37	0.39	0.41	0.43	0.45
0.890	2.948	3.203	2.921	2.911	2.771	2,851	0.890	2.836	2.910	2.884	2.796	2.938	2.774
0.894	3.199	3.049	2.767	2.789	3.001	2,919	0.894	2.833	2.851	2.775	2.786	2.911	2.911
0.898	2.777	2.786	2.910	2.920	2.911	2,924	0.898	2.748	2.874	2.829	2.919	3.009	3.281
0.902	2.991	2.852	2.750	2.932	2.989	2,810	0.902	3.188	2.742	2.948	2.744	2.740	2.915
0.906	2.918	2.798	2.929	2.789	2.940	2,924	0.906	3.057	2.781	2.921	3.057	2.757	2.914
0.910	2.737	2.817	2.740	2.995	2.756	2,953	0.910	3.188	2.976	2.803	2.925	2.911	2.758

Table 3. Numerical statistics for Different Cooling Schedules (fat and t_1) and Hypersphere Radius (dx_1)

dx1 = 0.0090

fat1/t1	0,35			0,37			0,39			0,41			0,43			0.45		
	fmed	cv	pac	Fmed	cv	pac	fmed	cv	pac	fmed	cv	pac	fmed	cv	pac	fmed	cv	pac
0,890	4,6984	0,21	0,0681	4,0753	0,21	0,0714	4,4535	0,23	0,0829	5.2288	027	0,0765	4,9735	0,19	0,0657	4,686	0,22	0,0775
0,894	4,6829	0,23	0,0673	4,4424	0,22	0,0766	5,3171	0,22	0,0660	4.6654	0,26	0,0688	4,4400	0,22	0,0845	4,9206	0,26	0,0672
0,898	3,9496	0,15	0,0795	4,6459	0,21	0,0891	4,9494	0,28	0,0710	4.2105	0,18	0,0838	4,8231	0,25	0,0853	4,3262	0,20	0,0932
0,902	4,8763	0,24	0,0768	4,8066	0,21	0,0963	4,0992	0,18	0,0919	4.5930	0,27	0,0775	4,7847	0,24	0,0818	4,8984	0,24	0,0769
0,906	4,7196	0,23	0,0985	5,1365	0,23	0,0873	5,1278	0,25	0,0994	4.7537	0,25	0,0824	4,0357	0,16	0,1053	4,2161	0,12	0,0849
0,910	4,5884	0,27	0,0965	4,9983	025	0,0856	4,3211	0,28	0,0881	4.0987	0,15	0,1070	4,6472	0,22	0,1138	3,8025	0,16	0,0931

Table 3. Numerical statistics for Different Cooling Schedules (fat and t_1) and Hypersphere Radius (dx_1) (cont.)

dx1 = 0.0096

fat1/t1	0,35			0,37			0,39			0,41			0,43			0.45		
	fmed	cv	pac	Fmed	cv	pac	fmed	cv	pac	fmed	cv	pac	fmed	cv	pac	fmed	cv	pac
0,890	4,2482	0,21	0,06	4,9998	0,26	0,081	4,3243	0,18	0,0663	5,2288	0,27	0,0765	4,585	0,25	0,0828	4,6517	0,23	0,081
0,894	4,6683	0,18	0,0747	4,7626	0,26	0,0808	5,0872	0,25	0,0779	4,179	0,19	0,0762	4,4747	0,26	0,072	4,8899	0,28	0,0799
0,898	4,5541	0,19	0,0899	4,7751	0,24	0,0758	4,9271	0,25	0,0769	4,1083	0,15	0,0735	4,9021	0,25	0,0689	4,8023	0,25	0,0962
0,902	4,2946	0,23	0,0914	4,5997	0,21	0,0769	4,2511	0,21	0,0894	4,6152	0,27	0,0740	4,5465	0,19	0,0915	5,1714	0,25	0,0779
0,906	5,1428	0,28	0,0808	4,6553	0,25	0,0100	4,558	0,22	0,081	5,0013	0,25	0,1035	4,9839	0,26	0,0776	3,7793	0,14	0,0964
0,910	4,7151	0,25	0,1096	4,1704	0,15	0,0965	4,1693	0,20	0,0826	4,7023	0,23	0,0857	4,4489	0,18	0,0929	4,3738	0,20	0,0865

