Genetic Algorithm Implementation in Maximum Entropy Principal Method to Predict Spray Characteristics

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Abstract: Solving of nonlinear equations is a prominent problem in science. In this study, the genetic algorithm as a general tool for solving optimum problems is used to determine velocity and droplet size distribution. Prediction of velocity and droplet size is done based on Maximum entropy principle. There are various theories on solving of nonlinear equations by use of genetic algorithm. Therefore, by coupling of one of these theories with Maximum entropy principle equations, the velocity and droplet size distribution will be calculated. Results show that the new method is indeed very effective.

1. Introduction

Genetic algorithm (GA) is a searching and heuristic technique for optimization of linear and nonlinear problems. GA introducing concepts such as inheritance and mutations in natural sciences uses the evolutionary algorithms to solve intricate problems. GA was innovated by John Holland and later, this method achieved actual position with Goldenberg’s attempt [1]. More recently, however, genetic algorithms have been employed to an increasing number of engineering problems in the areas of heat transfer and fluid mechanics. They also have been applied to basic heat transfer problems, Davalos and Rubinsky [2, 3, 4, 5, 6, 7], multiphase flow functions estimation, Akin and Demiral [8].

The main purpose of GA is to preserve the desired results closer to exact solution and discard the poor results. In this work, we applied GA to solve highly nonlinear transcendental equation introduced in maximum entropy principle method. The MEP method emerged in the late 80’s. The MEP method is defined based on probability distribution function for size as well as velocity of droplets in a spray. In this method, the droplet size and velocity distribution function is predicted using conservation equations coupled by maximum entropy principle. To eliminate the need for experimental data in MEP method, the source terms are calculated by analytical theories like instability of liquid sheet.

In pre-works, the traditional Newton-Raphson method was applied to solve highly nonlinear MEP equations.

As the Newton-Raphson has a local search method to find the solution, it is sensitive to initial guess and the Newton-Raphson solution cannot accurately converge as GA solution can in MEP.

2. Genetic Algorithm (GA)

The basic concepts of Genetic Algorithm method are introduced for solving numerical problems [9]. For this aim, it is necessary to introduce some definitions [10].

Gene: The basic unit capable of transmitting characteristics from one generation to the next such as droplet size as a variable in a specific node.

Chromosome: The structure carrying genes determines the characteristics of organism. This structure inherits the intrinsic property from its parents. Population: A group of chromosomes.

Parents: The candidates to generate next generation. Usually in GA, the primary population of chromosomes is introduced as candidates for optimization and the progress proceeds toward the final solution by introducing some abstract concepts.

Crossover is the most fundamental operator to generate new generation. Crossover selects genes from parent heat transfer problems, Davalos and Rubinsky [2, 3, 4, 5, 6, 7], multiphase flow functions estimation, Akin and Demiral [8]. The main purpose of GA is to preserve the desired results closer to exact solution and discard the poor results. In this work, we applied GA to solve highly nonlinear transcendental equation introduced in maximum entropy principle method. The MEP method emerged in the late 80’s. The MEP method is defined based on probability distribution function for size as well as velocity of droplets in a spray. In this method, the droplet size and velocity distribution function is predicted using conservation equations coupled by maximum entropy principle. To eliminate the need for experimental data in MEP method, the source terms are calculated by analytical theories like instability of liquid sheet.

In this work, two-point crossover operator is used in order to prevent unreasonable children. Parents’ chromosomes break from two points, and offspring chromosome is generated from the crossover of the first part of parents as seen in Fig. (1). Mutation is another important GA operator altering one part of chromosome randomly. After crossover is performed, mutation takes place. The main purpose of mutation is to prevent positioning all solutions into a local optimum of solved problem. Mutation
Algorithm is started with a set of solutions (represented by chromosomes) called population. We are motivated by a hope the new population will be better than the old one. Solutions selected to form new solutions (offspring) are evaluated according to their fitness: the more qualified they are, the more chances to reproduce. In other words, the weaker chromosomes are doomed to be annihilated. The motor of GA makes a primary population by a procedure. Anybody will be tested based on a set of data and the most deserving of them (perhaps 10 percent of the best) remain and the other data discarded. A probability number of connection is usually introduced in genetic algorithm. This number is bounded between 0.6 and 1 defining the probability of child creation. The deserved parents mate together and exchange their DNA elements and fertilized chromosomes are randomly promoted by mutation. Generally, the GA tends continuously to reproduce the fittest generations based on cost function. These processes continue until we achieve the most valuable member of population.

3. Maximum entropy principle (MEP)

Generally, the prediction of velocity and droplet size distribution on spray process is a complex process. This mechanism depends on many variables and it is based on a sophisticated structure. In the first phase of atomization process entitled primary breakup, the process is modeled by hydrodynamic instability theory and known as a deterministic process. While the second phase of atomization process called secondary breakup is a stochastic and randomly process.

