



Analysis of Water Application Planning (WAP) Model Using Modified Genetic Algorithm (GA)

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ABSTRACT

The water application planning (WAP) model is designed to minimise the amount of water used by industries using water reuse, recycling, and regeneration (for both reuse and recycling). The design of WAP becomes a complex task when multiple contaminants are treated in the same plant with the use of multiple regeneration units. The modelling approach used was based on the concept of superstructure. The Genetic Algorithm (GA) which is an adaptive meta-heuristic search algorithm premised on the evolutionary ideas of natural selection and genetics, was used to find the solution to the modelled WAP problem. In order to increase the efficiency in obtaining the solutions of the model, the hybrid function was added to the GA, and the results obtained were compared with and without hybrid function. The behaviour of GA in solving WAP problems (with and without hybrid function) and the computing time to obtain the WAP model results was determined. The results show that there is a high efficiency in using the GA for solving the WAP problems (to minimise the total water consumption of the industrial processes). The GA produces results of the WAP problem in a short time of 3.4 to 10.1 seconds for the 2 to 10 industrial processes using a population size of 10 and 90% of the trial time, the optimum results were achieved.

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INTRODUCTION

The two major approaches in addressing water application planning (WAP) problems can be categorised as insight-based techniques and model-based optimisation methods. The former (insight-based technique) typically involves a water pinch analysis (WPA) technique that offers good insights with low computational burden, yet often at the expense of requiring significant problem simplification as demonstrated by previous studies (Wang and Smith, 1995; El-hawagi *et al.*, 2003; and Foo, 2009).

On the other hand, model-based optimisation approach allows handling of WAP problems in their full complexity by

considering different contaminants and objective functions. Some of the objective functions include minimising the quantity of freshwater use, minimising the quantity of wastewater produced, minimising the quantity of wastewater reused by other processes by considering their level of contaminants and the possible interconnections of the processes in the given industry and regeneration units. A model-based optimisation handles multiple contaminants, various constraints and integrates different types of processes involved in any given industry in selecting a reasonable reuse or regeneration reuse options.



The major challenges of model-based optimisation are high computational burden to achieve optimality, and it does not guarantee global optimum, which is the required best result and the lowest value (the global minimum) that depends on the objective function (Bagajewicz and Savelski, 2001; Chaturvedi *et al.*, 2016).

The design of water application planning (WAP) is a complex task, especially when multiple contaminants are treated in the same plant with the decision about the use of many regeneration units. This problem has been identified in previous studies (Gunaratnam *et al.*, 2005; Feng *et al.*, 2007 and Boix *et al.*, 2011). The analysis of the literature shows that there is need to formulate a generic framework that considers one or several objective functions and has a robust approach in solving large WAP problems. The mathematical representation of WAP with multiple contaminants is in the class of nonlinear programming (NLP) (Liu *et al.*, 2015), and the use of mathematical stochastic optimisation was verified to be effective in solving NLP formulation problems. Doyle and Smith (1997) described linear and non-linear formulations of the water reuse problem with multiple contaminants, which was combined with the previous method of Wang and Smith (1995) to provide a graphical representation of the problem. However, they use solution from the linear model to provide an initialization for a nonlinear optimisation solution. Tsai and Chang (2001) developed a mathematical programming model for modified water usage and treatment networks (WUTNs) design problem and solved it by identifying the optimal cost and least consumption using genetic algorithm (GA). Tan and Cruz (2004) applied stochastic optimisation based techniques to water network synthesis problems, while Tan *et al.* (2009) considered membrane separation-based water regenerators for total water