Table 3. Numerical statistics for Different Cooling Schedules (fat and t_1) and Hypersphere Radius (dx_1) (cont.)

dx1=0.0102

fat1/t1	0,35			0,37			0,39			0,41			0,43			0.45		
	fmed	cv	pac	Fmed	cv	pac	fmed	cv	pac	fmed	cv	pac	fmed	cv	pac	fmed	cv	pac
0,890	4,6946	0,27	0,0703	4,9787	0,26	0,0769	5,0406	0,24	0,0709	4,6129	0,27	0,0757	4,4995	0,26	0,0624	4,7796	0,28	0,061
0,894	4,8417	0,27	0,0838	4,8011	0,2	0,0805	4,8226	0,26	0,087	4,7128	0,22	0,0758	4,7163	0,26	0,0656	4,6976	0,25	0,0679
0,898	4,5358	0,21	0,0657	4,2	0,2	0,0645	4,2866	0,21	0,0802	4,1849	0,20	0,0810	4,2315	0,19	0,0846	4,7963	0,2	0,0785
0,902	4,4274	0,19	0,0686	3,9124	0,22	0,0824	4,2413	0,17	0,0813	3,91	0,19	0,095	4,6948	0,29	0,0776	5,2847	0,25	0,0895
0,906	4,4778	0,16	0,0863	4,773	0,24	0,0907	4,0179	0,19	0,0794	4,6708	0,26	0,0797	4,6194	0,29	0,0925	4,0143	0,11	0,0102
0,910	4,6268	0,25	0,0957	4,0217	0,17	0,0961	4,4477	0,24	0,0820	5,3266	0,26	0,0889	4,4761	0,27	0,1134	5,4277	0,27	0,0905

Table 3. Numerical statistics for Different Cooling Schedules (fat and t_1) and Hypersphere Radius (dx_1) (cont.)

dx1=0.0108

fat1/t1	0,35			0,37			0,39			0,41			0,43			0.45		
	fmed	cv	pac	Fmed	cv	pac	fmed	cv	pac	fmed	cv	pac	fmed	cv	pac	fmed	cv	pac
0,890	3,8563	0,20	0,0574	4,7255	0,24	0,0702	3,8322	0,13	0,0612	4,3298	0,21	0,07	4,697	0,24	0,0825	4,1786	0,18	0,0728
0,894	4,0405	0,20	0,06	4,8005	0,21	0,0763	3,7605	0,14	0,0738	4,6306	0,29	0,0637	4,0574	0,21	0,0665	4,4701	0,23	0,0786
0,898	4,3944	0,23	0,0632	3,6065	0,11	0,0738	5,1434	0,26	0,0798	4,0973	0,13	0,0895	5,4481	0,27	0,0871	4,3637	0,22	0,0826
0,902	3,8994	0,11	0,0846	4,3782	0,28	0,0673	4,2801	0,18	0,0759	4,6001	0,25	0,0852	4,8334	0,21	0,076	4,1649	0,17	0,0941
0,906	4,7545	0,24	0,0921	4,8376	0,22	0,0873	3,8506	0,15	0,078	4,3896	0,18	0,0901	4,3235	0,24	0,0925	4,551	0,24	0,01
0,910	4,8189	0,27	9,7229	3,6806	0,15	0,0925	4,2434	0,17	0,0794	4,1607	0,23	0,0954	4,3153	0,2	0,0893	4,4925	0,2	0,01

Table 3. Numerical statistics for Different Cooling Schedules (fat and t_1) and Hypersphere Radius (dx_1) (cont.)