The governing equations of breakup in the first stage of secondary atomization include mass, momentum, and energy conservation equations known as MEP equations. The result of MEP equations solution is velocity and droplet size distribution not unique and may be non-physical. To close the set of MEP equations, a neglected physical constraint should be introduced. The maximum entropy is a fundamental law governing in the nature and the solution of every physical problem should be satisfied implicitly or explicitly this universal law.

The MEP method to predict size and velocity distribution of droplets was first developed by Sellens and Brzustowski in 1986 Takin and Li made the MEP method more detailed by considering the conservation equations and the effect of surface tension, [11, 12]. Dumouchel continued to improve his pioneers rout to predict the spray characteristics, [13, 14]. Recently, Movahednejad using the theory of liquid sheet stability modified the MEP equations and introduced a new source term of momentum equations in MEP [15, 16].

Shannon stated the form of entropy based on information theory as [11,12,16].

\[
S = -\kappa \sum f \ln(f) 
\]

Where \( s \) is the statement of statistical thermodynamic entropy, \( \kappa \) is the Boltzmann's constant and \( f \) is the probability density function of the event. Besides maximizing of thermodynamic entropy, the conservation equations including mass, momentum, and energy should be satisfied in sheet or jet breakup. Consider spherical droplets, the conservation equations including continuity, momentum, and energy are introduced based on probability density function as bellows.
\[
\int_{D_{\text{min}}}^{D_{\text{max}}} \int_{u_{\text{min}}}^{u_{\text{max}}} f D^3 dD du = 1 + \bar{s}_n
\]  
\[\text{Eq.(2)}\]

\[
\int_{D_{\text{min}}}^{D_{\text{max}}} \int_{u_{\text{min}}}^{u_{\text{max}}} f D u D^2 dD du = 1 + \bar{s}_nu
\]  
\[\text{Eq.(3)}\]

\[
\int_{D_{\text{min}}}^{D_{\text{max}}} \int_{u_{\text{min}}}^{u_{\text{max}}} f \left( D^3 u^2 + \frac{B D^2}{H} \right) dD du = 1 + \bar{s}_e
\]  
\[\text{Eq.(4)}\]

Where \( H \) is the shape of the velocity distribution, equal unity for uniform velocities and \( B \) is defined as,
\[
B = \frac{12}{W_e}
\]  
\[\text{Eq.(5)}\]

Weber is defined as Weber number. According to the PFD definition, the following equation is also satisfied
\[
\int_{D_{\text{min}}}^{D_{\text{max}}} \int_{u_{\text{min}}}^{u_{\text{max}}} f D^3 dD du = 1
\]  
\[\text{Eq.(6)}\]

It is worthy to note that Eqs. (2-4) and (6) are non-dimensionalized by \( D_{\text{min}} \) and \( U_f \) known as mean diameter and the potential velocity of liquid sheet, respectively.

Based on Lagrange multipliers method, maximizing Shanon entropy in Eq. (1) coupled by conservation laws in Eqs. (2-4) and (6) conducts to the following pdf function
\[
f = f_0 \exp \left[ -\frac{1}{\lambda} - \frac{1}{\tilde{\lambda}} \frac{\tilde{D}}{D} - \frac{1}{\lambda} \frac{\tilde{D}}{D} + \frac{1}{\lambda} \frac{\tilde{D}}{D} + \frac{B}{H} \right]
\]  
\[\text{Eq.(7)}\]

Since the initial formation of the liquid sheet is dictated by linear instability somewhere near the breakup zone, the primary function of \( f_0 \) can be expressed as
\[
f_0 = \begin{cases} 
\frac{m \tilde{D}}{\lambda} & \tilde{D} < \tilde{D}_c \\
\frac{1}{\lambda} (\tilde{D}) & \tilde{D} > \tilde{D}_c 
\end{cases}
\]  
\[\text{Eq.(8)}\]

As it can be seen from the equations, the solution domains are changed from \( D_{\text{min}} \) to \( D_{\text{max}} \) and from \( u_{\text{min}} \) to \( u_{\text{max}} \). The variations of \( D \) and \( u \) in the domain are independent. In addition, the solution of probability function in other points, other than \( D_{\text{min}} \) to \( D_{\text{max}} \) and from \( u_{\text{min}} \) to \( u_{\text{max}} \), is equal to zero. Therefore, it can to use boundary of probability function from 0 to \( \infty \). In addition, the parameter that be seen in the primary function is \( \omega \) or temporal growth rate. this parameter can be calculated from instability theory [15,16].

