

Received: 15 March, 2021

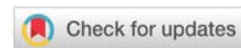
Accepted: 06 April, 2021

Published: 07 April, 2021

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**Keywords:** Chlorine contact plug flow reactor; Genetic algorithm; Nonlinear condition; Simulated annealing algorithm; Pattern search algorithm and microbial load

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## Research Article

# Presenting a novel approach for designing chlorine contact reactors by combination of genetic algorithm with nonlinear condition functions, simulated annealing algorithm, pattern search algorithm and experimental efforts

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## Abstract

Nowadays, water supplies face critical conditions in terms of quality and quantity. Furthermore, growth in population along with their needs require an increasing level of water-related resources. Consequently, the potential application of purified wastewater supplies can be considered in agriculture, industry, and irrigation of green spaces. Hence the necessity of disinfection and reduction of microbial load in the outlet sewage of water treatment plants are so clear for all designers and operators. Chlorine contact reactors are one of the major pillars of any wastewater treatment plant, whether urban or industrial. A new method is presented in this study based on the optimization of the dispersion amount in a Chlorine Contact Plug Flow Reactor (CCPFR) using single-objective Genetic Algorithm (GA) and nonlinear condition functions, Simulated Annealing Algorithm (SAA) and Pattern Search Algorithm (PSA). Then, it is attempted to assess the hydraulic behavior of the reactor and the microbial load removal performance using statistical, probabilistic and experimental practices. This research was done in a case study of Mashhad city's wastewater treatment plant. The results of presented study illustrate that GA model has the best outcomes for designing CCPFR and the desired reactor with a depth of 2.45m, width of 1.23m, length of 24.8m, a number of 15 channels, and a retention time of 87 minutes is able to reduce a population of 300000 microorganisms (MPN/100 ml) at the entry to 274 (MPN/100 ml) at the exit. As per this method, investment cost of CCPFR is reduced around 30 percentages in comparison of traditional computation system.

## Introduction

Since the beginning of the 1900s until the early 1970s, wastewater treatment was majorly carried out with the purpose

of separating colloidal particles and suspended floating matter, purifying biological decomposable material, and removing pathogenic microorganisms [1]. Following the approval of Federal Water Pollution Control Act of 1972 in the US, a set

of general changes were introduced in wastewater treatment processes. When the act was passed, the US Environmental Protection Agency (EPA) necessitated the application of advanced secondary treatment with the purpose of adjusting pH parameters, the extent of Biological Oxygen Demand (BOD), total suspended solids, and fecal coliforms for wastewater treatment plants in 1973 [2]. The agency also enabled different states to edit and compile their own criteria including disinfection indices for wastewater treatment plans [1-4]. As a result, certain states in the US nowadays use standard ranges of 5000-2.2 (MPN (Most Probable Number)/ 100ml) and 10000-2.2 (MPN/ 100ml) for fecal and total coliforms, respectively. The most common standard for receiving water is up to 300 (MPN/ 100ml) for fecal coliforms [2-6]. Currently, the most common method in Iran involves using chlorine for disinfection due to its low cost and relatively suitable microbe removal power and survival rate. During the disinfection process, there are five general mechanisms that disable microorganisms and damage their cellular structure; these mechanisms include damaging cell walls, changing cell permeability, changing the colloidal properties of protoplasm, changing DNA or RNA, and preventing enzyme activities [7]. Oxidizing chemicals such as chlorine prevents enzyme activities in microorganisms. In other words, oxidizing substances destroy the geometrical structure of enzymes to prevent microorganisms from using food materials (substrates) through enzymes [8]. A key unit in designing wastewater treatment plants is chlorine contact tanks as a microbial control system. The purpose of designing this reactor is to offer sufficient contact time between chlorine and sewage mass in order to destroy microorganism structures. Subsequently, this Plug Flow Reactor (PFR) requires particularly detailed design and systematic calculations [9]. PFR systems are commonly used for chlorine contact tanks in order to provide longitudinal mixing and sufficient retention time for contact between chlorine and the fluid. In this system, the injected chlorine is dispersed across the sewage flow through three mechanisms including diffusion mass transfer, advection, and dispersion [10-14].