dx1=0.0114

fat1/t1	0,35			0,37			0,39			0,41			0,43			0,45		
	fmed	Cv	pac	Fmed	cv	pac	fmed	cv	pac	fmed	cv	pac	fmed	cv	pac	fmed	cv	pac
0,890	4,2674	0,24	0,0708	4,1821	0,17	0,0712	4,2603	0,26	0,0668	4,2341	0,18	0,0733	5,0169	0,22	0,0632	4,2427	0,23	0,063
0,894	4,325	0,19	0,0734	4,6924	0,28	0,0582	3,9223	0,22	0,0608	5,0213	0,24	0,059	4,8369	0,25	0,075	5,1462	0,27	0,0788
0,898	4,8927	0,28	0,0666	4,4996	0,27	0,066	4,4487	0,22	0,0775	3,5198	0,12	0,0768	4,4805	0,23	0,0791	4,4652	0,22	0,0904
0,902	4,0178	0,23	0,0803	4,1179	0,15	0,0734	5,1263	0,26	0,0709	4,7889	0,28	0,0811	4,4735	0,22	0,086	4,7425	0,24	0,0767
0,906	4,6535	0,30	0,0811	4,6031	0,24	0,0731	4,1462	0,18	0,0966	4,3897	0,29	0,0723	4,488	0,19	0,1032	4,5883	0,27	0,0998
0,910	3,8285	0,13	0,0748	4,2079	0,18	0,0748	3,7662	0,15	0,08	4,6385	0,25	0,1022	3,9312	0,22	0,0842	4,4446	0,24	0,0961

Table 3. Numerical statistics for Different Cooling Schedules (fat and t_1) and Hypersphere Radius (dx_1) (cont.)

dx1=0.0120

fat1/t1	0,35			0,37			0,39			0,41			0,43			0.45		
	fmed	Cv	pac	Fmed	cv	pac	fmed	cv	pac	fmed	cv	pac	fmed	cv	pac	fmed	cv	pac
0,890	3,7888	0,0993	0,0569	4,4334	0,26	0,0664	4,841	0,25	0,0604	4,6189	0,28	0,0585	4,6781	0,24	0,0673	5,1359	0,27	0,0609
0,894	4,0840	0,26	0,0575	5,1534	0,31	0,0584	3,8635	0,18	0,0631	5,0213	0,24	0,059	4,8369	0,25	0,075	4,2603	0,24	0,0732
0,898	4,736	0,30	0,0628	4,6709	0,25	0,0633	4,3236	0,24	0,0614	5,0302	0,25	0,0744	4,2543	0,14	0,0814	4,044	0,12	0,0893
0,902	4,2644	0,21	0,0815	4,3841	0,24	0,0691	4,1997	0,17	0,0925	3,8135	0,19	0,0694	4,0508	0,22	0,0685	4,6819	0,28	0,0851
0,906	4,7067	0,24	0,0943	3,6528	0,15	0,0747	3,7339	0,18	0,0853	4,2191	0,24	0,103	4,9973	0,28	0,0732	4,6427	0,25	0,0896
0,910	4,7729	0,21	0,096	3,8123	0,13	0,0886	4,7311	0,21	0,0845	4,4041	0,22	0,0944	4,3239	0,21	0,0937	3,791	0,12	0,0842

APENDIX- Random Functions generation

The joint distribution function of *n* normal, random and independent variables, N(0,1), is defined by:

$$f_{\mathbf{Z}}(\mathbf{z}) = \frac{1}{(2\pi)^{n/2}} \exp[-\frac{1}{2}(z_1^2 + ... + z_n^2)] . \quad (A.1)$$

The function (A1) has the property of having a constant density over the surface of the hyperspheres, with the following form:

$$z_1^2 + ... + z_n^2 = r^2 . \quad (A2)$$

Using the distribution function defined in (A1), by means of a transformation of variables, one can derive a method for generating random vectors randomly distributed in the hypersphere surface, with a unit radius. (Alagar, 1976). Applying a polar transformation to (A1), results in (Kendall, 1961):

$$f_{R,\Theta}(r,\theta\ ) = \frac{1}{(2\pi)^{n/2}} \exp(-\frac{1}{2}r^2)\, r^{n-1} \prod_{i=2}^{n-1} \mathrm{sen}^{i-1}\theta_i . \quad (A.3)$$

(A3) was found by aplying the following spheric polar transformation to the variable **Z**.

$$z_i = r\cos\theta_{i-1} \prod_{j=i}^{n} \mathrm{sen}\,\theta_j , \qquad i=1,...,n, \quad (A.4)$$

with:

$\cos\theta_0 = \mathrm{sen}\,\theta_n = 1$, $0 \le \theta_1 < 2\pi$, and $0 \le \theta_i \le \pi$ for i=2,...,n−1.