network synthesis. Prakotpol and Srinophakun (2004) developed a genetic algorithm (GA) with WPA-based program (GA Pinch) to solve the wastewater minimisation problem. Lavric *et al.* (2005) applied GA optimisation to water systems with multiple contaminants and several contaminated sources. They generate an overall optimal water network topology with respect to the minimum source water usage that considers all constraints. Moreover, Tudor and Lavric (2010) solved a detailed model of an integrated water/wastewater network (IWWN) using genetic algorithms to obtain the best topology. Moreover, Karuppiah and Grossmann (2006) proposed a piecewise-affine relaxation of non-convex terms in the solution of water network analysis, and Bagajewicz and Savelski (2001) proposed a planning model and method of obtaining a global optimum result with piecewise-affine relaxation enhanced with bound contraction and also considered pre-treatment for water network synthesis. Sujak *et al.* (2015) created a model for the design of optimal total water network (OTWN). Sharma and Rangaiah (2016) proposed designing, retrofitting, and revamping water networks in petroleum refineries using multi-objective optimisation. Boix *et al.* (2011) described the multi-objective optimisation of industrial water networks with multiple contaminants. Chaturvedi *et al.* (2016) demonstrate the analysis of effect of multiple water sources in a flexible-schedule batch water network.

However, despite all the above mentioned significant achievements in water network analysis research that utilizes optimisation-based modelling techniques and computational strategies, there are some challenges in the issues of non-convexity (which leads to the presence of multiple local optimal solutions), nonlinearity (which is due to considering multi-contaminant and regeneration technologies as nonlinear mixed with linear objective function),

simultaneous optimisation of the interactions of rigorous design models for wastewater treatment technologies and multiple water-using units, enabling faster numerical solutions, development of easy-to-understand optimisation-based formulations, uncertainty (posed by the data obtained from the industry), the parameters involved in the analysis of the problems, and obtaining the best result, alternative methods for optimisation under uncertainty such as hybrid stochastic optimisation and extension of the solution to resource recovery systems.

However, the use of stochastic mathematical optimisation algorithm improves the potential future directions in water application planning analysis and assists in the development of feasible, cleaner, and more economic industrial water networks (IWN) that drastically reduce freshwater consumption as well as wastewater, and ensure reasonable costs and efficient productivity (Prakotpol and Srinophakun; 2004). As such, the challenges and uncertainties highlighted above can be handled by using stochastic mathematical algorithm optimisation method known as genetic algorithm (GA), which is a robust stochastic optimisation method. The aim of this research is to determine the behaviour of GA with and without hybrid function in obtaining the solution to WAP

problems and determine the time taken by a standard desktop computer to execute the programme.

MATERIALS AND METHODS

The WAP Superstructure

The way to model an integrated water application planning (WAP) problem is based on the concept of superstructure (Yeomans and Grossmann, 1999; Savelski and Bagajewicz, 2000). Ramos et al. (2014) explained that from a given number of regeneration units and processes, all possible connections between them may exist, except recycling to the same unit. This constraint forbids self-recycles on process and regeneration units, although the latter is often relevant in some chemical processes. Considering each process within an industry to have a certain freshwater flow rate, output water from other processes or regenerated water, the output from the process will have effluent with a certain level of pollutants that can be discharged, recycled, or regenerated for reuse. The regeneration units can interchange the effluent for efficient treatment. This system can be represented as the superstructure of the company without a detailed explanation of the physical and chemical phenomena that occur in each process. The super structure is shown in Figure 1.