Neglecting mass transfer between droplets and gaseous medium, mass source term is considered to zero in Eqs. (2). As well, momentum and energy source terms are calculated by following equations.
\[
\bar{S}_m = \frac{1}{2} C_f \rho (U-1)^2 L_b
\]  
\[\text{Eq.(9)}\]

\[
\bar{S}_e = C_f \rho (U-1)^3 L_b
\]  
\[\text{Eq.(10)}\]

Where \( C_f \) is the drag coefficient of planar sheet defined as bellow.
\[
C_f = \begin{cases} 
1.328 \sqrt{\text{Re}} & \text{Re} \leq 10^5 \\
0.0312 \frac{\sqrt{\text{Re}}}{\text{Re}^{1.5}} & \text{Re} > 10^5
\end{cases}
\]  
\[\text{Eq.(11)}\]

In the previous works such as Li and Kim et al., momentum exchange between the gas stream and the droplets were neglected [17], but Movahednejad et al. modified momentum source term by considering the drag force on droplets calculated as follows [15].
\[
R = \frac{1}{2} C_D U_f^2 \rho_d A
\]  
\[\text{Eq.(12)}\]

Where the drag coefficient \( C_D \) is defined as:
\[
C_D = \begin{cases} 
24 / \text{Re} & \text{Re} < 0.2 \\
18.5 / \text{Re} & 0.2 \leq \text{Re} < 500 \\
0.44 & 500 \leq \text{Re} < 10^3
\end{cases}
\]  
\[\text{Eq.(13)}\]

To apply the drag force on droplets, the conservation equations of (2-4) as well as (6) are initially solved to determine velocity and droplet size distribution. Then, modified momentum source term will be upgraded to consider the drag. Upgrading continues to conduct the accurate solution.

If the graph under surface of probability function versus droplet velocity be calculated, the number density of droplets on the basis of dimensionless droplet size will be determined. Therefore, to compute the number density of droplets versus dimensionless droplet size, the droplet size distribution can be calculated as Eq. (14).
\[
\frac{dN}{dD} = \int_{u_{\text{min}}}^{u_{\text{max}}} f du
\]  
\[\text{Eq.(14)}\]
4. The solution of MEP equation by GA

Generally, Newton-Raphson method was used simultaneously solve MEP equations in previous studies [15, 16, 18].

The main problem in using Newton-Raphson method is drastic degree of dependency on the initial guess to find the solution [19]. But various studies have shown the genetic algorithm (GA) is one of the most eligible methods to solve highly nonlinear equations with global minimization characteristic after transmuting MEP equations to the minimizing problem [19, 20]. Nikos E. Mastorakis studied the problem of solving nonlinear equations by genetic algorithm for different objective functions defined as [20].

\[
Q(x) = \sum_{i=1}^{n} f_i^2(x_1, x_2, \ldots, x_n) \quad (15)
\]

\[
Q(x) = \sum_{i=1}^{n} \text{abs}\left[ f_i(x_1, x_2, \ldots, x_n) \right] \quad (16)
\]

\[
Q(x) = \sum_{i=1}^{n} f_i(x_1, x_2, \ldots, x_n) \quad (17)
\]

Where \( f_i(x) \) are MEP equations presented in Eqs. (2-4) and Eqs. (6) with arranging in left hand side as following strongly nonlinear exponential equations, Pourrajabian et al. offered the absolute function as the best cost function to solve nonlinear equation [21]. Finally, MEP equations will be solved by objective function definition as Eq. (16) and nonlinear constraints as eq. (2-13) to determine the velocity and droplet size distribution.

5. Results and Validation

To validate the results of GA, the solution should be compared with Newton-Raphson method. To assess the maximum entropy principle for determination of PDF, the procedure is evaluated for pressure swirl atomizer of Mitra [18]. The spray characteristics are presented in Table 1.

Table (2) shows the results of Newton-Raphson method and GA. The values of \( f_i - f_d \) represent the residual of nonlinear MEP equations, according to Eqs 2-6 and \( Q(x) \) is defined as the objective function according to Eq. 15. Also, the pdf function of velocity and droplet size distribution between two methods is compared as can be seen in figure 3. Figure 4 as well shows the number density of droplets versus dimensionless droplet size in different weber number.

<table>
<thead>
<tr>
<th>Case</th>
<th>We</th>
<th>( \rho )</th>
<th>( U )</th>
<th>( L_0 )</th>
<th>( D_{30(m)} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>50</td>
<td>0.01</td>
<td>4</td>
<td>151</td>
<td>157</td>
</tr>
<tr>
<td>2</td>
<td>150</td>
<td>0.001</td>
<td>4</td>
<td>75</td>
<td>86</td>
</tr>
<tr>
<td>3</td>
<td>500</td>
<td>0.001</td>
<td>4</td>
<td>23</td>
<td>43</td>
</tr>
</tbody>
</table>
a) Newton-Raphson method

b) Genetic Algorithm method

Fig. 3. The pdf function of droplet size and velocity distribution for $We = 50; U = 4; \rho = 0.001$