As per reviewed researches, designing and computing the optimum Chlorine Contact Plug Flow Reactor (CCPFR) is considered serious problem in planning the wastewater treatment plants. While, the classical systems cannot cover optimum conditions and application of evolutionary algorithms can be useful for satisfying economical purposes. This research gap can be fill by presenting a novel method for computing the dimensional aspects and microbial performance evaluation of CCPFR.

In this study, it is attempted to (i) present a method for designing a chlorine contact reactor using single-objective Genetic Algorithm (GA) and nonlinear condition function, Simulated Annealing Algorithm (SAA) and Pattern Search Algorithm (PSA), (ii) assess the behavior of the designed reactor using probability distribution functions and microbial load elimination and (iii) economic appraisal of GA, SAA and PSA algorithms performance for designing CCPFR.

## Materials and Methods

### Calculation relations for reactor design

First, the capacity of pump dosing systems should be indicated. To this end, the values recommended by the literature are used. Calculations related to this section are presented in Equation 1 [15-18].

$$Cl_{2-\max} \left( \frac{kg}{day} \right) = [\max \text{ injection dose}]' k_{\max}' Q_{ave}$$

$$Cl_{2-\text{ave}} \left( \frac{kg}{day} \right) = [\text{ave injection dose}]' Q_{ave} \quad (1)$$

Next, the design process takes place according to the flow dispersion model. The design stages in this part are presented in Equation 2. The ultimate purpose of this section is to indicate the extent of dispersion to assess the reactor's functional system [19-21].

$$\text{depth} = x_1, \text{width} = x_2, \text{number of channel} = x_3, \text{HRT} = t$$

$$L(m) = \frac{k_{\max} \times Q_{ave}}{\text{number of channel}} \times \text{HRT} \times \frac{1}{\text{width} \times \text{depth}}$$

$$\text{Velocity} \left( \frac{m}{s} \right) = \frac{k_{\max} \times Q_{ave}}{\text{width} \times \text{depth}}$$

$$\text{reynolds number} = \frac{4 \times \text{velocity} \times R}{\nu}, \nu = 1.003 \times 10^{-6} \frac{m^2}{s}, R = \frac{\text{width} \times \text{depth}}{2 \times (\text{width} + \text{depth})}$$

$$\text{Dispersion Coefficient} = 0.01 \times \nu \times (\text{reynolds number})^{0.875}$$

$$\text{dispersion} = \frac{D}{uL} = \frac{Dt}{L^2} \quad (2)$$

### Application of genetic algorithm in reactor design

In this section, parameters including depth ( $X_1$ ), width ( $X_2$ ) and number ( $X_3$ ) of channels were defined as the variables for the optimization equation. However, the extent of standard dispersion according to design standards in CCPFR should be within a range of 0-0.015. Consequently, the optimization error function can be expressed based on the sum of squared errors as shown in Equation 3. Likewise, the specification of GA, PSA and SAA are depicted in Equation 4 until 6, correspondingly.

$$\text{Cost Function} = \min \left( \frac{0.01 \cdot n \cdot \left( \frac{2Q_{ave} k_{\max}}{(x_1 + x_2)} \right)^{0.875} \cdot t}{\left( \frac{Q_{ave} k_{\max} t}{x_1 x_2 x_3} \right)} - 0.015 \right)^2 \quad (3)$$

Mutation Rate = 0.01

Cross Over Probability = 0.8

Initial Population = 50

Number of Iteration = 50 (4)

Temperature Update Function © Exponential temperature function

Reannealing Interval = 100

Initial Temperature = 120

Number of Iteration = 50

(5)

Poll Method ® GPS Positive basis N2

Expansion Factor = 4

Mesh Initial Size = 3

Contraction Factor = 0.5

Mesh Tolerance = 1e-6 (6)

Next, the length of the reactor is defined as a nonlinear condition function of the three aforementioned variables (For GA and PSA), demonstrated in Equation 7. As per main design references [1], the suggested value of reactor's length ( $L_{empirical}$ )

should be more than  $L_{theory} (\frac{Q_{ave} k_{max} t}{x_1 x_2 x_3})$ . In the all equations,  $Q_{ave}$ ,

$k_{max}$  and  $t$  are equal to mean flow of wastewater, maximum coefficient of wastewater regime and hydraulic retention time in each design, respectively.