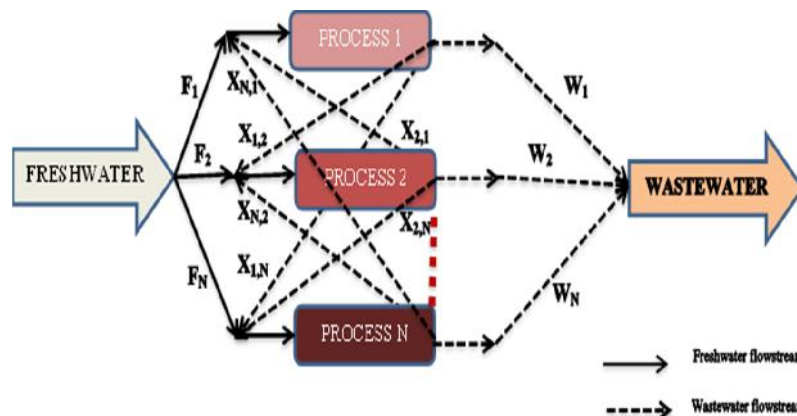


Figure 1: Superstructure for WAP problem



The values of superstructure variables for a given process condition are determined so as to minimise the total cost, subject to constraints derived from material balances and interrelationships among water-using units and wastewater-treating units. The optimisation problem was solved by using the Complex method, which was illustrated by its application to the WAP in a petroleum refinery. Mann and Liu (1999) introduced another superstructure method to formulate the water network as linear (LP) and nonlinear programming (NLP) for multiple contaminant systems. This superstructure model presents serious numerical difficulties in solving nonlinear programming (NLP) and non-convex mixed integer nonlinear programming (MINLP), owing to the non-guarantee of their optimum result. But the procedure can be used efficiently for single-component problems, and if the concentration of the contaminant is low. Examples from Wang and Smith (1995) and Olesen and Polley (1997) were used to substantiate the above claim. The details of the adopted procedure were from Savelski and Bagajewicz (2001).

However, it is quite often found that connections between certain processes are not allowed or must be imposed due to design or retrofit strategies. For example: heating and cooling limitations may render certain connections beneficial or undesirable, very low flow rate interconnections may also be discarded due to economic or controllability reasons. Finally, distance and space limitations may become decision variables as well. When imposing such restrictions on any of the previous cases, we can expect either feasible or infeasible solutions. Infeasibility may arise if no network can be found for the fresh water flow rate fixed at its minimum target.

Limits on the inlet and outlet concentrations of the pollutant are imposed a-priori on each process, and a fixed load of contaminants is used. These

inlet and outlet concentration limits account for corrosion, fouling, maximum solubility, etc.

The objective function for the sum of freshwater flow rates at the entrance of all the processes can be expressed as equation 1.

$$F = M \sum_{i=1}^n F_i \dots \dots \dots (1)$$

Where, F is the total freshwater flow rate, F_i is the freshwater flow for each process 'i' to 'n' (the number of processes).

The Linear Constraint functions are:

- i. The constraint of the water mass balance of all processes (equation 2):

$$F_i + \sum_{j \neq i} X_{i,j} - W_i - \sum_{j \neq i} X_{j,i} = 0 \dots \dots (2)$$

- ii. The constraint of the contaminant mass balance of all processes (equation 3) $\sum_{j \neq i} C_{j,o} X_{i,j} + \Delta M_i - C_{i,o} (W_i + \sum_{j \neq i} X_{j,i}) = 0 \dots (3)$

The nonlinear constraint function for the maximum contaminant inlet concentration is (equation 4):

$$\frac{C_{j,i}}{\sum_{j \neq i} C_{j,o} X_{i,j} + F_i} \leq C_{i,i}^m \dots \dots (4)$$

Where: $X_{i,j}$, is the wastewater flow from process 'i' to 'j'; $C_{i,o}$ and $C_{j,o}$ are the maximum outlet contaminant concentrations limits for the processes 'i' and 'j', and W_i is the wastewater flowrate out of the system.

The above systems of Equations 1 to 4 are derived based on the superstructure in Figure 1. They are simultaneously solved using mathematical programming by demanding the minimisation of equation 1 subject to constraints 2 to 4. The minimum freshwater use obtained can then be used to determine the total cost of obtaining freshwater by multiplying the value with the unit cost of freshwater.

Genetic Algorithm (GA)

The GA is an adaptive meta-heuristic search algorithm premised on the evolutionary ideas of natural

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selection and genetics. They represent an intelligent exploitation of a random search within a defined search space to provide solutions to a problem that consistently outperforms other methods (Srinivasa *et. al.* 2014). Davis (1991) has identified three main advantages of GAs in optimization: First, they generally find nearly global optima in complex spaces. Second, genetic algorithms do not require any form of smoothness, that is, they can handle nonlinearity and discontinuity. Third, considering their ability to find global optima, GA's are fast, especially when tuned to the domain on which they are operating. Advantageous features of GAs in solving large-scale, nonlinear optimization problems are that they can be used with continuous or discrete parameters require no simplifying assumptions about the problem, and they do not require the computation of derivative information during the optimization (Haupt and Haupt, 2004). Therefore, it is considered in this research to be the most appropriate method for the solution to WAP problem.