Table 2. The results of Newton-Raphson method for solving MEP equations

<table>
<thead>
<tr>
<th>N</th>
<th>Algorithm</th>
<th>$f_1$</th>
<th>$f_2$</th>
<th>$f_3$</th>
<th>$f_4$</th>
<th>$Q(x)$</th>
<th>Iteration</th>
<th>Time</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>N-R</td>
<td>0.00290</td>
<td>-0.38340</td>
<td>-0.44800</td>
<td>-0.57200</td>
<td>1.40100</td>
<td>75</td>
<td>135s</td>
</tr>
<tr>
<td></td>
<td>GA</td>
<td>0.00000</td>
<td>0.00000</td>
<td>0.00000</td>
<td>0.00000</td>
<td>0.00010</td>
<td>6</td>
<td>165(min)</td>
</tr>
<tr>
<td></td>
<td>N-R</td>
<td>-0.36770</td>
<td>-0.40190</td>
<td>-0.45740</td>
<td>-0.54200</td>
<td>1.76990</td>
<td>44</td>
<td>66s</td>
</tr>
<tr>
<td></td>
<td>GA</td>
<td>0.00001</td>
<td>0.00000</td>
<td>0.00010</td>
<td>0.00010</td>
<td>0.00023</td>
<td>5</td>
<td>295min</td>
</tr>
<tr>
<td></td>
<td>N-R</td>
<td>-0.74000</td>
<td>-0.61650</td>
<td>-0.64640</td>
<td>-0.67400</td>
<td>2.67830</td>
<td>61</td>
<td>103s</td>
</tr>
<tr>
<td></td>
<td>GA</td>
<td>0.00001</td>
<td>0.00000</td>
<td>0.00010</td>
<td>0.00010</td>
<td>0.00023</td>
<td>5</td>
<td>295min</td>
</tr>
</tbody>
</table>

Table 3. The performance conditions of GA-method

<table>
<thead>
<tr>
<th>character</th>
<th>population</th>
<th>fitness scaling</th>
<th>cross over</th>
<th>Migration</th>
<th>Function tolerance</th>
<th>stall generation</th>
</tr>
</thead>
<tbody>
<tr>
<td>data</td>
<td>30</td>
<td>Top</td>
<td>two point</td>
<td>Both</td>
<td>1e-11</td>
<td>100</td>
</tr>
</tbody>
</table>

5.1 Validation

In addition, the solution will be compared with the experimental results of Li X et al. [12]. The genetic algorithm is converging after 5 generation. The value of $Q(x)$ function for this case study is equal to $Q(x) = 0.00012589$ for GA. Fig. 5 compares the result of numerical method with experimental result. The findings illustrates the GA predicts size distribution droplet better than Newton-Raphson method. Also, the arrangements that be used in GA-method are presented in Table 3.

Also, fig. 6 compares the droplets number density between experimental work and numerical results. This figure shows that the results of GA-method is improved other than NR-method.

6. Summary

In this paper, Genetic Algorithm is applied to solve nonlinear exponential MEP equations to improve the rate of convergence as well as solution accuracy. Traditional Newton-Raphson method is a way to examine a local minimum of functions and does not calculate the global minimum of functions. Therefore, if the primary selections of initial candidate are not close to the answer, the result may be not to converge to the correct solution. In the genetic algorithm, due to the exhaustive search in the solutions domain, the global minimums of functions are calculated. Therefore, it doesn’t need to introduce the initial guess being close to the solutions domain. Generally, GA is a suitable method for solving of strongly nonlinear equations such as MEP equations. But, setting the method parameters has a particular importance.

Although, the computational cost will grow by selection of GA parameters as more precisely and broader, but the accuracy of solutions significantly will increase.
a) Genetic Algorithm method

b) Newton-Raphson method

c) Experimental work [12]

Fig. 5. The pdf function for droplet size and velocity distribution

Fig. 6. The number density of droplets versus dimensionless droplet size
References


NOMENCLATURE

\[ C_D \]  Modify drag force 
\[ f \]  Probability function 
\[ S \]  Shannon entropy 
\[ C_F \]  Drag coefficient 
\[ Q(x) \]  Objective function 
\[ S_{m} \]  Mass source term 
\[ \bar{D} \]  Dimensionless drop diameter 
\[ R \]  Modify drag force 
\[ S_{mu} \]  Momentum source term 
\[ D_{10} \]  Mean diameter 
\[ Re \]  Reynolds number 
\[ S_{e} \]  Energy source term 
\[ u \]  Axial velocity(m/s) 
\[ We \]  Weber number 
\[ \lambda \]  Lagrange multiplier 
\[ \mu \]  Density 
\[ U \]  Mean velocity 
\[ MEP \]  Maximum entropy principle 
\[ \rho \]  Density