Applying the transformation (A.4) to the function (A.38) and making r=1, one obtains:

$$f_{\Theta}(\theta\ ) = \frac{\Gamma(n/2)}{2\pi^{\,n/2}} \prod_{i=2}^{n-1} \mathrm{sen}^{i-1}\theta_i . \quad (A.5)$$

Integrating the function A3, in relation to the variable *r*, from 0 to +∞, it is verified that the result equals the expression (A5), that represents the distribution function of the random vectors over the hypersphere surface, with unit radius and *n* dimensions.
Generating n normal unitary **Z** random variables, the vector:

$$\mathbf{X} = \mathbf{Z}/r , \quad (A.6)$$

is uniformly distributed over the hypersphere surface with dimension *n* and unitary radius.

The method proposed by Box and Muller in 1958 (Hammersley and Handscomb, 1979), can be used for the generation of normal random variables:

$$x_1 = (-2\ln u)^{1/2}\cos 2\pi v \quad \text{and} \quad x_2 = (-2\ln u)^{1/2}\,\mathrm{sen}\,2\pi v , \quad (A7)$$

with u and v as uniform random numbers between 0 and 1.

Press and others (1992) present a version of this generator where it's not necessary to calculate the sine and cosine functions. Considering u' e v' as uniform random numbers in the interval [-1,1], the following relation can be defined:

$$u = u'^2 + v'^2 , \quad \text{with } u<1, \quad (A.8)$$

$$u' = u^{1/2}\cos 2\pi v \qquad \text{and} \qquad v' = u^{1/2}\text{sen}\, 2\pi v\,. \tag{A.9}$$

It can be shown that:

$$f_{U,V}(u,v) = \pi\, f_{U',V'}(u',v') = \pi/4\,, \quad \text{and} \tag{A.8}$$

$$f_{U,V}(u,v \mid u<1) = f_{U,V}(u,v)/P[U<1] = 1\,. \tag{A.9}$$

arriving at the following expressions:

$$x_1 = (-\frac{2}{u}\ln u)^{1/2}u' \quad \text{and} \quad x_2 = (-\frac{2}{u}\ln u)^{1/2}v'\,, \qquad \text{with} \quad u = u'^2 + v'^2 < 1\,. \tag{A.10}$$

References

Aarts, E. and Korst, J., 1989, "Simulated Annealing and Boltzmann Machines", Wiley, 272p.

Alagar, V.S., 1976, "The Distribution of the Distance between Random Points". J. Appl. Prob. 13, 558.

Burn, D.H., and Yulanti, J.S., 2001, "Waste-Load Allocation Using Genetic Algorithms", Journal of Water Resources Planning and Management ASCE, Vol. 127, No. 2, pp. 121-129.

Chang, N.B, Chen, H.W. and Yang, C.H., 1997, "Water Pollution Control in River Basin by Interactive Fuzzy Interval Multiobjective Programming", Journal of the Environmental Engineering Division ASCE, Vol. 123, No. 12, pp. 1208-1216.

Carmichael, J.J. and Strzepek, K.M., 2000, "A Multiple-Organic-Pollutant Simulation/Optimization Model of Industrial and Municipal Wastewater Loading to a Riverine Environment", Water Resources Research, Vol. 36, No. 5, pp. 1325-1332.

Cerny, V. 1985, "AThermodynamical Approach to the Traveling Salesman Problem", J. Optimization Theory and Applications, 45, pp. 41-51.

Chang, S.Y., Brill Jr., E.D., and Hopkins, L.D. 1982, "Use of Mathematical Models to Generate Alternative Solutions to Water Resources Planning Problems", Water Resources Research, Vol. 18, No. 1, pp. 58-64.