GA mimics the natural selection process that drives biological evolution in solving both constrained and unconstrained optimisation problems. The GA repeatedly modifies a population of individual solutions. At each step, it selects individuals randomly from the current population to be parents and uses them to produce the children for the next generation. Over successive generations, the population "evolves" toward an optimal solution. The GA can be applied to solve a variety of optimisation problems that are not well suited for standard optimisation algorithms, including problems in which the objective function is discontinuous, non-differentiable, stochastic, or highly nonlinear. It can address problems of mixed-integer programming, where some components are restricted to be integer-valued. It works with a coding of the parameter set, not the parameters themselves. It searches from a population

of points, not a single point. It uses objective function information, not derivatives or other auxiliary knowledge, and it uses probabilistic transition rules not deterministic rules. Therefore, it is considered the best option for optimisation of the WAP problem in this research.

The GA uses selection, crossover, and mutation rules at each step to create the next generation from the current population. Selection rules select the individuals called parents that contribute to the population at the next generation. Crossover rules combine two parents to form children for the next generation, and mutation rules apply random changes to individual parents to form children.

The GA differs from a classical, derivative-based, optimisation algorithm in that it generates a population of points at the end of each computational procedure, selects the next population by computation that uses random number generators, while the best point in the population approaches an optimal solution. This makes it a renowned technique for avoiding local optima in improving the search space of any mathematical problem.

Genetic Algorithm (GA) in MATLAB

MATLAB is a technical computing environment that provides a framework to develop tailored algorithms for advanced analyses and data visualisation. Its language provides interfaces to other programming languages, including FORTRAN and C, which enables the sharing of ideas and the development of solutions.

MATLAB gives immediate access to high-performance numerical computing with more than 600 mathematical, statistical, and engineering functions. This functionality is extended with add-on and signal processing toolboxes and interactive graphical capabilities for creating plots, images, surfaces, and volumetric representations.



MATLAB software (MATLAB R2016a) was used to implement the steps used in the solution of GA; as such, some adjustments were adopted to obtain the best result. The collections of routines, written mostly in m-files, which implement the most important functions in genetic algorithms, are used to solve the optimisation model in MATLAB. Tarek *et. al.* (2006) observed that incorporating a search method within a genetic algorithm can improve the search performance under the condition that their roles cooperate to achieve the optimisation goal. Therefore, to further improve the diversity and convergence of the solutions of the WAP obtained by MATLAB, a hybrid function was incorporated. The crossover and mutation operators combine to improve the search ability of the algorithm and produce the best solution, which further provides an optimum solution with a hybrid function.

Method for the Hybrid Approach

Incorporating a hybrid within a GA can improve search performance under the condition that their roles cooperate to achieve the optimisation goal (Tarek *et al.*, 2006). The gradient-based local deterministic optimisation function, known as the sequential quadratic programming (SQP) algorithm, was used as a hybrid function for single-objective WAP problem. In single-objective GA, the hybrid function starts at the best point returned by the GA.

The method combines the principles of GA and the SQP algorithm, which performs the computation of the Hessian of the objective function and its nonlinear constraints. The hybrid function prevents the GA from being stuck in the local minimum solution of the WAP problem.

The Hessian for an unconstrained problem is the matrix of the second derivatives of the objective function *f*, as shown in Equation 5.

$$H \quad H_i = \frac{d^2f}{d_i d_j} \dots\dots\dots (5)$$

The Hessian for a constrained problem is the Hessian of the Lagrangian. For an objective function *f*, non-linear inequality constraint vector *c*, and nonlinear equality constraint vector *C_{eq}*, the Lagrangian is given by Equation 6.

$$L = f + \sum_i \lambda_i c_i + \sum_j \lambda_j c_{e_j} \dots\dots\dots (6)$$

λ_i are Lagrange multipliers. The Hessian of the Lagrangian is shown in Equation 7.

$$H = \nabla^2 L = \nabla^2 f + \sum_i \lambda_i \nabla^2 c_i + \sum_j \lambda_j \nabla^2 c_{e_j} \dots\dots\dots (7)$$

MATLAB software provides SQP as “*fmincon*”, which minimise the constraint function based on a powerful concept in optimisation known as trust regions. “*fmincon*” uses a Hessian as an input function. The Hessian in this case is the matrix of the second derivatives of the nonlinear constraint functions of the WAP model.