$$(\frac{Q_{ave} k_{max} t}{x_1 x_2 x_3}) - L_{empirical} \leq 0 \tag{7}$$

In this study, the entire calculations were carried out using MATLAB® 2013b software and Optim Tool [22]. Furthermore, given the experiences gained from previous design attempts, minimum and maximum limits should be considered for  $X_1$ ,  $X_2$ ,  $X_3$ , and  $E_{empirical}$  variables. According to the literature, the hydraulic retention time (HRT= $t$ ) was selected in a range of 90-120 minutes at the beginning of the design process [23]; then, the accuracy of the choice is controlled using statistical functions and hydraulic examinations. Subsequently, the hydraulic retention time at the beginning of the design is considered as 120 minutes.

### Examining the hydraulic behavior of the reactor

The designed tank should then be assessed in terms of hydraulics and performance conditions of the reactor. Prior to the examining this factor, it should be pointed out that a performance similar to that of CCPFR could be created by serializing a large number of CMR reactors. Péclet number was used to provide equivalence among reactors (Equation 8) [24]. Likewise, probability of passed flow in channel is computed by Equation 9.

$$\text{number of CMR} = \frac{P_e}{2} = \frac{1}{2d} \tag{8}$$

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$$E(q) = \frac{n}{(n-1)!} (nq)^{n-1} e^{-nq}$$

$\theta$  = Time(fractional),  $n$  = Number of seri reactor  
 $E(\theta)$  = Passage distribution of flow  
 $F$  = Percentage of passed flow =  $\int_0^{\theta} E(\theta)$  (9)

### Experimental efforts

For evaluation of each designed system based on GA, PSA and SAA, some experiments for assessment of microbial load elimination are done in the Lab. In each run, Total Coliform removal is appraised and all experiments are performed as per standard method for the examination of water and wastewater [25]. The algorithm of experimental efforts is illustrated in Figure 1. Whereas, outcomes of each algorithm are assessed in adjustable water channel in the hydraulic (For implementation of patterns) and microbial (For microbial load elimination) Labs. The scheme of adjustable water channel and real picture of channel are demonstrated in Figures 2,3, respectively. Likewise, all hydraulic and microbial experiments are done in Ferdowsi university of Mashhad, Iran and Reyhan Azma, Mashhad, Iran, correspondingly. Hydraulic experiments are completed based on each algorithm (GA, SAA, PSA, classical model) with three repetitions (All hydraulic efforts were equal to twelve tests). Also, for evaluation of microbial load elimination, all microbial culturing has done in three repetitions in each run. In this investigation, all materials such as chlorine (Sodium Hypochlorite) and cultural environment (Mc Cankey agar) are