Cunha, M.C. and Souza, J., 1999, "Water Distribution Network Design Optimization: Simulated Annealing Approach", Journal of Water Resources Planning and management ASCE, Vol. 125, No. 4, pp. 215-221.

Cunha, M.C. and Ribeiro, L. 2004, "Tabu Search Algorithms for Water Network Optimization", European Journal of Operational Research, Vol. 157, pp. 746-758.

Cunha, M. C., Pinheiro, L., Afonso, P. and Souza, J., 2004, "Decision-aid Models for the Implementation of the Water Framework Directive", DMUCE, CD Edition, Porto, 10p.

Deininger, R.A. 1965, "Water Quality Management: The Planning of Economically Optimum Pollution Control Systems", Proc. First Annual Water Resources Conf., Chicago, Ill., American Water Resources Association, pp. 254-282.

Ecker, J. 1975, "A Geometric Programming Model for Optimal Allocation of Stream Dissolved Oxygen", Management Science, 21, pp- 658-668.

Hammersley, J.M., Handscomb, D.C., 1979, "Monte Carlo Methods". Chapman and Hall, London.

Kendall, M.G., 1979, "A Course in the Geometry of *n* Dimensions", Charles Griffin & Company Limited, London.

Kerri, K.D. 1966, "A Dynamic Model for Water Quality Control", Journal of the Water Pollution Control Federation, Vol.39, No.5, pp. 772-786.

Kirkpatrick, S., Gellat, C. and Vecchi, M., 1983, "Optimization by Simulated Annealing", Sci., Vol. 220, No. 4958, pp. 671-680.

Koonin, S.E., Meredith, D.C., 1993, "Computational Physics", Fortran Version, Addison-Wesley Publishing Company, Inc., Reading.

Liebman, J.C and Lynn, W.R., 1966, "The Optimal Allocation of Stream Dissolved Oxygen", Water Resources Research, Vol.2, , No. 3, pp. 581-591. Converse, A.O., 1972, "Optimum Number and Location of Treatment Plants", Journal of the Water Pollution Control Federation, Vol.44, No.8, pp. 1629-1636.

Metropolis, N., Rosenbluth, A.W., Rosenbluth, M.N., Teller, A.H., 1953, "Equation of state calculations by fast computing machines", J. Chem. Phys. 21 (6), 1087.

McNamara, J.R. 1976, "An Optimization Model for Regional Water Quality Management", Water Resources Research, Vol. 12, No. 2, pp. 125-134.

Mujumdar, P.P. and Vemula, V.R.S., 2004, "Fuzzy Waste Load Allocation Model: Simulation-Optimization Approach", Journal of Computing in Civil Engineering ASCE, Vol. 18, No. 2, pp. 120-131.

Nakamura, M. and Brill, Jr. E.D., 1979, "Generation and Evaluation of Alternative Plans for Regional Wastewater Systems: An Imputed Value Method", Water Resources Research, Vol. 15, No. 4, pp. 750-756.

Ong, S.L. 1983, “Capacity Expansion for Regional Wastewater Treatment Systems”, Ph.D. Dissertation, University of Toronto.

Press, W.H., Flannery, B.P., Teukolsky, S.A., Vetterling, W.T., 1992, Numerical Recipes in Pascal. Cambridge University Press, Cambridge.

ReVelle, C., Loucks, D.P., and Lynn, W.R. 1967, “A Management Model for Water Quality Control”, Journal of the Water Pollution Control Federation, Vol.39, No.7, pp. 1164-1183.

Rossmann, L.A. 1978, “Planning Time-Phased Regional Treatment Systems”, Journal of the Environmental Engineering Division ASCE, 104(EE4), pp. 685-700.

Souza, J., Ribeiro A., Cunha, M.C., Antunes, A. 2002, “An Optimization Approach to Waste Water Systems Planning at the Regional Level”, Journal of Hydroinformatics, Vol. 4, No. 2, pp-115-123.

Zhu, Z. and ReVelle, C. 1988, “A Siting Model for Regional Wastewater Treatment Systems: The Chain Configuration Case”, Water Resources Research, Vol. 24, No.1, pp. 137-144.