Population Size Analysis of Single Contaminant Water Reuse without Regeneration for 2 to 10 Industrial Processes

The population size parameter of the genetic algorithm (GA) and the time taken by the single contaminant water reuse model that does not include regeneration was analysed for 2 to 10 industrial processes, using different examples from the literature. Increasing the population size enables the GA to search for more points and thereby obtain a better result. However, the larger the population size, the longer it takes GA to compute each generation. The number of variables for single contaminant water reuse without regeneration is equal to n^2+n , where *n* is the number of industrial processes involved in the analysis. To compare the

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time to achieve the optimum result for the solution of the WAP model using the GA with and without hybrid, different population sizes from 3 to 1000 were used.

Moreover, the intention is to experiment with different sets of population size to determine the value that returns optimal result without taking a prohibitive amount of time for the algorithm to execute.

The hybrid function “*fmincon*” was added to the GA analysis to improve its performance in obtaining the final result. The population size used was categorised into three groups. The first group is the range of 3 to 10, in steps of 1. The second group is the range of 10 to 100 in steps of 10, while the third group is 100 to 1000 in steps of 100. The three groups were used for the model containing 2 to 10 industrial processes. The maximum, minimum, and median time taken to run the model using GA without hybrid function for all the three population size groups were determined

(Table 1). The time-based performance measures of algorithms are not normally distributed; therefore, the median is used as a measure of central tendency.

The Pearson's correlation coefficient (Equation 8) was used to measure the linear correlation between the time taken with and without hybrid function y and x , respectively.

$$R_x = \frac{n \sum x_i y_i - \sum x_i \sum y_i}{\sqrt{n \sum x_i^2 - (\sum x_i)^2} \sqrt{n \sum y_i^2 - (\sum y_i)^2}} \dots \dots \dots (8)$$

Where: R_{xy} is the Pearson's correlation coefficient, n is the number of runs, x_i are the individual average time taken (without hybrid function) points indexed with i , and y_i are the individual average time taken (with hybrid function) points indexed with i .

Each set of the population size was used to run the model for 2 to 10 number of industrial processes. The analysis leads to getting an estimate of the running time as a function of the population size used in solving the GA, as shown in Table1.

Table 1: Categorisation of population size groups and the time of the model runs

Group	Population Range	Time of run for 2 to 10 number of industrial processes (s)		
		Minimum	Median	Maximum
First	3 to 10	3.0	5.7	10.1
Second	10 to 60	3.6	8.5	18.7
	70 to 100	7.2	15.9	25.3
Third	100	11.2	19.5	25.3
	200	53.2	70.0	90.1
	300	141.0	176.8	218.0
	400	354.1	369.8	548.0
	500	806.6	879.7	1151.3
	600	1570.7	1932.1	2286.5
	700	2871.2	3175.8	3534.9
	800	6468.2	6805.2	7292.3
	900	10632.0	11236.1	11719.8
1000	16141.2	16180.7	16978.3	

RESULTS AND DISCUSSION

For the first group considered (in Table 1) 3 to 10 population size, the time taken to run the model without hybrid function is similar to that with the hybrid

function incorporated in the GA for analysis. The second group for 10 to 100 population sizes, the time is different by 2s, when the hybrid function is included in the running of the GA for all the

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industrial processes. However, for the third group of 100 to 1000 population sizes, each population category exhibited a different time range with clear differences. The population size of 100 has a median of 19.6s with a hybrid function. The population sizes of 200, 300, 400, and 500 have a median of 63.6, 190.0, 399.8, and 908.7s with a hybrid function, respectively.