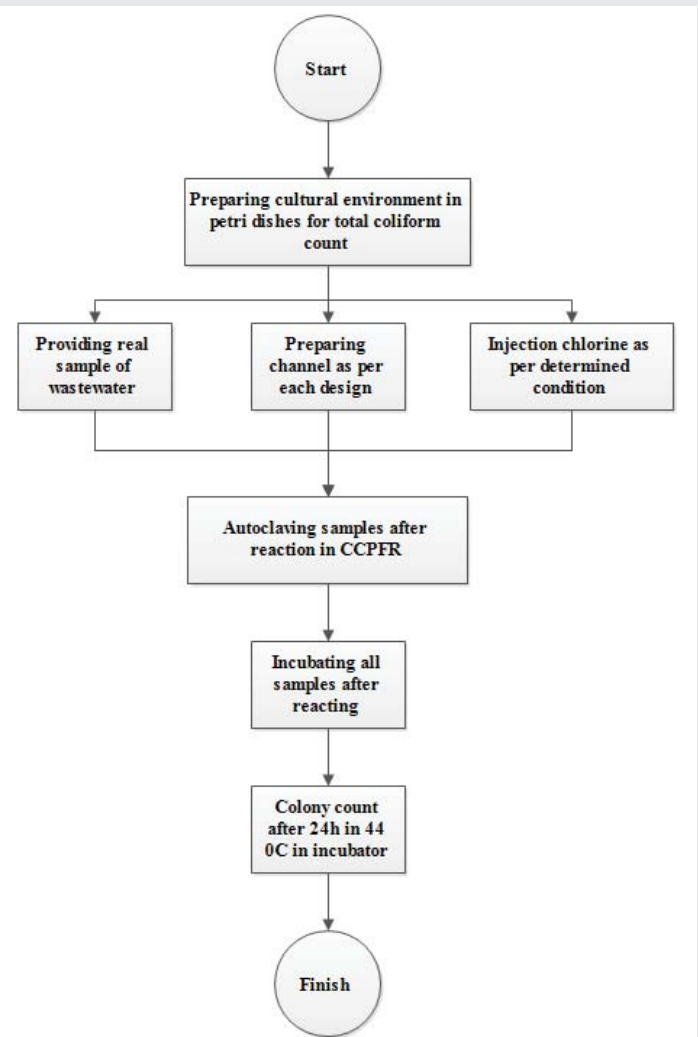


Figure 1: Executive plan of microbial tests in present research.

purchased from Merck, Germany. All microbial experiments are calculated with  $\pm 0.25$  S.D.

## Results and Discussions

To carry out analyses beyond the presented scenario, an average discharge of 3000 m<sup>3</sup>/day and maximum coefficient of 2.75 were considered as per real condition of Mashhad city wastewater treatment plant. Accordingly, GA, PSA and SSA were performed using predetermined limits shown in Figure 4 until Figure 6, correspondingly. The outcomes of designed CCPFR by each algorithm and classical computation is summarized in Table 1. As per Figures 4-6, SSA is tended to optimum conditions faster than other algorithms (around 10 iteration). While GA and PSA tend to optimum situation around 20 and 40 iterations, but, it is not powerful reason for determination of performance of design for each computational method.

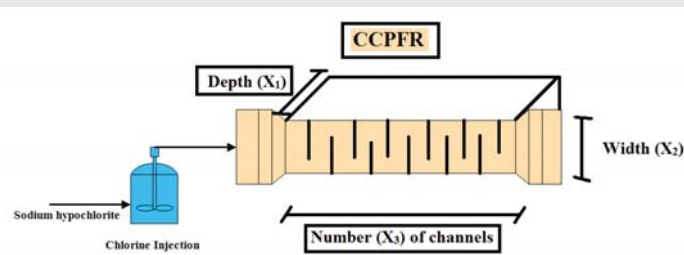


Figure 2: Scheme of hydraulic and microbial experiments in present research.



Figure 3: Real picture of Lab in present research.

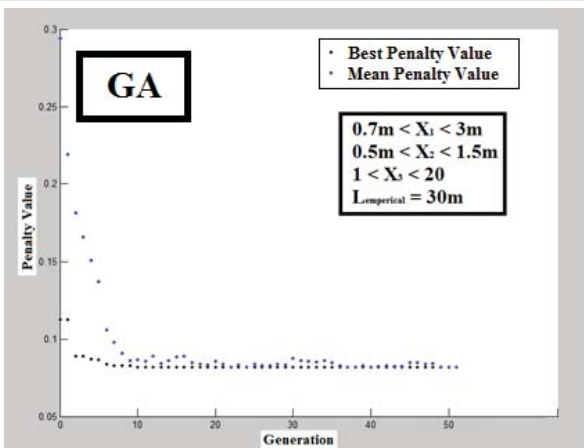


Figure 4: Optimal convergence of target function values in various generations of the GA.

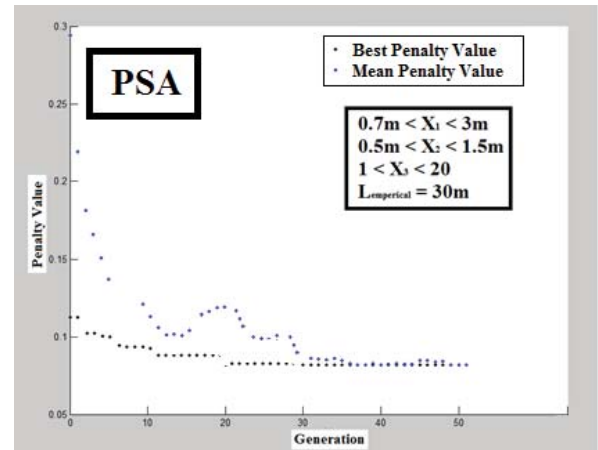


Figure 5: Optimal convergence of target function values in various generations of the PSA.

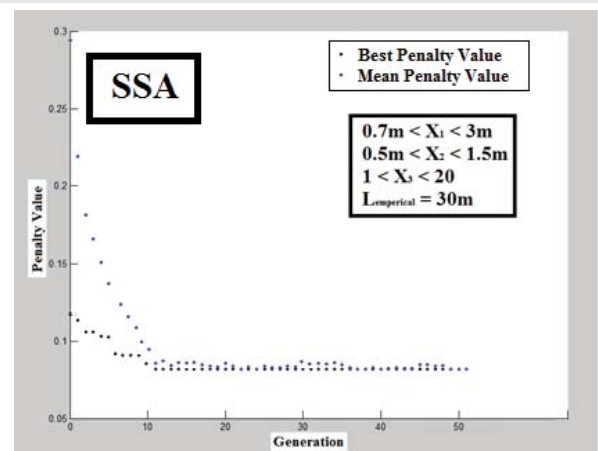


Figure 6: Optimal convergence of target function values in various generations of the SSA.

Table 1: The results of designed CCPFR by GA, PSA, SAA and classical computations.

Computations method	Depth (m)	Width (m)	Number of channels
GA	2.45	1.23	15
PSA	3.5	1.45	19
SAA	3	2.1	16
Classical method	4.5	2.5	25

Based on outcomes of Table 1, the cost of each mathematical model for designing CCPFR is illustrated in Figure 7. According to Figure 7, GA, PSA and SSA can reduce the CCPFR investment cost equal to 30%, 15% and 22% respectively, in comparison of classical computation. It is worth noting that all economic computations are computed based on material and construction usages as per Iranian markets in 2021.

Calculations regarding the hydraulic behavior of chlorine contact reactor were carried out flow passing in each design. The extent of changes in probability function of E (Teta) which is based on the probability of a certain percentage of flow passing through the reactor for GA, PSA and SAA are demonstrated in Figure 8. In the following, values of cumulative passage percentage of the flow (F) from the reactor as per GA, PSA and SAA are expressed in Figure 9. Based on Figures 8,9

for scrutinizing the performance of flow passing, it is clear that GA is tend to maximum efficiency in the minimum time in comparison of other methods.

In the final part of designing the disinfection system using chlorine, the extent of residual microorganisms were assessed using the Segregated Flow Model (SFM) method and experimental efforts [26-28]. Plus, for evaluation of microbial load elimination, all measurements and residual microbial load detections were done in the last point of channel. The outputs of analyses as per GA, PSA, SAA and classical computations for CCPFR design are demonstrated in Figure 10. According to Figure 10, in 87 min after reaction time passing, all

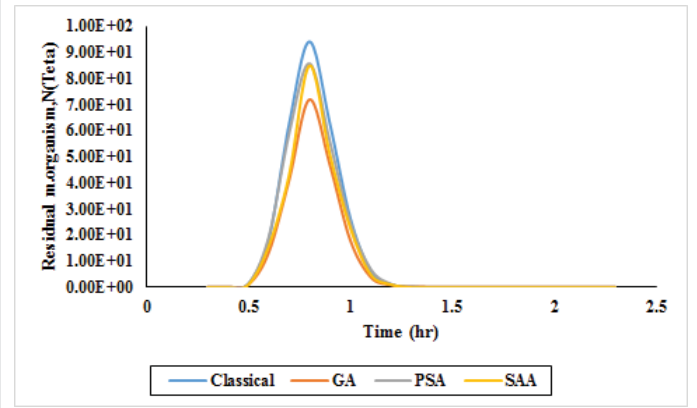


Figure 10: The extent of residual microorganisms in CCPFR for GA, PSA, SAA and classical computations.

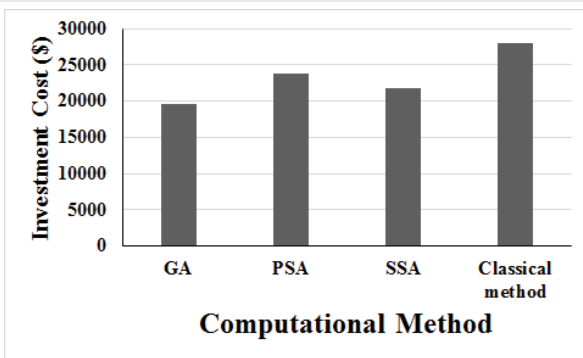


Figure 7: Economical evaluation of GA, PSA, SAA and classical method for designing CCPFR.

computation outcomes present the best performance, but, GA have shown minimum residual total coliform in the mentioned time. Therefore, GA has the best performance for designing CCPFR in comparison of PSA, SSA and classical calculations.