The median time taken for the population size range of 3 to 100 with and without hybrid function included in running the GA for the solution of 2 to 10

industrial processes WAP problem are shown in Figures 2 and 3, respectively. The trend lines of the two graphs indicate a similar exponential relationship, as shown in Equations 9 and 10.

$$Y = 0.08x^2 - 0.6x + 6.4 \dots \dots (9)$$

$$Y = 0.085x^2 - 0.7x + 6.6 \dots \dots (10)$$

The Pearson's correlation coefficient of the two variations of time, with and without hybrid function is 0.95. This indicates a strong correlation between the two data.

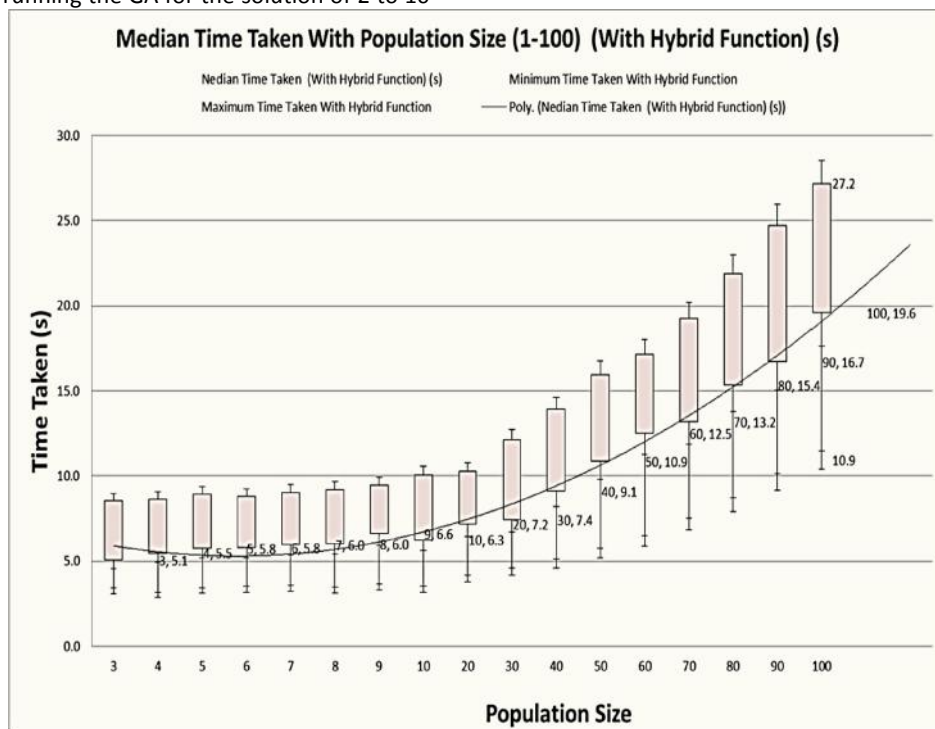


Figure 2: Median time for Population 3-100 without hybrid function included in running the GA for the solution of 2 to 10 industrial processes WAP problem.