The results of calculations illustrate that the number of residual microorganisms during hydraulic retention time for GA (in high level of performance) was 274 (with initial number of 300000) per 100 ml of MPN, which is acceptable given common standard values as per Environmental Protection Agency standards [29]. Rauen, et al. (2012) have presented a novel method for designing CCPFR based on Computational Fluid Dynamics (CFD). The results showed that CFD can be useful for simulating E(Teta) and F values with high accuracy [30]. Also, Hart and Vogiatzis (1982) have expressed modified CCPFR with cross-baffles for enhancing the performance of microbial load elimination. The declared investigation illustrated that with application of baffles, urban standards can be satisfied [31].

### Conclusion

Considering the second use of purified wastewater supplies for applications such as agriculture, industry, and irrigation, the disinfection of outlet sewage from wastewater treatment plants has been necessitated. A number of various calculation methods are used for hydraulic design and dimensions of CCPFR at wastewater treatment plants. The present study offers a new method for designing CCPFR using GA, PSA, SAA and classical computations. Then, the hydraulic and functional behavior of the designed reactor was assessed and examined using the statistical reactor assessments and experimental efforts. The results showed that GA can optimize the investment cost of CCPFR equal to 30% and it was the minimum value between all computation systems. The GA based reactor in question with a depth of 2.45m, width of 1.23m, and length of 24.8m with 15 channels and hydraulic retention time of 87 minutes is capable of reducing microorganism population from 300000 (MPN/ 100ml) at the entry to 274 (MPN/ 100ml) at the outlet. The mentioned outcomes were acceptable from point view of EPA standards. The outcomes have shown that all GA, SAA and PSA are acceptable based on EPA standard, but GA results can present the most optimum condition in comparison of other ones.

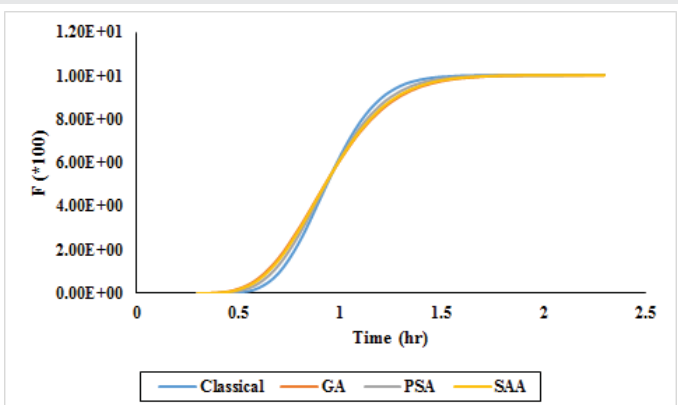


Figure 8: Probable distribution of passed flow (E(Teta)) in CCPFR in percentage for GA, PSA, SAA and classical computations.

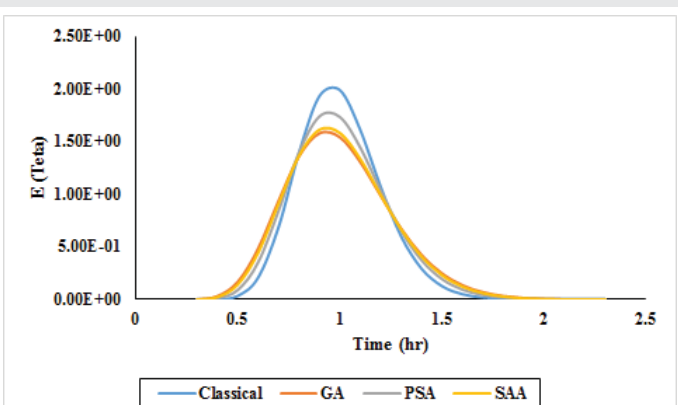


Figure 9: Cumulative percentage of passed flow (F) in CCPFR for GA, PSA, SAA and classical computations.

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