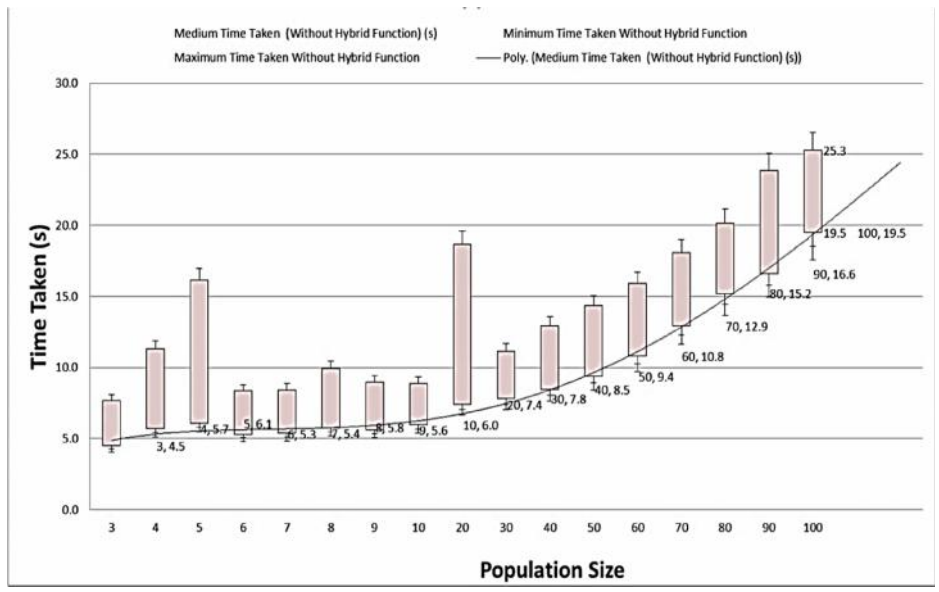


Figure 3: Median Time for Population 3 to 100 with hybrid function included in running the GA for the solution of 2 to 10 industrial processes WAP problem.

Figure 4 shows the percentage of the optimum result obtained for the solution of 2 to 10 industrial processes WAP problem using the population size of 3 to 1000 with and without hybrid function included in running the GA.

Observation of the objective function results for the different industrial processes from 2 to 10 obtained indicates that a population size of 10 gives the highest percentage of the optimum result, which is 90%.

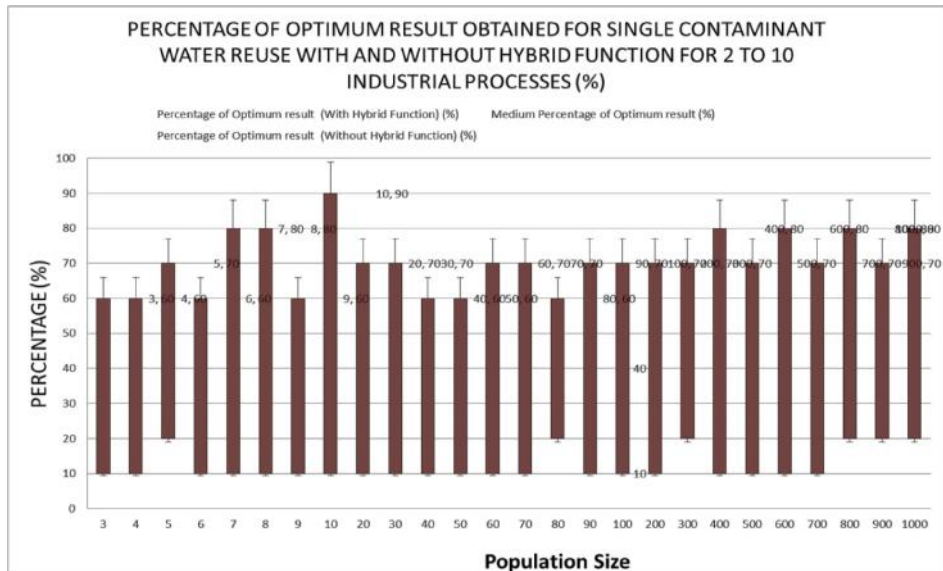


Figure 4: Percentage of the optimum result obtained for the solution of 2 to 10 industrial processes WAP problem using the population size of 3-1000 with and without hybrid function included in running the GA.

However, running the GA with and without hybrid function takes almost the same time, but analysis of the population size of 3 to 1000 indicates a median difference of 50% in the number of times GA with hybrid gives the optimum result.

Running the model for two industrial processes indicates that, once the population size is more than the number of variables, which in this case is 6, the GA with hybrid achieved the optimum result. However, the model gets stuck in the local optimum for up to a population size of 40 without a hybrid function.

Running the model for 3, 5, 6, and 7 industrial processes indicates that the GA with hybrid achieved optimum results for almost all population sizes, but gets stuck in the local optimum for all the population sizes without hybrid function.

Running the model for 4 industrial processes indicates that, once the population size is more than 3, the GA with hybrid achieved optimum results for the population size range from 4 to 20 and 200 to 1000, but gets stuck in the local optimum for the remaining population sizes and for all without hybrid function. This indicates that a population size of less than 3 cannot be used in the solution of the WAP problem.

Running the model for eight industrial processes indicates that only the population sizes of 4, 5, 6, 10, 50, 60, 100, 600, and 800 for the GA with hybrid achieved optimum results, but get stuck in the local optimum for all the population sizes of GA without hybrid function.

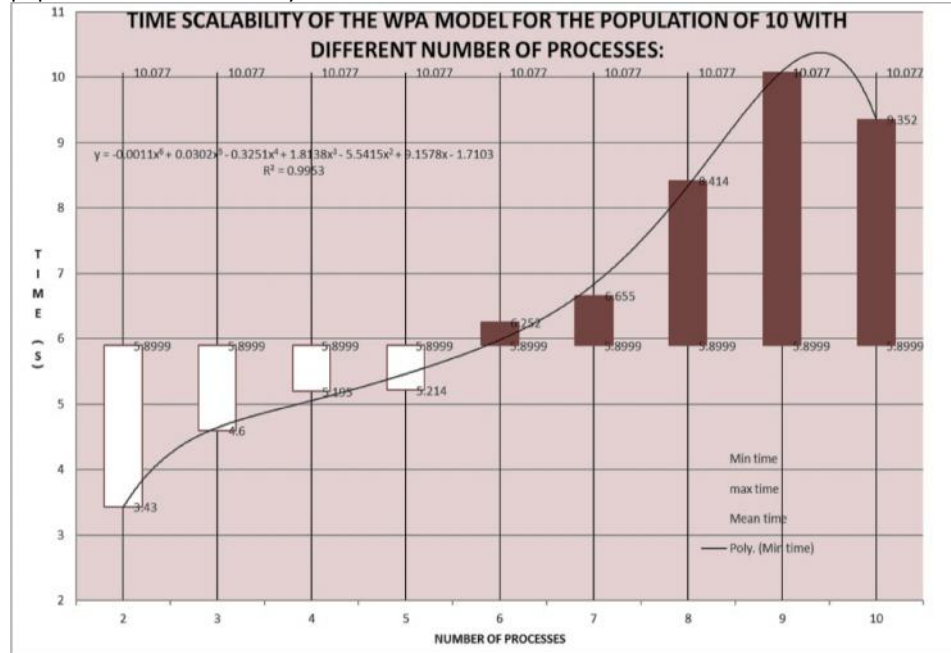


Figure 5: Time Scalability of the GA for the solution of 2 to 10 industrial processes WAP problem for population size of 10.

Running the model for nine industrial processes indicates that only a population size of 10 for the GA with hybrid achieved the optimum result, and the population sizes of 5 and 80 of GA

without hybrid function, but gets stuck in the local optimum for all the remaining population sizes of GA with and without hybrid function. Running the model for ten industrial processes indicates that



there is no difference in the results obtained with or without hybrid.

The time scalability of the GA for the solution of 2 -10 industrial processes WAP problem for a population size of 10 is shown in Figure 5. The population size of 10 produces algorithm results of the WAP problem in a short time of 3.4 to 10.1 seconds for the 2 to 10 industrial processes and 90% of the trial time, the optimum result is achieved.

CONCLUSION

The modelling approach of WAP problems using superstructure was presented, and the analysis of the model was carried out using the GA method to solve the different WAP problems. In order to improve the performance of GA in obtaining the final result, a hybrid function was incorporated within it. The behaviour of GA with and without hybrid function and the computer time for obtaining the WAP solution for different population sizes were compared. The hybrid used for single-objective GA optimisation is 'fmincon'. The population sizes were varied from 3 to 1000 for the single contaminant water reuse model that does not include regeneration for 2 to 10 industrial processes, using different examples from the literature. For the first population size group of 3 to 10, the median time taken for the solution of the model is 6s for the 2 to 10 industrial processes. For the second group of 10 to 100, the solution is obtained within an average time of 10s for a population size of 10 to 60, and it runs for an average time of 15s for a population size of 70 to 100. For the third group of 100 to 1000, each population category exhibited a different time range with clear differences.

Observation of the fitness function results for different industrial processes from 2 to 10 obtained with and without hybrid function indicates that the population size of 10 gives the highest percentage of the optimum result, which is 90%.

The analysis shows the increase in efficiency of the GA and the statistics of the computer time for different numbers of industrial processes using the data obtained from previous WAP studies.

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